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Operator Algebras and Quantum Statistical Mechanics 2

Equilibrium States.
Models in Quantum Statistical Mechanics

Second Edition

Springer

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To
Trygve Bratteli,
Samuel Robinson,
and
Harold Ross

Preface to the Second Edition

Fifteen years have passed since completion of the first edition of this book and much has happened. Any attempt to do justice to the new developments would necessitate at least one new volume rather than a second edition of the current one. Fortunately other authors have taken up the challenge of describing these discoveries and our bibliography includes references to a variety of new books that have appeared or are about to appear. We consequently decided to keep the format of this book as a basic reference for the operator algebraic approach to quantum statistical mechanics and concentrated on correcting, improving, and updating the material of the first edition. This in itself has not been easy and changes occur throughout the text. The major changes are a corrected presentation of Bose–Einstein condensation in Theorem 5.2.30, insertion of a general result on the absence of symmetry breaking in Theorem 5.3.33A, and an extended description of the dynamics of the X–Y model in Example 6.2.14. The discussion of phase transitions in specific models, in Sects. 6.2.6 and 6.2.7, has been expanded with the focus shifted from the classical Ising model to genuine quantum situations such as the Heisenberg and X–Y models. In addition the Notes and Remarks to various subsections have been considerably augmented.

Since our interest in the subject of equilibrium states and models of statistical mechanics has waned considerably in the last fifteen years it

would have been impossible to prepare this second edition without the support and encouragement of many of our friends and colleagues. We are particularly indebted to Charles Batty, Michiel van den Berg, Tom ter Elst, Dai Evans, Mark Fannes, Jürg Fröhlich, Taku Matsui, André Verbeure, and Marinus Winnink for information and helpful advice, and we apologize for often ignoring the latter. We are especially grateful to Aernout van Enter and Reinhard Werner for counselling us on recent developments and giving detailed suggestions for revisions.

Oslo and Canberra 1996

Ola Bratteli
Derek W. Robinson

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States in Quantum Statistical Mechanics

5.1. Introduction

In this chapter, and the following one, we examine various applications of C^*-algebras and their states to statistical mechanics. Principally we analyze the structural properties of the equilibrium states of quantum systems consisting of a large number of particles. In Chapter 1 we argued that this leads to the study of states of infinite-particle systems as an initial approximation. There are two approaches to this study which are to a large extent complementary.

The first approach begins with the specific description of finite systems and their equilibrium states provided by quantum statistical mechanics. One then rephrases this description in an algebraic language which identifies the equilibrium states as states over a quasi-local C^*-algebra generated by subalgebras corresponding to the observables of spatial subsystems. Finally, one attempts to calculate an approximation of these states by taking their limit as the volume of the system tends to infinity, the so-called thermodynamic limit. The infinite-volume equilibrium states obtained in this manner provide the data for the calculation of bulk properties of the matter under consideration as functions of the thermodynamic variables. By this we mean properties such as the particle density, or specific heat, as functions of the temperature and chemical potential, etc. In fact, the infinite-volume data provides a much more detailed, even microscopic, description of the equilibrium phenomena although one is only generally interested in the bulk properties and their fluctuations. Examination of the thermodynamic limit also provides a test of the scope of the usual statistical mechanical formalism. If this formalism is rich enough to describe phase transitions, then at certain critical values of the thermodynamic parameters there should be a multiplicity of infinite-volume limit states arising from slight variations of the external interactions or boundary conditions. These states would correspond to various phases and mixtures of these phases. In such a situation it should be possible to arrange the limits such that phase separation takes place and then the equilibrium states would also provide information concerning interface phenomena such as surface tension.

The second approach to algebraic statistical mechanics avoids discussion of the thermodynamic limit and attempts to characterize and classify the equilibrium states of the infinite system as states over an appropriate C^*-algebra. The elements of the C^*-algebra represent kinematic observables, i.e., observables at a given time, and the states describe the instantaneous states of the system. For a complete physical description it is necessary to specify the dynamical law

governing the change with time of the observables, or the states, and the equilibrium states are determined by their properties with respect to this dynamics. The general nature of the dynamical law can be inferred from the usual quantum-mechanical formalism and it appears that there are various possibilities. Recall that for finite quantum systems the dynamics is given by a one-parameter group of *-automorphisms of the algebra of observables,

$$A \mapsto \tau_t(A) = e^{itH} A e^{-itH} \quad ,$$

where H is the selfadjoint Hamiltonian operator of the system. Thus it appears natural that the dynamics of the infinite system should be determined by a continuous one-parameter group of *-automorphisms τ of the C^*-algebra of observables. This type of dynamics is certainly the simplest possible and it occurs in various specific models, e.g., the noninteracting Fermi gas, some of which we examine in the sequel. Nevertheless, it is not the general situation. The difficulty is that a group of this kind automatically defines a continuous development of every state of the system. But this is not to be expected for general infinite systems in which complicated phenomena involving the local accumulation of an infinite number of particles and energy can occur for certain initial states. Thus it is necessary to examine weaker forms of evolution. For example, one could assume the dynamics to be specified as a group of automorphisms of the von Neumann algebras corresponding to a subclass of states over the C^*-algebra. Alternatively one could adopt an infinitesimal description and assume that the evolution is determined by a derivation which generates an automorphism group only in certain representations. Each of these possible structures could in principle be verified in a particular model by a thermodynamic limiting process and each such structure provides a framework for characterizing equilibrium phenomena. To understand the type of characterization which is possible it is useful to refer to the finite-volume description of equilibrium.

There are various possible descriptions of equilibrium states, which all stem from the early work of Boltzmann and Gibbs on classical statistical mechanics, and which differ only in their initial specification. The three most common possibilities are the microcanonical ensemble, the canonical ensemble, and the grand canonical ensemble. In the first, the energy and particle number are held fixed; in the second, states of various energy are allowed for fixed particle number; and in the third, both the energy and the particle number vary. Each of these descriptions can be rephrased algebraically but the grand canonical description is in several ways more convenient. Let $\mathfrak{H}$ be the Hilbert space of states for all possible energies and particle numbers of the finite system, and H and N, the selfadjoint Hamiltonian and number operators, respectively. The Gibbs grand canonical equilibrium state is defined as a state over $\mathscr{L}(\mathfrak{H})$, or $\mathscr{L}\mathscr{C}(\mathfrak{H})$, by

$$\omega_{\beta,\mu}(A) = \frac{\mathrm{Tr}_{\mathfrak{H}}(e^{-\beta K} A)}{\mathrm{Tr}_{\mathfrak{H}}(e^{-\beta K})} \quad ,$$

where $K = H - \mu N$, $\mu \in \mathbb{R}$, and it is assumed that $e^{-\beta K}$ is a trace-class operator. Typically H is lower semi-bounded and the trace-class property is valid for all $\beta > 0$. The parameters β and μ correspond to the inverse temperature of the system, in suitable units, and the chemical potential, respectively, and therefore this description is well-suited to a given type of material at a fixed temperature. Now if the generalized evolution τ is defined by

$$A \in \mathscr{L}(\mathfrak{H}) \mapsto \tau_t(A) = e^{itK} A e^{-itK} \in \mathscr{L}(\mathfrak{H}) \ ,$$

then the trace-class property of $e^{-\beta K}$ allows one to deduce that the functions

$$t \mapsto \omega_{\beta,\,\mu}(A\tau_t(B))$$

are analytic in the open strip $0 < \operatorname{Im} t < \beta$ and continuous on the boundaries of the strip. Moreover, the cyclicity of the trace gives

$$\omega_{\beta,\,\mu}(A\tau_t(B))|_{t=i\beta} \ = \ \omega_{\beta,\,\mu}(BA) \ .$$

This is the KMS condition which we briefly described in Chapter 1 and which will play an important role throughout this chapter. One significance of this condition is that it uniquely determines the Gibbs state over $\mathscr{L}\mathscr{C}(\mathfrak{H})$, i.e., the only state over $\mathscr{L}\mathscr{C}(\mathfrak{H})$ which satisfies the KMS condition with respect to τ at the value β is the Gibbs grand canonical equilibrium state. This can be proved by explicit calculation but it will in fact follow from the characterization of extremal KMS states occurring in Section 5.3. It also follows under quite general conditions that the KMS condition is stable under limits. Thus for a system whose kinematic observables form a C^*-algebra $\mathfrak{A}$ and whose dynamics is supposed to be given by a continuous group of *-automorphisms τ of $\mathfrak{A}$, it is natural to take the KMS condition as an empirical definition of an equilibrium state.

Prior to the analysis of KMS states we introduce the specific quasi-local C^*-algebras which provide the quantum-mechanical description of systems of point particles and examine various properties of their states and representations. In particular we discuss the equilibrium states of systems of non-interacting particles. This analysis illustrates the thermodynamic limiting process, utilizes the KMS condition as a calculational device, and also provides a testing ground for the general formalism which we subsequently develop.

In the latter half of the chapter we discuss attempts to derive the KMS condition from first principles.

5.2. Continuous Quantum Systems. I

5.2.1. The CAR and CCR Relations

There are two approaches to the algebraic structure associated with systems of point particles in quantum mechanics. The first is quite concrete and physical. One begins with the Hilbert space of vector states of the particles and subsequently introduces algebras of operators corresponding to certain particle observables. The second approach is more abstract and consists of postulating certain structural features of a C^*-algebra of observables and then proving uniqueness of the algebra. One recovers the first point of view by passing to a particular representation. We discuss the first concrete approach in this subsection and then in Section 5.2.2 we examine the abstract formulation.

The quantum-mechanical states of n identical point particles in the configuration space $\mathbb{R}^\nu$ are given by vectors of the Hilbert space $L^2(\mathbb{R}^{n\nu})$. If the number of particles is not fixed, the states are described by vectors of the direct sum space

$$\mathfrak{F} = \bigoplus_{n \geq 0} L^2(\mathbb{R}^{n\nu}) \ ,$$

i.e., sequences $\psi = \{\psi^{(n)}\}_{n \geq 0}$, where $\psi^{(0)} \in \mathbb{C}$, $\psi^{(n)} \in L^2(\mathbb{R}^{n\nu})$ for $n \geq 1$, and the norm of ψ is given by

$$\|\psi\|^2 = |\psi^{(0)}|^2 + \sum_{n \geq 1} \int dx_1 \cdots dx_n |\psi^{(n)}(x_1, \ldots, x_n)|^2 \ .$$

There is, however, a further restriction imposed by quantum statistics.

If $\psi \in \mathfrak{F}$ is normalized, then

$$d\rho(x_1, \ldots, x_n) = |\psi^{(n)}(x_1, \ldots, x_n)|^2 dx_1 \cdots dx_n$$

is the quantum-mechanical probability density for ψ to describe n particles at the infinitesimal neighborhood of the points $x_1, \ldots, x_n$. The normalization of ψ corresponds to the normalization of the total probability to unity. But in microscopic physics identical particles are indistinguishable and this is reflected by the symmetry of the probability density under interchange of the particle coordinates. This interchange defines a unitary representation of the permutation group and the symmetry is assured if the ψ transform under a suitable subrepresentation. There are two cases of paramount importance.

The first arises when the components $\psi^{(n)}$ of each ψ are symmetric under interchange of coordinates. Particles whose states transform in this manner are called *bosons* and are said to satisfy *Bose (–Einstein) statistics*. The second case corresponds to anti-symmetry of the $\psi^{(n)}$ under interchange of each pair of coordinates. The associated particles are called *fermions* and are said to satisfy *Fermi (–Dirac) statistics*. Thus to discuss these two types of particle one must examine the Hilbert subspaces $\mathfrak{F}_\pm$, of $\mathfrak{F}$, formed by the $\psi = \{\psi^{(n)}\}_{n\geq 0}$ whose components are symmetric (the + sign) or anti-symmetric (the – sign). These subspaces are usually called Fock spaces but we will also use the term for more general direct sum spaces.

To describe particles which have internal structure, e.g., an intrinsic angular momentum, or spin, it is necessary to generalize the above construction of Fock space.

Assume that the states of each particle form a complex Hilbert space $\mathfrak{h}$ and let $\mathfrak{h}^n = \mathfrak{h} \otimes \mathfrak{h} \otimes \cdots \otimes \mathfrak{h}$ denote the n-fold tensor product of $\mathfrak{h}$ with itself. Further introduce the *Fock space* $\mathfrak{F}(\mathfrak{h})$ by

$$\mathfrak{F}(\mathfrak{h}) = \bigoplus_{n\geq 0} \mathfrak{h}^n \ ,$$

where $\mathfrak{h}^0 = \mathbb{C}$. Thus a vector $\psi \in \mathfrak{F}(\mathfrak{h})$ is a sequence $\{\psi^{(n)}\}_{n\geq 0}$ of vectors $\psi^{(n)} \in \mathfrak{h}^n$ and $\mathfrak{h}^n$ can be identified as the closed subspace of $\mathfrak{F}(\mathfrak{h})$ formed by the vectors with all components except the nth equal to zero.

In order to introduce the subspaces relevant to the description of bosons and fermions we first define operators $P_\pm$ on $\mathfrak{F}(\mathfrak{h})$ by

$$P_+(f_1 \otimes f_2 \otimes \cdots \otimes f_n) = (n!)^{-1} \sum_\pi f_{\pi_1} \otimes f_{\pi_2} \otimes \cdots \otimes f_{\pi_n} \ ,$$

$$P_-(f_1 \otimes f_2 \otimes \cdots \otimes f_n) = (n!)^{-1} \sum_\pi \varepsilon_\pi f_{\pi_1} \otimes f_{\pi_2} \otimes \cdots \otimes f_{\pi_n}$$

for all $f_1, \ldots, f_n \in \mathfrak{h}$. The sum is over all permutations $\pi; (1, 2, \ldots, n) \mapsto (\pi_1, \pi_2, \ldots, \pi_n)$ of the indices and ε_π is one if π is even and minus one if π is odd. Extension by linearity yields two densely defined operators with $\|P_\pm\| = 1$ and the $P_\pm$ extend by continuity to bounded operators of norm one. The P_+ and P_- restricted to $\mathfrak{h}^n$, are the projections onto the subspaces of $\mathfrak{h}^n$ corresponding to the one-dimensional unitary representations $\pi \mapsto 1$ and $\pi \mapsto \varepsilon_\pi$ of the permutation group of n elements, respectively. The *Bose-Fock space* $\mathfrak{F}_+(\mathfrak{h})$ and the *Fermi-Fock space* $\mathfrak{F}_-(\mathfrak{h})$ are then defined by

$$\mathfrak{F}_\pm(\mathfrak{h}) = P_\pm\, \mathfrak{F}(\mathfrak{h})$$

and the corresponding n-particle subspaces $\mathfrak{h}^n_\pm$ by $\mathfrak{h}^n_\pm = P_\pm\, \mathfrak{h}^n$. We also define a *number operator* N on $\mathfrak{F}(\mathfrak{h})$ by

$$D(N) = \left\{ \psi;\ \psi = \{\psi^{(n)}\}_{n\geq 0},\ \sum_{n\geq 0} n^2 \|\psi^{(n)}\|^2 < +\infty \right\}$$

and

$$N\psi = \{n\psi^{(n)}\}_{n\geq 0}$$

for each $\psi \in D(N)$. It is evident that N is selfadjoint since it is already given in its spectral representation. Note that e^{itN} leaves the subspaces $\mathfrak{F}_{\pm}(\mathfrak{h})$ invariant. We will also use N to denote the selfadjoint restrictions of the number operator to these subspaces.

The peculiar structure of Fock space allows the amplification of operators on $\mathfrak{h}$ to the whole spaces $\mathfrak{F}_{\pm}(\mathfrak{h})$ by a method commonly referred to as *second quantization*. This is of particular interest for selfadjoint operators and unitaries.

If H is selfadjoint operator on $\mathfrak{h}$, one can define H_n on $\mathfrak{h}^n_{\pm}$ by setting $H_0 = 0$ and

$$H_n(P_{\pm}(f_1 \otimes \cdots \otimes f_n)) = P_{\pm}\left(\sum_{i=1}^{n} f_1 \otimes f_2 \otimes \cdots \otimes Hf_i \otimes \cdots \otimes f_n\right)$$

for all $f_i \in D(H)$, and then extending by continuity. The direct sum of the H_n is essentially selfadjoint because (1) it is symmetric and hence closable, (2) it has a dense set of analytic vectors formed by finite sums of (anti-) symmetrized products of analytic vectors of H. The selfadjoint closure of this sum is called the second quantization of H and is denoted by $d\Gamma(H)$. Thus

$$d\Gamma(H) = \overline{\bigoplus_{n \geq 0} H_n} \ .$$

The simplest example of this second quantization is given by choosing $H = \mathbb{1}$, one then has

$$d\Gamma(\mathbb{1}) = N \ .$$

If U is unitary, U_n is defined by $U_0 = \mathbb{1}$ and by setting

$$U_n(P_{\pm}(f_1 \otimes f_2 \otimes \cdots \otimes f_n)) = P_{\pm}(Uf_1 \otimes Uf_2 \otimes \cdots \otimes Uf_n)$$

and extending by continuity. The second quantization of U is denoted by $\Gamma(U)$, where

$$\Gamma(U) = \bigoplus_{n \geq 0} U_n \ .$$

Note that $\Gamma(U)$ is unitary. The notation $d\Gamma$ and Γ is chosen because if $U_t = e^{itH}$ is a strongly continuous one-parameter unitary group, then

$$\Gamma(U_t) = e^{itd\Gamma(H)} \ .$$

Next we wish to describe two C^*-algebras of observables associated with bosons and fermions, respectively. Both algebras are defined with the aid of particle *"annihilation"* and *"creation" operators* which are introduced as follows. For each $f \in \mathfrak{h}$ we define operators $a(f)$, and $a^*(f)$, on $\mathfrak{F}(\mathfrak{h})$ by initially setting $a(f)\psi^{(0)} = 0, a^*(f)\psi^{(0)} = f$, $f \in \mathfrak{h}$, and

$$a(f)(f_1 \otimes f_2 \otimes \cdots \otimes f_n) = n^{1/2}(f, f_1) f_2 \otimes f_3 \otimes \cdots \otimes f_n \ ,$$

$$a^*(f)(f_1 \otimes f_2 \otimes \cdots \otimes f_n) = (n+1)^{1/2} f \otimes f_1 \otimes \cdots \otimes f_n \ .$$

Extension by linearity again yields two densely defined operators and if $\psi^{(n)} \in \mathfrak{h}^n$, one easily calculates that

$$\|a(f)\psi^{(n)}\| \leq n^{1/2}\|f\|\|\psi^{(n)}\|, \qquad \|a^*(f)\psi^{(n)}\| \leq (n+1)^{1/2}\|f\|\,\|\psi^{(n)}\| \ .$$

Thus $a(f)$ and $a^*(f)$ have well-defined extensions to the domain $D(N^{1/2})$ of $N^{1/2}$ and

$$\|a^{\#}(f)\psi\| \leq \|f\|\,\|(N+1)^{1/2}\psi\|$$

for all $\psi \in D(N^{1/2})$, where $a^{\#}(f)$ denotes either $a(f)$ or $a^*(f)$. Moreover, one has the adjoint relation

$$(a^*(f)\varphi, \psi) = (\varphi, a(f)\psi)$$

for all $\varphi, \psi \in D(N^{1/2})$. Finally, we define annihilation and creation operators $a_\pm(f)$ and $a_\pm^*(f)$ on the Fock spaces $\mathfrak{F}_\pm(\mathfrak{h})$ by

$$a_\pm(f) = P_\pm\, a(f) P_\pm\,, \qquad a_\pm^*(f) = P_\pm\, a^*(f) P_\pm \ .$$

The relations

$$(a_\pm^*(f)\varphi, \psi) = (\varphi, a_\pm(f)\psi), \qquad \|a_\pm^*(f)\psi\| \leq \|f\|\,\|(N+1)^{1/2}\psi\|$$

follow from the corresponding relations for $a(f)$ and $a^*(f)$. Moreover,

$$a_\pm(f) = a(f)P_\pm, \qquad a_\pm^*(f) = P_\pm\, a^*(f)$$

because $a(f)$ leaves the subspaces $\mathfrak{F}_\pm(\mathfrak{h})$ invariant. Note that the maps $f \mapsto a_\pm(f)$ are anti-linear but the maps $f \mapsto a_\pm^*(f)$ are linear.

The physical interpretation of these operators is the following. Let $\Omega = (1, 0, 0, \ldots)$, then Ω corresponds to the zero-particle state, the *vacuum*. The vectors

$$\psi_\pm(f) = a_\pm^*(f)\Omega$$

identify with elements of the one-particle space $\mathfrak{h}$ and hence $a_\pm^*(f)$ "creates" a particle in the state f. The vectors

$$\begin{aligned}\psi_\pm(f_1, \ldots, f_n) &= (n!)^{-1/2} a_\pm^*(f_1) \cdots a_\pm^*(f_n)\Omega \\ &= P_\pm(f_1 \otimes \cdots \otimes f_n)\end{aligned}$$

are n-particle states which arise from successive "creation" of particles in the states $f_n, f_{n-1}, \ldots, f_1$. Similarly the $a_\pm(f)$ reduce the number of particles, i.e., they annihilate particles. Note that if $f_i = f_j$ for some pair i, j with $1 \leq i < j \leq n$, then

$$\psi_-(f_1, \ldots, f_n) = P_-(f_1 \otimes \cdots \otimes f_n) = 0$$

by anti-symmetry. Thus it is impossible to create two fermions in the same state. This is the celebrated *Pauli principle* which is reflected by the operator equation

$$a_-^*(f)a_-^*(f) = 0 \ .$$

This last relation is the simplest case of the commutation relations which link the annihilation and creation operators.

One computes straightforwardly that

$$[a_+(f), a_+(g)] = 0 = [a_+^*(f), a_+^*(g)] \ ,$$

$$[a_+(f), a_+^*(g)] = (f,g)\mathbb{1} \ ,$$

and

$$\{a_-(f), a_-(g)\} = 0 = \{a_-^*(f), a_-^*(g)\} \ ,$$

$$\{a_-(f), a_-^*(g)\} = (f,g)\mathbb{1} \ ,$$

where we have again used the notation $\{A,B\} = AB + BA$. The first relations are called the *canonical commutation relations* (CCRs) and the second the *canonical anti-commutation relations* (CARs).

Although there is a superficial similarity between these two sets of algebraic rules, the properties of the respective operators are radically different. In applications to physics these differences are thought to be at the root of the fundamentally disparate behaviors of Bose and Fermi systems at low temperatures. In order to emphasize these differences we separate the subsequent discussion of the CARs and CCRs but before the general analysis we give an example of the creation and annihilation operators for point particles.

EXAMPLE 5.2.1. If $\mathfrak{h} = L^2(\mathbb{R}^\nu)$, then $\mathfrak{F}_\pm(\mathfrak{h})$ consists of sequences $\{\psi^{(n)}\}_{n\geq 0}$ of functions of n variables $x_i \in \mathbb{R}^\nu$ which are totally symmetric ($+$ sign) or totally antisymmetric ($-$ sign). The action of the annihilation and creation operators is given by

$$(a_\pm(f)\psi)^{(n)}(x_1,\ldots,x_n) = (n+1)^{1/2} \int dx\, \overline{f(x)}\psi^{(n+1)}(x,x_1,\ldots,x_n) \ ,$$

$$(a_\pm^*(f)\psi)^{(n)}(x_1,\ldots,x_n) = n^{-1/2} \sum_{i=1}^{n} (\pm 1)^{i-1} f(x_i)\psi^{(n-1)}(x_1,\ldots,\hat{x}_i,\ldots,x_n) \ ,$$

where $\hat{x}_i$ denotes that the i th variable is to be omitted. Note that as the maps

$$f \mapsto a_\pm(f), \qquad f \mapsto a_\pm^*(f)$$

are anti-linear and linear, respectively, one may introduce operator-valued distributions, i.e., fields $a_\pm(x)$, and $a_\pm^*(x)$, such that

$$a_\pm(f) = \int dx\, \overline{f(x)}\, a_\pm(x) \ , \qquad a_\pm^*(f) = \int dx\, f(x) a_\pm^*(x) \ ,$$

and then the action of these fields is given by

$$(a_\pm(x)\psi)^{(n)}(x_1,\ldots,x_n) = (n+1)^{1/2}\, \psi^{(n+1)}(x,x_1,\ldots,x_n) \ ,$$

$$(a_\pm^*(x)\psi)^{(n)}(x_1,\ldots,x_n) = n^{-1/2} \sum_{i=1}^{n} (\pm 1)^{i-1} \delta(x-x_i)\psi^{(n-1)}(x_1,\ldots,\hat{x}_i,\ldots,x_n) \ .$$

In terms of these fields the number operator N is formally given by

$$N = \int dx\, a_\pm^*(x) a_\pm(x) \ .$$

5.2.1.1 The CAR Relations. We next analyze the properties of the creation and annihilation operators obeying the CAR relations on the Fock space $\mathfrak{F}_-(\mathfrak{h})$. We simplify notation by dropping the suffix minus on the operators.

Proposition 5.2.2. *Let $\mathfrak{h}$ be a complex Hilbert space, $\mathfrak{F}_-(\mathfrak{h})$ the Fermi Fock space, and $a(f)$ and $a^*(g)$ the corresponding annihilation and creation operators on $\mathfrak{F}_-(\mathfrak{h})$. It follows that*

(1) $$\|a(f)\| = \|f\| = \|a^*(f)\|$$

for all $f \in \mathfrak{h}$, and hence $a(f)$ and $a^*(g)$ have bounded extensions.

(2) *If $\Omega = (1,0,0,\ldots)$ and $\{f_\alpha\}$ is an orthonormal basis of $\mathfrak{h}$, then*

$$\psi(f_{\alpha_1},\ldots,f_{\alpha_n}) = a^*(f_{\alpha_1})\cdots a^*(f_{\alpha_n})\Omega$$

is an orthonormal basis of $\mathfrak{F}_-(\mathfrak{h})$ when $\{f_{\alpha_1},\ldots,f_{\alpha_n}\}$ runs over the finite subsets of $\{f_\alpha\}$.

(3) *The set of bounded operators $\{a(f),\, a^*(g);\, g \in \mathfrak{h}\}$ is irreducible on $\mathfrak{F}_-(\mathfrak{h})$.*

Proof. (1) One has

$$(a^*(f)a(f))^2 = a^*(f)\{a(f),\, a^*(f)\}a(f) = \|f\|^2 a^*(f)a(f)$$

and hence

$$\|a(f)\|^4 = \|(a^*(f)a(f))^2\| = \|f\|^2\|a^*(f)a(f)\| = \|f\|^2\|a(f)\|^2 \ .$$

As $a(f) \neq 0$ for $f \neq 0$ one concludes that

$$\|a(f)\| = \|f\| = \|a^*(f)\| \ .$$

(2) This follows easily from the observation that

$$\psi(f_{\alpha_1},\ldots,f_{\alpha_n}) = (n!)^{1/2} P_-(f_{\alpha_1}\otimes\cdots\otimes f_{\alpha_n}) \ .$$

(3) Let T be a bounded operator in the commutant of $\{a(f), a^*(g); f, g \in \mathfrak{h}\}$, then

$$\begin{aligned}(\psi(f_{\alpha_1},\ldots,f_{\alpha_n}),\quad & T\psi(g_{\beta_1},\ldots,g_{\beta_m}))\\ &= (T^*\Omega, a(f_{\alpha_n})\cdots a(f_{\alpha_1})a^*(g_{\beta_1})\cdots a^*(g_{\beta_m})\Omega)\\ &= (T^*\Omega,\Omega)(\psi(f_{\alpha_1},\ldots,f_{\alpha_n}),\, \psi(g_{\beta_1},\ldots,g_{\beta_m})) \ .\end{aligned}$$

To establish the last equality one considers the three cases $n > m$, $n < m$, and $n = m$, separately. In the first case both expressions are zero because the $a(f)$ annihilate more particles than the $a^*(g)$ create. In the second case both expressions are again zero by complex conjugation. In the third case $a(f_{\alpha_n})\cdots a^*(g_{\beta_m})\Omega$ is a multiple of Ω and the desired equality follows once more. Thus $T = (\Omega, T\Omega)\mathbb{1}$ and irreducibility is a consequence of Proposition 2.3.8.

5.2.1.2. The CCR Relations. The main qualitative difference between fermions and bosons is the absence of a Pauli principle for the latter particles. There is no bound on the number of particles which can occupy a given state. This is quantitatively reflected by the unboundedness of the Bose annihilation and creation operators. If, for example, $\psi^{(n)}$ is the n-fold tensor product of $f \in \mathfrak{h}$ with itself, then the annihilation operator satisfies

$$\|a(f)\psi^{(n)}\| = n^{1/2}\|\psi^{(n)}\|\|f\|$$

(we omit the suffix plus on the operators). This unboundedness leads to a large number of technical difficulties which are absent for fermions. These problems can be partially avoided by consideration of bounded functions of the operators $a(f)$ and $a^*(g)$.

It is convenient to introduce a family of operators $\{\Phi(f), f \in \mathfrak{h}\}$ by

$$\Phi(f) = 2^{-1/2}(a(f) + a^*(f)) \ ,$$

Note that if $\Pi(f) = \Phi(if)$, then

$$\Pi(f) = -i\,2^{-1/2}(a(f) - a^*(f)) \ ,$$

Thus

$$a(f) = 2^{-1/2}(\Phi(f) + i\Pi(f)), \qquad a^*(f) = 2^{-1/2}(\Phi(f) - i\Pi(f)) \ ,$$

and the $a(f)$ and $a^*(f)$ can be recuperated from the $\Phi(f)$. Thus for functional purposes it suffices to examine the latter operators. Their basic properties are most easily examined on the subspace $F(\mathfrak{h}) \subset \mathfrak{F}_+(\mathfrak{h})$ formed by the finite-particle vectors, i.e., the $\psi = \{\psi^{(n)}\}_{n\geq 0}$ which have only a finite number of nonvanishing components.

Proposition 5.2.3. *Let $\mathfrak{h}$ be a complex Hilbert space, $\mathfrak{F}_+(\mathfrak{h})$ the Bose Fock space, and $a(f)$ and $a^*(g)$ annihilation and creation operators satisfying the canonical commutation relations. Define Φ by*

$$\Phi(f) = 2^{-1/2}(a(f) + a^*(f))$$

for all $f \in \mathfrak{h}$. It follows that

(1) *For each $f \in \mathfrak{h}, \Phi(f)$ is essentially selfadjoint on $F(\mathfrak{h})$ and if $\|f_\alpha - f\| \to 0$, then $\|\Phi(f_\alpha)\psi - \Phi(f)\psi\| \to 0$ for all $\psi \in D(N^{1/2})$.*
(2) *If $\Omega = (1, 0, 0, \ldots)$ then the linear span of the set $\{\Phi(f_1)\cdots\Phi(f_n)\Omega; f_i \in \mathfrak{h}, n = 0, 1, \ldots\}$ is dense in $\mathfrak{F}_+(\mathfrak{h})$.*
(3) *For each $\psi \in D(N)$ and, $f, g \in \mathfrak{h}$ one has*

$$(\Phi(f)\Phi(g) - \Phi(g)\Phi(f))\psi = i\,\mathrm{Im}(f, g)\psi \ .$$

Proof. (1) The operator $\Phi(f)$ is densely defined, and symmetric, hence closable. To establish essential selfadjointness it suffices to prove that $\Phi(f)$ has a dense set of analytic vectors. But if $\psi^{(n)} \in \mathfrak{h}_+^n$, then $\psi^{(n)} \in D(\Phi(f)^m)$ for all m and $\Phi(f)\psi^{(n)} \in \mathfrak{h}_+^{n+1} \oplus \mathfrak{h}_+^{n-1}$. The estimates

$$\|a(f)\psi^{(n)}\| \le (n+1)^{1/2}\|\psi^{(n)}\|\|f\|, \qquad \|a^*(f)\psi^{(n)}\| \le (n+1)^{1/2}\|\psi^{(n)}\|\|f\|$$

then imply that

$$\|\Phi(f)^m\psi^{(n)}\| \le 2^{m/2}(n+m)^{1/2}(n+m-1)^{1/2}\cdots(n+1)^{1/2}\|\psi^{(n)}\|\|f\|^m .$$

Therefore

$$\sum_{m\ge 0}\frac{|t|^m}{m!}\|\Phi(f)^m\psi^{(n)}\| \le \sum_{m\ge 0}\frac{(\sqrt{2}|t|)^m}{m!}\left(\frac{(n+m)!}{n!}\right)^{1/2}\|f\|^n\|\psi^{(n)}\| < +\infty$$

for all $t \in \mathbb{C}$. It immediately follows that each ψ in the dense set $F(\mathfrak{h})$ is an analytic vector for $\Phi(f)$.

The continuity follows because

$$\begin{aligned}\|(\Phi(f_\alpha)-\Phi(f))\psi\| &\le 2^{-1/2}\|a(f_\alpha - f)\psi\| + 2^{-1/2}\|a^*(f_\alpha - f)\psi\| \\ &\le 2^{1/2}\|f_\alpha - f\|\|(N+1)^{1/2}\psi\|\end{aligned}$$

(2) The linear spans of $\{\Phi(f_1)\cdots\Phi(f_n)\Omega; f_i \in \mathfrak{h}, n \ge 0\}$ and $\{a^*(f_1)\cdots a^*(f_n)\Omega; f_i \in \mathfrak{h}, n \ge 0\}$ are identical. But the latter is dense by the same arguments used in Proposition 5.2.2.

(3) This is immediate from the canonical commutation relations.

Next we consider the unitary groups generated by the operators $\Phi(f)$, but henceforth we use this symbol to denote the selfadjoint closure of the previous $\Phi(f)$.

Proposition 5.2.4. *For each $f \in \mathfrak{h}$ let $\Phi(f)$ denote the selfadjoint operator*

$$\Phi(f) = 2^{-1/2}\,\overline{(a(f)+a^*(f))}\,.$$

Moreover let $W(f)$ denote the unitary operator $\exp\{i\Phi(f)\}$. *It follows that*

(1) *For each pair $f, g \in \mathfrak{h}$, $W(f)D(\Phi(g)) = D(\Phi(g))$ and*

$$W(f)\Phi(g)W(f)^* = \Phi(g) - \operatorname{Im}(f,g)\mathbb{1}\,.$$

(2) *For each pair $f, g \in \mathfrak{h}$*

$$W(f)W(g) = e^{-i\operatorname{Im}(f,g)/2}W(f+g)\,,$$

(3) *The set $\{W(f); f \in \mathfrak{h}\}$ is irreducible on $\mathfrak{F}_+(\mathfrak{h})$.*

(4) *If $\|f_\alpha - f\| \to 0$, then*

$$\|(W(f_\alpha) - W(f))\psi\| \to 0$$

for all $\psi \in \mathfrak{F}_+(\mathfrak{h})$

(5) *For each $f \in \mathfrak{h}\backslash\{0\}$*

$$\|W(f) - \mathbb{1}\| = 2\,.$$

Proof. (1) Each $\psi_\alpha \in F(\mathfrak{h})$ is analytic for $\Phi(f)$ and one can define $\Phi(g)W(f)^*$ on ψ_α by power-series expansion. This expansion yields the identity

$$\Phi(g)W(f)^*\psi_\alpha = W(f)^*(\Phi(g) - \mathrm{Im}(f, g)\mathbb{1})\psi_\alpha$$

and consequently

$$\|\Phi(g)W(f)^*(\psi_\alpha - \psi_\beta)\| \leq \|\Phi(g)(\psi_\alpha - \psi_\beta)\| + |\mathrm{Im}(f, g)|\|\psi_\alpha - \psi_\beta\| .$$

But $F(\mathfrak{h})$ is a core for $\Phi(g)$. Thus if $\psi \in D(\Phi(g))$, one may choose the ψ_α such that $\psi_\alpha \to \psi$ and $\Phi(g)\psi_\alpha \to \Phi(g)\psi$. It immediately follows that $\Phi(g)W(f)^*\psi_\alpha$ converges and therefore $W(f)^*\psi \in D(\Phi(g))$ and $\Phi(g)W(f)^*\psi_\alpha \to \Phi(g)W(f)^*\psi$. Thus $D(\Phi(g))$ is invariant under each $W(f)$ and

$$\Phi(g)W(f)^* = W(f)^*(\Phi(g) - \mathrm{Im}(f, g)\mathbb{1})$$

on $D(\Phi(g))$.

(2) For $\psi \in F(\mathfrak{h})$ one can exploit the invariance of $D(\Phi(g))$ under $W(f+g)^*$, etc., and the closedness of each $\Phi(f)$ to derive the identity

$$\begin{aligned}
&\frac{d}{dt}W(tf)W(tg)W(t(f+g))^*\psi \\
&\quad = W(tf)[i\Phi(f), W(tg)]W(t(f+g))^*\psi \\
&\quad = -it\,\mathrm{Im}(f, g)W(tf)W(tg)W(t(f+g))^*\psi \ .
\end{aligned}$$

Integration then gives the following identity between bounded operators

$$W(f)W(g)W(f+g)^* = \mathbb{1} - i\int_0^1 dt\ t\,\mathrm{Im}(f, g)W(tf)W(tg)W(t(f+g))^* \ .$$

Iteration of this identity immediately yields

$$W(f)W(g)W(f+g)^* = e^{-i\,\mathrm{Im}(f,g)/2}$$

which is equivalent to the stated result.

(3) If T is a bounded operator which commutes with each $W(f)$, then $TD(\Phi(f)) \subseteq D(\Phi(f))$ and $\Phi(f)T\psi = T\Phi(f)\psi$ for each $\psi \in D(\Phi(f))$ because $\Phi(f)$ is the infinitesimal generator of $t \in \mathbb{R} \mapsto W(tf)$. But $a(f) = 2^{-1/2}(\Phi(f) + i\Phi(if))$ and so T commutes with $a(f)$ in the same manner and irreducibility follows by the same calculation used for the CARs in Proposition 5.2.2.

(4) $F(\mathfrak{h})$ is a core of $\Phi(f)$ and $\|(\Phi(f_\alpha) - \Phi(f))\psi\| \to 0$ for all $\psi \in F(\mathfrak{h})$ by Proposition 5.2.3. Therefore, it follows from Theorem 3.1.28 that $W(f_\alpha)$ converges strongly to $W(f)$.

(5) It follows from part (1) that

$$W(itf)\Phi(f)W(itf)^* = \Phi(f) - t\|f\|^2\mathbb{1}$$

for all $t \in \mathbb{R}$. Thus the spectrum of $\Phi(f)$ must be the whole real line. Now consider the unitary group $W(tf)$ and its spectral representation

$$W(tf) = \int dE(\lambda)e^{it\lambda} \ .$$

For each $\psi \in \mathfrak{F}_+(\mathfrak{h})$ one has

$$4\|\psi\|^2 - \|W(f)\psi - \psi\|^2 = 2\int d(\psi, E(\lambda)\psi)(1 - \cos\lambda) \ .$$

Thus if $E([\pi + \varepsilon, \pi - \varepsilon])\psi = \psi$ with $0 < \varepsilon < \pi/2$

$$\left|4 - \|W(f) - \mathbb{1})\psi\|^2/\|\psi\|^2\right| \leq 2|1 - \cos\varepsilon|$$

and hence $\|W(f) - \mathbb{1}\| = 2$.

The operators $W(f)$ introduced in the above proposition are usually called *Weyl operators* and the commutation relations

$$W(f)W(g) = e^{-i\,\mathrm{Im}(f,g)/2}W(f+g) = e^{-i\,\mathrm{Im}(f,g)}W(g)W(f)$$

are called the *Weyl form of the canonical commutation relations.*

5.2.2. The CAR and CCR Algebras

In the last subsection we derived the canonical commutation and anti-commutation relations and constructed the Weyl operators associated with the former. To complete this discussion we next examine the abstract C^*-algebras generated by elements satisfying the CARs or the Weyl form of the CCRs. It will result that these algebras are uniquely determined by the appropriate form of commutation relation.

Again we divide the discussion into two separate parts.

5.2.2.1. The CAR Algebra. The foregoing Fock space construction established the existence of bounded operators satisfying the CARs. The next result characterizes the abstract properties of the C^*-algebra generated by these operators.

Theorem 5.2.5. *Let $\mathfrak{h}$ be a pre-Hilbert space with closure $\bar{\mathfrak{h}}$ and let $\mathfrak{A}_i$, $i = 1, 2$, be two C^*-algebras generated by the identity $\mathbb{1}$ and elements $a_i(f)$, $f \in \mathfrak{h}$, satisfying*

(1) $f \mapsto a_i(f)$ *is antilinear,*
(2) $\{a_i(f), a_i(g)\} = 0$,
(3) $\{a_i(f), a_i(g)^*\} = (f, g)\mathbb{1}$

for all $f, g \in \mathfrak{h}$, $i = 1, 2$.

It follows that there exists a unique *-isomorphism $\alpha : \mathfrak{A}_1 \mapsto \mathfrak{A}_2$ such that

$$\alpha(a_1(f)) = a_2(f)$$

for all $f \in \mathfrak{h}$. Thus there exists a unique, up to *-isomorphism, C^*-algebra $\mathfrak{A} = \mathfrak{A}(\mathfrak{h}) = \mathfrak{A}(\bar{\mathfrak{h}})$ generated by elements $a(f)$, satisfying the canonical anti-commutation relations over $\mathfrak{h}$.

Furthermore

(1) $\|a(f)\| = \|f\|$ *for all $f \in \bar{\mathfrak{h}}$.*
(2) *If $\mathfrak{h}$ is n dimensional, where $n < +\infty$, then $\mathfrak{A}(\mathfrak{h})$ is isomorphic with the C^*-algebra of $2^n \times 2^n$ complex matrices.*
(3) *$\mathfrak{A}(\mathfrak{h})$ is separable if, and only if, $\mathfrak{h}$ is separable.*
(4) *$\mathfrak{A}(\mathfrak{h})$ is simple.*
(5) *If U is a bounded linear operator on $\mathfrak{h}$ and V a bounded antilinear operator satisfying*

$$V^*U + U^*V = 0 = UV^* + VU^* \ ,$$

$$U^*U + V^*V = \mathbb{1} = UU^* + VV^* \ ,$$

*then there exists a unique *-automorphism γ of $\mathfrak{A}(\mathfrak{h})$ such that*

$$\gamma(a(f)) = a(Uf) + a^*(Vf)$$

and in this case

$$\gamma^{-1}(a(f)) = a(U^*f) + a^*(V^*f) \ .$$

PROOF. (1) The proof that $\|a_i(f)\| = \|f\|$ is identical to the proof given in Proposition 5.2.2. It is a direct consequence of the CARs.

(2) Assume that $\mathfrak{h}$ is finite dimensional, and let $\{f_1, \ldots, f_n\}$ be an orthonormal basis for $\mathfrak{h}$. If $f \mapsto a(f)$ are operators satisfying the CARs, define

$$e_{11}^{(k)} = a(f_k)a^*(f_k), \qquad e_{12}^{(k)} = V_{k-1}a(f_k) \ ,$$
$$e_{21}^{(k)} = V_{k-1}a^*(f_k), \qquad e_{22}^{(k)} = a^*(f_k)a(f_k) \ .$$

for $k = 1, \ldots, n$ where

$$V_k = \prod_{i=1}^{k}(\mathbb{1} - 2a^*(f_i)a(f_i))$$

and we use the standard notation $a^*(f) = a(f)^*$. It follows from the CARs that $\{e_{ij}^{(k)}\}_{i,j=1,2}$ are n families of mutually commuting 2×2 matrix units,

$$e_{ij}^{(k)} e_{lm}^{(k)} = \delta_{jl} e_{im}^{(k)} \ ,$$
$$k \neq g \Rightarrow e_{ij}^{(k)} e_{lm}^{(g)} = e_{lm}^{(g)} e_{ij}^{(k)} \ .$$

Moreover, they generate the same algebra as the $a(f)$ since

$$a(f_k) = \left(\prod_{i=1}^{k-1}(e_{11}^{(l)} - e_{22}^{(l)})\right) e_{12}^{(k)} \ .$$

Hence this algebra is the algebra of $2^n \times 2^n$ matrices, and this establishes property (2), and the proposition when $\mathfrak{h}$ is finite dimensional.

When $\mathfrak{h}$ is infinite dimensional, construct an orthonormal basis $\{f_\alpha\}$ for $\mathfrak{h}$. For each finite dimensional subset of $\{f_\alpha\}$ we may construct matrix units as above, and as $\|a(f)\| = \|f\|$ it follows by continuity that the C^*-algebra generated by the $a(f)$ is unique and is, in fact, generated by an increasing net of full matrix algebras. Moreover, $\mathfrak{A}(\mathfrak{h}) = \mathfrak{A}(\bar{\mathfrak{h}})$.

The separability statement (3) is immediate from the construction of $\mathfrak{A}(\mathfrak{h})$ above, and the simplicity follows from Corollary 2.6.19 or can be proved as follows: since $\{a(f), a^*(f)\} = \|f\|^2\mathbb{1}$, it follows that $\pi(a(f)) \neq 0$ for all representations of π of $\mathfrak{A}(\mathfrak{h})$, and hence π is faithful by the uniqueness of $\mathfrak{A}(\mathfrak{h})$. Hence $\mathfrak{A}(\mathfrak{h})$ has no non-trivial closed two-sided ideals. Statement (5) follows by applying the first statement of the Proposition on $a_1(f) = a(f)$, $a_2(f) = a(Uf) + a^*(Vf)$.

Note that from statement (2) of the theorem and the construction of $\mathfrak{A}(\mathfrak{h})$ it follows that this algebra is a UHF algebra (see Example 2.6.12).

The transformations described in part (5) of the theorem are often called *Bogoliubov transformations*.

We next investigate local structure of the CAR algebra $\mathfrak{A}(\mathfrak{h})$ over a Hilbert space $\mathfrak{h}$.

Proposition 5.2.6. *Let $\mathfrak{A}(\mathfrak{h})$ be the CAR algebra over a Hilbert space $\mathfrak{h}$, and let I be a net of closed nonempty subspaces of $\mathfrak{h}$, ordered by inclusion such that:*

(1) *If $M \in I$, there exists an $N \in I$ such that $M \perp N$.*
(2) *If $M \perp N$ and $M \perp K$, there exists an $L \in I$ such that $M \perp L$ and $N, K \subseteq L$.*
(3) $\mathfrak{h} = \overline{\bigcup_{M \in I} M}$.

Let $\mathfrak{A}(M) \subseteq \mathfrak{A}(\mathfrak{h})$ be the sub-C^*-algebra generated by $\{a(f); f \in M\}$ for each $M \in I$. Then $(\mathfrak{A}(\mathfrak{h}), \{\mathfrak{A}(M)\}_{M \in I})$ is a quasi-local algebra in the sense of Definition 2.6.3, *with $\sigma(a(f)) = -a(f)$ for all $f \in \mathfrak{h}$.*

Proof. First, if $M_1 \subseteq M_2$, we evidently have $\mathfrak{A}(M_1) \subseteq \mathfrak{A}(M_2)$, and, second, as any $A \in \mathfrak{A}(\mathfrak{h})$ can be approximated by finite polynomials in $a(f)$ and $a^*(g)$, it follows from the relation $\|a(f)\| = \|f\|$ and assumption (3) that $\mathfrak{A}(\mathfrak{h}) = \overline{\bigcup_{M \in I} \mathfrak{A}(M)}$. Third, the $\mathfrak{A}(M)$ have a common identity by definition. Finally, let σ be the unique *-automorphism of $\mathfrak{A}$ such that $\sigma(a(f)) = -a(f)$ for all $f \in \mathfrak{H}$. This automorphism exists by applying Theorem 5.2.5 part (5) to $U = -1$ and $V = 0$. Then $\sigma^2 = \imath$ and $\sigma(\mathfrak{A}(M)) = \mathfrak{A}(M)$ for all $M \in I$. Each element $A \in \mathfrak{A}(M)$ can be uniformly approximated by a sequence of polynomials P_n in the $a(f)$ and $a^*(g)$ with $f, g \in M$. But if A is even, it follows that the $(P_n + \sigma(P_n))/2$ also converge to $A = (A + \sigma(A))/2$. But $(P_n + \sigma(P_n))/2$ is an even polynomial in the $a(f)$ and $a^*(g)$. By a similar reasoning odd elements can be approximated by odd polynomials. Hence it suffices to prove the commutation relations for polynomials. But noting that A^2 and B commute if A and B anti-commute, these follow directly from the CARs.

EXAMPLE 5.2.7. Let $\mathfrak{h} = L^2(\mathbb{R}^\nu)$ and, for each bounded open set $\Lambda \subseteq \mathbb{R}^\nu$, define $\mathfrak{A}_\Lambda$ as the C^*-subalgebra generated by $\{a(f) : f \in L^2(\Lambda)\}$. It follows that the CAR algebra $\mathfrak{A}(\mathfrak{h})$ is a quasi-local algebra with respect to this generating net. In particular

$$\mathfrak{A}(\mathfrak{h}) = \overline{\bigcup_{\Lambda} \mathfrak{A}_\Lambda} \ .$$

We conclude by mentioning an equivalent way of describing the CAR algebra which is analogous to the description of the CCRs in terms of the operators $\{\Phi(f); f \in \mathfrak{h}\}$.

One defines a family of elements $B(f); f \in \mathfrak{h}$ by

$$B(f) = 2^{-1/2}(a(f) + a^*(f))$$

then

$$a(f) = 2^{-1/2}(B(f) + iB(if)) \ ,$$

i.e., the $a(f)$ can be recovered from the $B(f)$. But it follows from the CARs that

$$\{B(f), B(g)\} = \mathrm{Re}(f, g)$$

and conversely the CARs follow from these latter relations. Thus one is prompted to study the seemingly more general problem of an algebra $\mathfrak{A}$ generated by elements $B(f), f \in H$, satisfying

$$\{B(f), B(g)\} = s(f, g)$$

for all $f, g \in H$, where H is a real vector space and s is a real positive symmetric bilinear form over H. If in this context J is any operator such that

$$s(Jf, g) = -s(f, Jg), \quad J^2 = -1 \ ,$$

one can introduce annihilation, and creation operators $a_J(f)$ and $a_J^*(g)$ by

$$a_J(f) = 2^{-1/2}(B(f) + iB(Jf)), \ \ a_J^*(g) = 2^{-1/2}\big(B(g) - iB(Jg)\big)$$

and one has

$$\{a_J(f), a_J^*(g)\} = s(f, g) + is(f, Jg) \ ,$$

etc. Thus in comparison with the previous discussion $s(f, g)$ corresponds to the real part of (f, g) and $s(f, Jg)$ corresponds to the imaginary part.

Although this latter description seems more general we remark that if H is a real Hilbert space and if s is the nondegenerate inner product on H, then a J with the above properties exists if, and only if H has even (or infinite) dimension. In this case H is a complex Hilbert space and s is the real part of the inner product. One has the identification

$$(\lambda_1 + i\lambda_2)\xi = \lambda_1\xi + \lambda_2 J\xi$$

for all $\lambda_i \in \mathbb{R}$ and $\xi \in H$, and

$$(f, g) = s(f, g) + is(f, Jg) \ .$$

The J can be constructed by first choosing an orthonormal basis $\{\xi_1, \eta_1, \xi_2, \eta_2, \ldots\}$ of H and then defining J by

$$J\xi_i = \eta_i, \qquad J\eta_i = -\xi_i \ .$$

Finally we remark that if T is any real invertible operator such that

$$s(Tf, Tg) = s(f, g) \ ,$$

it follows that there exists a unique *-automorphism γ of $\mathfrak{A}$ such that

$$\gamma(B(f)) = B(Tf) \ .$$

A simple calculation shows that this corresponds to the Bogoliubov transformation of the $a_J(f)$ and $a_J^*(g)$, with

$$U = 2^{-1}(T - JTJ), \qquad V = 2^{-1}(T + JTJ) \ .$$

5.2.2.2. The CCR Algebra. Next we characterize the abstract properties of the C^*-algebra generated by the Weyl operators. Although this CCR algebra has many properties analogous to the CAR algebra the lack of norm continuity of the map $f \mapsto W(f)$ alters properties of density, separability, and quasi-locality.

We will slightly generalize the situation described in Section 5.2.1.2 and examine a family of Weyl operators $W(f)$ defined for elements f of a real linear space H equipped with a nondegenerate symplectic bilinear form σ, i.e., σ is a map from $H \times H$ into $\mathbb{R}$ such that

$$\sigma(f, g) = -\sigma(g, f)$$

for all $f, g \in H$, and if

$$\sigma(f, g) = 0$$

for all $f \in H$, then $g = 0$. For example, one could take H to be a complex pre-Hilbert space and σ to be given by

$$\sigma(f, g) = \mathrm{Im}(f, g)$$

and then one recuperates the CCR relations described previously.

In fact, the generalization is very slight because if σ is a nondegenerate symplectic bilinear form on H and there exists an operator J on H with the properties

$$\sigma(Jf, g) = -\sigma(f, Jg), \qquad J^2 = -1 \ ,$$

then H is a pre-Hilbert space with scalar multiplication and inner product defined by

$$(\lambda_1 + i\lambda_2)f = \lambda_1 f + \lambda_2 Jf, \qquad \lambda_i \in \mathbb{R}, \quad f \in H \ ,$$

$$(f, g) = \sigma(f, Jg) + i\sigma(f, g), \qquad f, g \in H \ ,$$

and clearly $\sigma(f, g) = \mathrm{Im}(f, g)$.

Note that if H is sequentially complete with respect to the topology defined by σ, a J with the above properties exists if, and only if, H does not have finite odd dimension. To construct J one first uses a procedure similar to the Gram–Schmidt orthogonalization procedure to find elements $\{\xi_i, \eta_i\}$ in H spanning a dense subspace and such that

$$\sigma(\xi_i, \xi_j) = \sigma(\eta_i, \eta_j) = 0 \ ,$$
$$\sigma(\xi_i, \eta_j) = \delta_{ij} \ .$$

Then one defines J by $J\xi_i = \eta_i$ and $J\eta_i = -\xi_i$ and extension by continuity.

In the following, when talking about the CCR algebra over a complex pre-Hilbert space H, it is always understood that σ is the imaginary part of the inner product.

Theorem 5.2.8. *Let H be a real linear space equipped with a nondegenerate symplectic bilinear form σ and let $\mathfrak{A}_i, i = 1, 2$, be two C^*-algebras generated by nonzero elements $W_i(f), f \in H$, satisfying*

(1) $W_i(-f) = W_i(f)^*$,
(2) $W_i(f)W_i(g) = e^{-i\sigma(f,g)/2}W_i(f+g)$ *for all* $f, g \in H$.

It follows that there exists a unique *-isomorphism $\alpha; \mathfrak{A}_1 \mapsto \mathfrak{A}_2$ such that

$$\alpha(W_1(f)) = W_2(f)$$

for all $f \in H$. Thus there exists a unique, up to *-isomorphism, C^*-algebra $\mathfrak{A} = \mathfrak{A}(H)$ generated by Weyl operators $W(f)$.

Furthermore

(1) $W(0) = \mathbb{1}$, $W(f)$, *is unitary for all* $f \in H$, *and* $\|W(f) - \mathbb{1}\| = 2$ *for all nonzero* $f \in H$.

(2) *If H is nonzero, then $\mathfrak{A}(H)$ is nonseparable.*
(3) *$\mathfrak{A}(H)$ is simple.*
(4) *If T is a real linear invertible operator on H such that*

$$\sigma(Tf, Tg) = \sigma(f, g)$$

for all $f, g \in H$, then there exists a unique *-automorphism γ of $\mathfrak{A}(H)$ such that

$$\gamma(W(f)) = W(Tf) \ .$$

PROOF. It follows from property (2) of the $W(f)$ that

$$W(f)W(0) = W(f) = W(0)W(f)$$

and

$$W(-f)W(f) = W(0) = W(f)W(-f) \ .$$

As the $W(f)$ are nonzero one concludes that $W(0)$ is the identity $\mathbb{1}$ and property (1) implies that $W(f)$ is unitary.

Next let us regard the linear space H as a discrete additive abelian group. The $W(f)$ give a unitary representation of H up to a phase, or multiplier $b(f, g) = \exp\{-i\sigma(f, g)/2\}$. It is subsequently of importance that $f \mapsto \chi_g(f) = b(f, g)$ is a character of H, e.g.,

$$b(f_1 + f_2, g) = b(f_1, g)b(f_2, g) \ .$$

Our aim is to prove that the C^*-algebras $\mathfrak{A}_i, i = 1, 2$, are *-isomorphic.

Consider the two representations R_b and R of H defined on $l^2(H)$ by

$$(R_b(g)F)(f) = b(f, g)F(f + g)$$

and

$$(R(g)F)(f) = F(f + g) \ .$$

One calculates that R_b is a unitary representation up to the multiplier b and R is a unitary representation in the usual sense. (Note that $W(g) = R_b(g)$ defines a representation of the CCRs and hence a CCR algebra exists.)

We may assume that $\mathfrak{A}_1$ and $\mathfrak{A}_2$ are faithfully represented on Hilbert spaces $\mathfrak{H}_1$ and $\mathfrak{H}_2$ and define new multiplier representations $W_i \times R$ on $l^2(H; \mathfrak{H}_i) = \mathfrak{H}_i \otimes l^2(H)$. An element $\psi \in l^2(H; \mathfrak{H}_i)$ is a function over H with values in $\mathfrak{H}_i$, and we set

$$((W_i \times R)(g)\psi)(f) = W_i(g)\psi(f + g) \ .$$

Then $W_i \times R$ is a multiplier representation of H with multiplier b, and we next show that $W_i \times R$ is quasi-equivalent to R_b. Define a unitary operator U_i on $l^2(H, \mathfrak{H}_i)$ by

$$(U_i\psi)(f) = W_i(f)\psi(f)$$

and then calculate that

$$\begin{aligned}(U_i(W_i \times R)(g)\psi)(f) &= W_i(f)((W_i \times R)(g)\psi)(f) \\ &= W_i(f)W_i(g)\psi(f + g) \\ &= b(f, g)W_i(f + g)\psi(f + g) \\ &= b(f, g)(U_i\psi)(f + g) = ((\mathbb{1}_i \otimes R_b(g))U_i\psi)(f) \ ,\end{aligned}$$

that is,

$$U_i(W_i \times R)(g)U_i^* = \mathbb{1}_i \otimes R_b(g) \ ,$$

where $\mathbb{1}_i$ is the identity on $\mathfrak{H}_i$. Let $\mathfrak{B}_i$ be the C^*-algebra generated by $\{(W_i \times R)(g); g \in H\}$. Then, by the above identity, there exists a *-isomorphism τ from $\mathfrak{B}_1$ onto $\mathfrak{B}_2$ such that

$$\tau((W_1 \times R)(g)) = (W_2 \times R)(g) \ .$$

Hence if we can find *-isomorphisms $\tau_i : \mathfrak{A}_i \mapsto \mathfrak{B}_i$ such that

$$\tau_i(W_i(g)) = (W_i \times R)(g) \ ,$$

the first statement of the theorem follows. But, setting $W = W_i$, this amounts to showing that

$$\left\| \sum_{i=1}^n \lambda_i (W \times R)(f_i) \right\| = \left\| \sum_{i=1}^n \lambda_i W(f_i) \right\|$$

for all $\lambda_i \in \mathbb{C}, f_i \in H$, and $n \geq 1$. The representation $W \times R$ is, via Fourier transform on $l^2(H)$, unitary equivalent to the representation $W \times \hat{R}$ on $l^2(\hat{H}; \mathfrak{H})$ defined by

$$((W \times \hat{R})(g)\psi)(\chi) = W(g)\chi(g)\psi(\chi), \ \ \chi \in \hat{H}$$

and hence

$$\left\| \sum_{i=1}^n \lambda_i (W \times R)(f_i) \right\| = \sup_{\chi \in \hat{H}} \left\| \sum_{i=1}^n \lambda_i \chi(f_i) W(f_i) \right\| \ .$$

Now, the set $\{\chi_g\}$ of $\chi \in \hat{H}$ of the form

$$\chi_g(f) = b(g, f)^2$$

is dense in $\hat{H}$, since it is a subgroup of $\hat{H}$ with annihilator zero. Moreover, $\chi_g(f)W(f) = W(g)W(f)W(g)^*$. Therefore

$$\begin{aligned} \left\| \sum_{i=1}^n \lambda_i (W \times R)(f_i) \right\| &= \sup_{g \in H} \left\| \sum_{i=1}^n \lambda_i \chi_g(f_i) W(f_i) \right\| \\ &= \sup_{g \in H} \left\| W(g) \left(\sum_{i=1}^n \lambda_i W(f_i) \right) W(g)^* \right\| = \left\| \sum_{i=1}^n \lambda_i W(f_i) \right\| \ . \end{aligned}$$

It follows that there exists a *-isomorphism $\alpha : \mathfrak{A}_1 \mapsto \mathfrak{A}_2$ such that

$$\alpha(W_1(f)) = W_2(f)$$

for all $f \in H$, and α is unique since the $W_i(f)$ generate $\mathfrak{A}_i$ as a C^*-algebra.

Let us next prove the four properties of $\mathfrak{A}(H)$ stated in the latter half of the theorem.

(1) At the beginning of the proof we established that each $W(f)$ is unitary and $W(0) = \mathbb{1}$. The CCRs now give

$$W(g)W(f)W(g)^* = e^{-i\sigma(g,f)}W(f)$$

and hence the spectrum of $W(f)$ is invariant under rotations. Hence the spectrum is equal to the circle and $\|W(f) - \mathbb{1}\| = 2$ by the spectral radius formula.

(2) Assume that $\mathfrak{A}(H)$ is separable and let $\{A_n\}_{n \geq 0}$ be a countable dense sequence of elements of $\mathfrak{A}(H)$. Thus for each $t \in \mathbb{R}$ and each $f \in H$ there must be an n_t such that

$$\|W(tf) - A_{n_t}\| < 1 \ .$$

But if $f \neq 0$ and $t_1 \neq t_2$, then $A_{n_{t_1}} \neq A_{n_{t_2}}$ because

$$\|W(t_1 f) - A_{n_{t_1}}\| < 1, \quad \|W(t_2 f) - A_{n_{t_1}}\| < 1$$

would imply

$$\|W((t_1 - t_2)f) - \mathbb{1}\| < 2$$

in contradiction to the first statement proved above. But as $\mathbb{R}$ is not countable A_n cannot be dense and this contradiction proves that $\mathfrak{A}(H)$ is nonseparable.

(3) Let π be a representation of $\mathfrak{A}(H)$, then by the first statement of the theorem there exists a *-isomorphism α from $\mathfrak{A}(H)$ onto $\pi(\mathfrak{A}(H))$ such that $\alpha(W(f)) = \pi(W(f))$ for all $f \in H$. But then $\alpha = \pi$ because $\mathfrak{A}(H)$ is generated by the $W(f)$. Hence the kernel of π is zero. But π was arbitrary and therefore $\mathfrak{A}(H)$ must be simple.

(4) This follows by applying the uniqueness statement to $W_1(f) = W(f)$ and $W_2(f) = W(Tf)$.

As in the CAR case, the transformations described in part (4) of the theorem are often called *Bogoliubov transformations*.

There is an important difference between this theorem and the corresponding result. Theorem 5.2.5, for the CARs. There is no statement analogous to $\mathfrak{A}(\mathfrak{h}) = \mathfrak{A}(\bar{\mathfrak{h}})$ and, and in fact, one has the following situation.

Proposition 5.2.9. *Let $\mathfrak{A}(H)$ be the CCR algebra over the real vector space H and let $\mathfrak{A}(M)$ be the C^*-subalgebra generated by $\{W(f); f \in M\}$ where M is a subspace of H.*

It follows that

$$\mathfrak{A}(M) = \mathfrak{A}(H)$$

if, and only if, $M = H$.

Proof. If $M \neq H$, consider the representation of $\mathfrak{A}(H)$ on $l^2(H)$ defined by

$$(W(g)F)(f) = b(f, g)F(f + g)\,,$$

i.e., the representation used in the proof of Theorem 5.2.8. Assume $g \in H \backslash M$ and let $\lambda_i \in \mathbb{C}, g_i \in M$, then

$$\left(\left(W(g) - \sum_{i=1}^{n} \lambda_i W(g_i)\right)F\right)(f) = b(f, g)\left(F(f + g) - \sum_{i=1}^{n} \lambda_i b(f, g_i - g)F(f + g_i)\right) \ .$$

Hence, if F is supported by M,

$$\left\|\left(W(g) - \sum_{i=1}^{n} \lambda_i W(g_i)\right)F\right\| \geq \|F\|$$

because the vector $f \mapsto F(f + g)$ is orthogonal to each of the vectors $f \mapsto b(f, g_i - g) \times F(f + g_i)$. This orthogonality follows because if $f + g_i \in \operatorname{supp} F \subseteq M$, then $f \in M - g_i = M$, and hence $f + g \notin M$. Therefore

$$\inf_{A \in \mathfrak{A}(M)} \|W(g) - A\| \geq 1$$

and hence $W(g) \notin \mathfrak{A}(M)$.

We now consider quasi-local structure on the CCR algebra.

Proposition 5.2.10. *Let H be a linear space with a nondegenerate symplectic bilinear form σ. If N and M are subspaces of H, define $N \perp M$ if and only if $\sigma(f, g) = 0$ for all $f \in N$ and $g \in M$. Let I be a net of nonempty subspaces of H, ordered by inclusion, such that:*

(1) *If $M \in I$, there exists an $N \in I$ such that $M \perp N$.*
(2) *If $M \perp N$ and $M \perp K$, there exists an $L \in I$ such that $M \perp L$ and $N, K \subseteq L$.*
(3) *$H = \bigcup_{M \in I} M$.*

Let $\mathfrak{A}(H)$ be the CCR algebra over H, and let $\mathfrak{A}(M)$ be the sub-C^*-algebras generated by $\{W(f); f \in M\}$ for each $M \in I$.

Then $(\mathfrak{A}(H), \{\mathfrak{A}(M)\}_{M \in I})$ is a quasi-local algebra in the sense of Definition 2.6.3, *with $\sigma = \imath$.*

PROOF. This is immediate from the relation

$$W(f)W(g) = e^{-i\sigma(f,g)}W(g)W(f)$$

for $f, g \in H$.

Although this statement on quasi-local structure is similar to Proposition 5.2.6, there is a distinction which arises from the phenomena described in Proposition 5.2.9 and which is illustrated by the following example.

EXAMPLE 5.2.11. Let H be the subspace of $L^2(\mathbb{R}^\nu)$ formed by the functions with compact support. Moreover, let

$$\sigma(f, g) = \mathrm{Im}(f, g) \ .$$

If Λ is a bounded open set of $\mathbb{R}^\nu$ and $\mathfrak{A}_\Lambda$ is the C^*-subalgebra of $\mathfrak{A}(H)$ generated by $\{W(f); f \in L^2(\Lambda)\}$ then $(\mathfrak{A}(H), \{\mathfrak{A}_\Lambda\}_{\Lambda \subset \mathbb{R}^\nu})$ is a quasi-local algebra in the sense of Definition 2.6.3. However, $\mathfrak{A}(H)$ is *not* equal to the CCR algebra over $L^2(\mathbb{R}^\nu)$ because of Proposition 5.2.9.

5.2.3. States and Representations

We continue the analysis of the CAR and CCR algebras with a discussion of various properties of states and representations of these algebras. Most of these properties are related to the existence of creation and annihilation operators and this causes a distinction between the CARs and CCRs. The CAR algebra contains creation and annihilation operators but these operators can only be affiliated with special representations of the CCR algebra. We begin with a discussion of these representations and associated states. We concentrate on the CCR algebra over a pre-Hilbert space $\mathfrak{h}$ and eschew the case of a real vector

space with symplectic form. As we have explained in Section 5.2.2.2 this latter case is barely more general.

There is a certain arbitrariness in the definition of the CCR algebra from the generators $\Phi(f)$ in Proposition 5.2.4, i.e., one could define this algebra by taking other functions of $\Phi(f)$ than $\lambda \to e^{it\lambda}$. In fact the C^*-subalgebra of the CCR algebra generated by $\{W(tf); t \in \mathbb{R}\}$ where $f \in \mathfrak{h}$ is a fixed nonzero element is isomorphic with the set of almost periodic functions on $\mathbb{R} = \sigma(\Phi(f))$, and there is no inherent reason not to operate with the set of continuous functions on $\mathbb{R}$ vanishing at infinity, or any other subalgebra of $C_b(\mathbb{R})$ which separates points of $\mathbb{R}$. A consequence of this analysis is that one is not too interested in general representations of the CCR algebra, but only representations where the generators of $t \mapsto W(tf)$ exist. These are the so-called regular representations.

A representation $(\mathfrak{H}, \pi)$ of the CCR algebra $\mathfrak{A}(\mathfrak{h})$, over the pre-Hilbert space $\mathfrak{h}$, is said to be *regular* if the unitary groups $t \in \mathbb{R} \mapsto \pi(W(tf))$ are strongly continuous for all $f \in \mathfrak{h}$. If π is regular, then one can introduce, on $\mathfrak{H}$, the selfadjoint infinitesimal generators $\Phi_\pi(f), f \in \mathfrak{h}$ of the groups $t \mapsto \pi(W(tf))$, $f \in \mathfrak{h}$, and then use these to define annihilation and creation operators.

Similarly a state ω over $\mathfrak{A}(\mathfrak{h})$ is said to be *regular* if the associated cyclic representation $(\mathfrak{H}_\omega, \pi_\omega, \Omega_\omega)$ is regular. Note that

$$\begin{aligned} &||(\pi_\omega(W(tf)) - \mathbb{1})\pi_\omega(W(g))\Omega_\omega||^2 \\ &\quad = 2 - e^{-it\,\mathrm{Im}(f,g)}\omega(W(tf)) - e^{it\,\mathrm{Im}(f,g)}\omega(W(-tf)) \end{aligned}$$

and hence it easily follows that ω is regular if, and only if, $t \in \mathbb{R} \mapsto \omega(W(tf)) \in \mathbb{C}$ is continuous for all $f \in \mathfrak{h}$. We use the notation $\Phi_\omega(f)$ to denote the infinitesimal generator of the unitary group $\pi_\omega(W(tf))$ associated with a regular state.

The simplest example of a regular state is the *Fock state* ω_F defined by the vacuum, or no-particle state, $\Omega = (1, 0, 0, \ldots) \in \mathfrak{F}_+(\mathfrak{h})$. One easily calculates that

$$\omega_F(W(f)) = (\Omega, W(f)\Omega) = e^{-||f||^2/4} \ .$$

Even if ω is a regular state, there are certain technical domain problems which complicate the introduction of annihilation and creation operators. These are handled, however, by the following quite straightforward result.

Lemma 5.2.12. Let $\mathfrak{A}(\mathfrak{h})$ be the *CCR algebra over the pre-Hilbert space* $\mathfrak{h}$ *and* ω *a regular state over* $\mathfrak{A}(\mathfrak{h})$. *For each* $f \in \mathfrak{h}$ *denote the infinitesimal generator of the unitary group* $t \mapsto \pi_\omega(W(tf))$ *by* $\Phi_\omega(f)$.

It follows that the operators $\{\Phi_\omega(f), \Phi_\omega(if), f \in M\}$ *have a common dense set of analytic vectors for every finite-dimensional subspace* $M \subseteq \mathfrak{h}$.

Moreover the annihilation and creation operators defined for each $f \in \mathfrak{h}$ by

$$D(a_\omega(f)) = D(\Phi_\omega(f)) \cap D(\Phi_\omega(if)) = D(a_\omega^*(f))$$

and

$$a_\omega(f) = 2^{-1/2}\big(\Phi_\omega(f) + i\Phi_\omega(if)\big), \quad a^*_\omega(f) = 2^{-1/2}\big(\Phi_\omega(f) - i\Phi_\omega(if)\big)$$

are densely defined, closed, $a_\omega(f)^* = a^*_\omega(f)$, *and*

$$||\Phi_\omega(f)\varphi||^2 + ||\Phi_\omega(if)\varphi||^2 = 2||a_\omega(f)\varphi||^2 + ||f||^2||\varphi||^2$$

for all $\varphi \in D(a_\omega(f))$.

PROOF. We may assume that M is a complex subspace. Let $\{f_j; j = 1, 2 \ldots, m\}$ be an orthonormal basis of M and define an operator R_n on $\mathfrak{H}_\omega$ *by*

$$R_n = \left(\frac{n}{\pi}\right)^m \int ds_1\, dt_1 \cdots ds_m dt_m e^{-n(s_1^2 + t_1^2 + \cdots + s_m^2 + t_m^2)} \pi_\omega\left(W\left(\sum_{j=1}^m (s_j + it_j) f_j\right)\right) .$$

It follows from rotational invariance that R_n is independent of the choice of basis. Moreover, if for $\psi \in \mathfrak{H}_\omega$ one defines ψ_n by $\psi_n = R_n\psi$ then $||\psi_n - \psi|| \to 0$ by a similar argument to that used to prove Proposition 2.5.22. But using

$$W(sf_j)W((s_j + it_j)f_j) = e^{-ist_j/2}W((s_j + s + it_j)f_j)$$

and a change of variable in the multiple integral defining R_n one calculates that ψ_n is analytic for each $\Phi_\omega(f_j)$. Hence ψ_n is analytic for each operator $\Phi_\omega(f)$, with $f \in M$.

It immediately follows that $a_\omega(f)$ and $a^*_\omega(f)$ are densely defined on $D(\Phi_\omega(f)) \cap D(\Phi_\omega(if))$. Moreover, $a_\omega(f)^* \supset a^*_\omega(f)$. Thus $a_\omega(f)$ has a densely defined adjoint which means that it is closable. Similarly $a^*_\omega(f)$ is closable. Now if $\varphi \in D(a_\omega(f))$, then

$$\begin{aligned} ||\Phi_\omega(f)\varphi||^2 + ||\Phi_\omega(if)\varphi||^2 &= (||(a_\omega(f) + a^*_\omega(f))\varphi||^2 + ||(a_\omega(f) - a^*_\omega(f))\varphi||^2)/2 \\ &= ||a_\omega(f)\varphi||^2 + ||a^*_\omega(f)\varphi||^2 . \end{aligned}$$

Moreover, by differentiation of the Weyl relations

$$(\Phi_\omega(f)\varphi, \Phi_\omega(if)\varphi) = (\Phi_\omega(if)\varphi, \Phi_\omega(f)\varphi) + i||f||^2||\varphi||^2$$

which gives

$$||a^*_\omega(f)\varphi||^2 = ||a_\omega(f)\varphi||^2 + ||f||^2||\varphi||^2 .$$

Combination of these two identities yields

$$||\Phi_\omega(f)\varphi||^2 + ||\Phi_\omega(if)\varphi||^2 = 2||a_\omega(f)\varphi||^2 + ||f||^2||\varphi||^2 .$$

But now assume that $\psi_n \in D(a_\omega(f)), ||\psi_n - \psi|| \to 0$, and $||a_\omega(f)(\psi_n - \psi_m)|| \to 0$. One may use the identity just derived with $\varphi = \psi_n - \psi_m$ to deduce that $||\Phi_\omega(f)(\psi_n - \psi_m)|| \to 0$ and $||\Phi_\omega(if)(\psi_n - \psi_m)|| \to 0$. But $\Phi_\omega(f)$ and $\Phi_\omega(if)$ are selfadjoint, and in particular closed, and hence $\psi \in D(\Phi_\omega(f)) \cap D(\Phi_\omega(if)) = D(a_\omega(f))$. Another application of the identity gives $||a_\omega(f)(\psi_n - \psi)|| \to 0$ and therefore $a_\omega(f)$ is closed. A similar argument is valid for $a^*_\omega(f)$.

It remains to prove that $a_\omega(f)^* = a^*_\omega(f)$. This will be deduced as a corollary of Corollary 5.2.15.

Our next aim is to establish criteria for a state to be normal with respect to the Fock representation, i.e., the defining representation of $\mathfrak{A}(\mathfrak{h})$ on the Fock

spaces $\mathfrak{F}_{\pm}(\mathfrak{h})$. In Section 2.6.2 we defined a state ω over an irreducible subalgebra $\mathfrak{A}$ of $\mathscr{L}(\mathfrak{H})$ to be normal if it is determined by a density matrix ρ in the form

$$\omega(A) = \mathrm{Tr}_{\mathfrak{H}}(\rho A) \ .$$

It follows from Theorem 2.4.25 that this is equivalent to the representation $(\mathfrak{H}_\omega, \pi_\omega, \Omega_\omega)$ being a direct sum of copies of the representation of $\mathfrak{A}$ on $\mathfrak{H}$. The condition of normality is of interest in applications because the normal states of the Fock representation correspond to convex combinations of finite-particle vector states. Thus the normal states are interpretable as the states with a finite number of particles. If the algebra is quasi-local, then the locally normal states, i.e., the states which are normal in restriction to the local generating algebras, correspond to states for which the local subsystems have a finite number of particles. Thus locally normal states can be used to describe infinite systems of particles for which the overall density is finite.

Basically the criterion for normality is the existence of a selfadjoint number operator but as this operator is almost always unbounded some care has to be taken in its definition. On Fock space the number operator N can be decomposed in terms of operators N_f of the form

$$N_f = a^*(f)a(f) \ .$$

It follows from the CARs and CCRs that these operators satisfy the relations

$$[N_f, a(g)] = -(g, f)a(f) \ ,$$
$$[N_f, a^*(g)] = (f, g)a^*(f)$$

and it is consistent with the interpretation of $a(f)$ and $a^*(g)$ as annihilation and creation operators that N_f measures the number of particles in the state $f \in \mathfrak{h}$. Moreover, one easily calculates that

$$(\psi, N\psi) = \sum_\alpha (\psi, N_{f_\alpha}\psi)$$

for $\psi \in D(N)$ where the sum is over an orthonormal basis of $\mathfrak{h}$. We will extend these relationships to other representations.

Notice that N_f is bounded for the CAR algebra but unbounded for the CCR algebra; thus we must first give a suitable definition of N_f for the CCR algebra and then find an appropriate definition of the sum of the N_f. We will use quadratic form techniques to handle both these problems. We need the following facts.

A *sesquilinear form* t over a Hilbert space $\mathfrak{H}$ is a function $\varphi, \psi \in D(t) \times D(t) \mapsto t(\varphi, \psi) \in \mathbb{C}$ where $D(t)$ is a subspace of $\mathfrak{H}$ and t is antilinear in φ and linear in ψ. The form is said to be *densely defined* if its domain $D(t)$ is dense, *symmetric* if

$$t(\varphi, \psi) = \overline{t(\psi, \varphi)}$$

for all $\varphi, \psi \in \mathfrak{H}$, and *positive* if

$$t(\psi, \psi) \geq 0$$

for all $\psi \in D(t)$. Positive forms are automatically symmetric.

Associated with each sesquilinear form t there is a *quadratic form* $t(\psi) = t(\psi, \psi)$. This quadratic form determines t by the polarization formula

$$t(\varphi, \psi) = \sum_{n=0}^{3} i^n t(\psi + i^n \varphi)/4 \ .$$

A positive quadratic form t is said to be *closed* whenever the conditions (1) $\psi_n \in D(t)$, (2) $\|\psi_n - \psi\| \to 0$, and (3) $t(\psi_n - \psi_m) \to 0$ imply that $\psi \in D(t)$ and $t(\psi_n - \psi) \to 0$. Alternatively, t is said to be *closable* if it has a closed extension and this is the case if, and only if, the conditions $\psi_n \in D(t)$, $\|\psi_n\| \to 0$ and $t(\psi_n - \psi_m) \to 0$ imply that $t(\psi_n) \to 0$.

Forms are important because if t is a densely defined, positive, closed, quadratic form, then there exists a unique positive selfadjoint operator T such that $D(t) = D(T^{1/2})$ and

$$t(\varphi, \psi) = (T^{1/2}\varphi, T^{1/2}\psi)$$

for all $\varphi, \psi \in D(t)$. In particular

$$t(\varphi, \psi) = (\varphi, T\psi)$$

for all $\varphi \in D(t)$ and $\psi \in D(T)$. This statement has an obvious converse and hence there is a one-to-one correspondence between forms t of this type and positive selfadjoint operators.

In applications the most sensitive point in the construction of positive operators from forms is the verification of closedness of the forms. But if S is a closed operator with dense domain $D(S)$, and one defines t by $D(t) = D(S)$ and

$$t(\varphi, \psi) = (S\varphi, S\psi) \ ,$$

it is evident that t is positive, densely defined, and closed. If T is the associated positive selfadjoint operator, then $T^{1/2}$ is nothing but the positive part of the polar decomposition of S, and $T = S^*S$.

If ω is a regular state over the CCR algebra $\mathfrak{A}(\mathfrak{h})$ on a pre-Hilbert space $\mathfrak{h}$, one can introduce closed annihilation and creation operators $a_\omega(f)$ and $a_\omega^*(f)$ on $\mathfrak{H}_\omega$ by Lemma 5.2.12. Let $n_{\omega, f}$ and $N_{\omega, f}$ be the positive form and the positive selfadjoint operator defined by $a_\omega(f)$, i.e.,

$$n_{\omega, f}(\psi) = \|a_\omega(f)\psi\|^2, \quad \psi \in D(a_\omega(f)) \ ,$$

$$N_{\omega, f} = a_\omega(f)^* a_\omega(f) \ .$$

We take $N_{\omega, f}$ as number operator for the one particle state $f \in \mathfrak{h}$. It is easy to check from the Weyl form of the CCRs and from Lemma 5.2.12 that one has

$$n_{\omega, f}(\psi) = \left(\|\Phi_\omega(f)\psi\|^2 + \|\Phi_\omega(if)\psi\|^2 - \|f\|^2\|\psi\|^2\right)\Big/2$$

It is natural to attempt to define a total number operator for the state ω by summing the $n_{\omega, f}$ over a complete orthonormal basis, but again the difficulty is whether the resulting quadratic form is closed. To handle this we first define an order relation between positive forms by $t_1 \geq t_2$ if $D(t_1) \subseteq D(t_2)$ and

$$t_1(\psi) \geq t_2(\psi)$$

for all $\psi \in D(t_1)$. This ordering defines an ordering of positive selfadjoint operators. If T_1 and T_2 are the selfadjoint operators determined by the positive, closed, densely defined forms t_1 and t_2, we write

$$T_1 \geq T_2$$

whenever

$$t_1 \geq t_2 \ .$$

This order relation is a generalization of the order for positive elements of a C^*-algebra discussed in Section 2.2.2 and has many properties in common with this latter order. In particular the same argument that established Proposition 2.2.13 shows that if T_1 and T_2 are two positive, invertible, operators and

$$T_1 \geq T_2 \geq 0 \ ,$$

then

$$(T_2 + \lambda \mathbb{1})^{-1} \geq (T_1 + \lambda \mathbb{1})^{-1}$$

for all $\lambda \geq 0$. In particular this means that $D(T_2^{-1/2}) \subseteq D(T_1^{-1/2})$ by the definition of the form ordering. Moreover, the discussion after Proposition 2.2.13 implies that

$$(T_2 + \lambda \mathbb{1})^{-1/2} \geq (T_1 + \lambda \mathbb{1})^{-1/2}$$

for all $\lambda > 0$. These points will be used in proving the following result.

Lemma 5.2.13. *Let t_α be a monotonically increasing net of positive, closed quadratic forms on a Hilbert space $\mathfrak{H}$ and define t by*

$$D(t) = \left\{ \psi; \psi \in \bigcap_\alpha D(t_\alpha), \sup_\alpha t_\alpha(\psi) < +\infty \right\} \ ,$$

$$t(\psi) = \sup_\alpha t_\alpha(\psi) \ .$$

It follows that t is a positive, closed, quadratic form.

If, moreover, t_α and t are densely defined, then the corresponding positive selfadjoint operators T_α and T satisfy

$$\lim_\alpha \|(e^{itT_\alpha} - e^{itT})\psi\| = 0$$

for all $\psi \in \mathfrak{H}$, uniformly for t in finite intervals of $\mathbb{R}$.

Proof. As the net is monotonic

$$t(\psi) = \lim_\alpha t_\alpha(\psi) \ .$$

Thus t is the limit of quadratic forms and it follows easily that it is itself a quadratic form. Moreover, it is positive.

Next assume $\psi_n \in D(t)$, $\|\psi_n - \psi\| \to 0$, and for $\varepsilon > 0$ there is an N_ε such that

$$t(\psi_n - \psi_m) < \varepsilon$$

for all $n, m > N_\varepsilon$. Therefore $t_\alpha(\psi_n - \psi_m) < \varepsilon$ for all α and as t_α is closed, $\psi \in D(t_\alpha)$ and $t_\alpha(\psi_n - \psi) \leq \varepsilon$ for all $n > N_\varepsilon$. But

$$t_\alpha((\psi - \psi_n) + \psi_n) + t_\alpha((\psi - \psi_n) - \psi_n) = 2t_\alpha(\psi_n) + 2t_\alpha(\psi - \psi_n)$$

and hence

$$t_\alpha(\psi) \leq 2t_\alpha(\psi_n) + 2\varepsilon \ .$$

Moreover

$$\sup_\alpha t_\alpha(\psi) \leq 2t(\psi_n) + 2\varepsilon < +\infty$$

and therefore $\psi \in D(t)$. But then

$$t(\psi_n - \psi) = \sup_\alpha t_\alpha(\psi_n - \psi) \leq \varepsilon$$

for all $n > N_\varepsilon$ and thus $t(\psi_n - \psi) \to 0$, i.e., t is closed.

Now consider the second statement. The forms t_α, and hence the operators $T_\alpha + \mathbb{1}$, are monotonically increasing. Therefore, the two families $(T_\alpha + \mathbb{1})^{-1}$ and $(T_\alpha + \mathbb{1})^{-1/2}$ are monotonically decreasing. Thus, by Lemma 2.4.19, $(T_\alpha + \mathbb{1})^{-1}$ converges strongly to a positive operator R and $(T_\alpha + \mathbb{1})^{-1/2}$ converges strongly to a positive operator which, by continuity, is $R^{1/2}$. It also follows from monotonicity that $R \geq (T + \mathbb{1})^{-1}$. This bound has two useful consequences. First, it shows that R is invertible, and its inverse R^{-1} is automatically selfadjoint. Second, it implies that $D((T + \mathbb{1})^{1/2}) \subseteq D(R^{-1/2})$.

Next introduce densely defined operators $B_\alpha = R^{1/2}(T_\alpha + \mathbb{1})^{1/2}$. If $\psi \in D(t_\alpha)$, then

$$\|B_\alpha \psi\|^2 = ((T_\alpha + \mathbb{1})^{1/2}\psi, R(T_\alpha + \mathbb{1})^{1/2}\psi) \leq \|\psi\|^2$$

by monotonicity. Hence B_α has a bounded extension with $\|B_\alpha\| \leq 1$ and B_α^* is bounded with $\|B_\alpha^*\| \leq 1$. It follows that $D(R^{-1/2})$, i.e., the range of $R^{1/2}$, lies in $D((T_\alpha + \mathbb{1})^{1/2})$ for each α. One also has

$$\lim_\alpha \|R^{1/2}(\mathbb{1} - B_\alpha^*)\psi\| = \lim_\alpha \|B_\alpha((T_\alpha + \mathbb{1})^{-1/2} - R^{1/2})\psi\| = 0$$

and hence $\mathbb{1} - B_\alpha$ converges weakly to zero on the range of $R^{1/2}$. As this range is dense, B_α and B_α^* converge weakly to $\mathbb{1}$. But the bound $\|B_\alpha^*\| \leq 1$ gives

$$\|(B_\alpha^* - \mathbb{1})\psi\|^2 \leq 2\|\psi\|^2 - (\psi, B_\alpha^*\psi) - (B_\alpha^*\psi, \psi) \to 0$$

and in particular $\|B_\alpha^*\psi\| \to \|\psi\|$. Therefore, if $\psi \in D(R^{-1/2})$, then

$$\begin{aligned} \lim_\alpha t_\alpha(\psi) + \|\psi\|^2 &= \lim_\alpha \|(T_\alpha + \mathbb{1})^{1/2}\psi\|^2 \\ &= \lim_\alpha \|B_\alpha^* R^{-1/2}\psi\|^2 = \|R^{-1/2}\psi\|^2 \end{aligned}$$

which simultaneously establishes that $\psi \in D(t) = D((T + \mathbb{1})^{1/2})$ and

$$t(\psi) + \|\psi\|^2 = \|(T + \mathbb{1})^{1/2}\psi\|^2 = \|R^{-1/2}\psi\|^2 \ .$$

But one has $D(R^{-1/2}) \subseteq D((T + \mathbb{1})^{1/2}) \subseteq D(R^{-1/2})$ and hence $T + \mathbb{1} = R^{-1}$. Thus we conclude that $(T_\alpha + \mathbb{1})^{-1}$ converges strongly to $(T + \mathbb{1})^{-1}$.

Finally, note that if $\psi = (\mathbb{1} + T)^{-1}\varphi \in D(T)$ and $\psi_\alpha = (\mathbb{1} + T_\alpha)^{-1}\varphi$, then $\psi_\alpha \to \psi$ and $T_\alpha\psi_\alpha = (\mathbb{1} - (\mathbb{1} + T_\alpha)^{-1})\varphi \to T\psi$. Therefore, the unitary groups generated by the T_α converge strongly to the group generated by T by Theorem 3.1.28.

Now let us return to the discussion of the number operator associated with a regular state ω over the CCR algebra on a pre-Hilbert space $\mathfrak{h}$. The finite-dimensional complex subspaces $F \subseteq \mathfrak{h}$ form a directed set when ordered by inclusion. If $\{f_i\}$ is an orthonormal basis for F, define

$$D(n_{\omega,F}) = \bigcap_{f \in F} D(a_\omega(f))$$

and

$$n_{\omega,F}(\psi) = \sum_i n_{\omega,f_i}(\psi) = \sum_i \|a_\omega(f_i)\psi\|^2 \ .$$

As any two orthonormal bases for F are related by a unitary matrix, it follows immediately that this definition of $n_{\omega,F}$ only depends on ω and F.

The $n_{\omega,F}$ form a monotonically increasing net of positive, closed, quadratic forms and their limit will be a positive, closed, quadratic form by Lemma 5.2.13. If this latter form is densely defined, then it uniquely determines a selfadjoint *number operator* N_ω on $\mathfrak{H}_\omega$. The following result shows that the existence of such an operator characterizes normality of ω. The main burden in the proof is the demonstration of algebraic properties of N_ω analogous to properties of the number operator on Fock space.

Theorem 5.2.14. *Let ω be a state over the CAR algebra, or a regular state over the CCR algebra, and let $\{a_\omega(f); f \in \mathfrak{h}\}$ denote the corresponding closed annihilation operators ($a_\omega(f) = \pi_\omega(a(f))$ is bounded in the CAR case). Define a positive, closed quadratic form on $\mathfrak{H}_\omega$ by*

$$n_\omega(\psi) = \sup_F n_{\omega,F}(\psi) \ ,$$

$$D(n_\omega) = \left\{\psi; \psi \in \bigcap_{f \in \mathfrak{h}} D(a_\omega(f)),\ n_\omega(\psi) < +\infty\right\} \ ,$$

where the supremum is over all finite-dimensional subspaces of $\mathfrak{h}$.

The following conditions are equivalent:

(1) *ω is normal with respect to the Fock representation.*
(2) *$D(n_\omega)$ is dense in $\mathfrak{H}_\omega$.*
(3) *$D(n_\omega)$ contains a vector which is cyclic for $\pi_\omega(\mathfrak{A}(h))$ in $\mathfrak{H}_\omega$.*

Moreover if these conditions are satisfied, then

$$\lim_F \|(e^{itN_{\omega,F}} - e^{itN_\omega})\psi\| = 0$$

uniformly for t in finite intervals of $\mathbb{R}$ where N_ω is the selfadjoint operator corresponding to the form n_ω and $N_{\omega,F}$ is the selfadjoint operator determined by the form $n_{\omega,F}$.

Proof. (1) $\Rightarrow$ (3): If ω is normal then by Theorem 2.4.26 $(\mathfrak{H}_\omega, \pi_\omega)$ is a countable direct sum of copies of the Fock representation since the Fock representation is

irreducible. Let $N_\omega = N \oplus N \oplus \cdots$ be a direct sum of copies of the Fock number operator and choose $\psi = \{\psi_n\}_{n\geq 0} \in \mathfrak{H}_\omega$ such that $\psi_n \in D(N)$, the ψ_n are mutually orthogonal, and $\psi \in D(N_\omega)$. Thus

$$\begin{aligned}(\psi, N_\omega \psi) &= \sum_{n\geq 0} (\psi_n, N\psi_n) \\ &= \sum_{n\geq 0} \sup_F \sum_{\{f_i\}\subseteq F} \|a(f_i)\psi_n\|^2 = \sup_F \sum_{\{f_i\}\subseteq F} \|a_\omega(f_i)\psi\|^2\end{aligned}$$

by direct calculation on Fock space. But the irreducibility of the Fock representation and the orthogonality of the components ψ_n ensure that ψ is cyclic for $\pi_\omega(\mathfrak{A}(\mathfrak{h}))$. Thus condition (3) is valid.

We next prove the implications (3) $\Rightarrow$ (2) $\Rightarrow$ (1) for the Weyl algebra. Subsequently, we comment on the easier case of the CAR algebra. The proof relies upon three observations which establish invariance of $D(n_\omega)$ under the Weyl operators and the commutation properties of the number operator N_ω determined by n_ω.

OBSERVATION 1

$$\begin{aligned}n_\omega(\psi) = \sup_{F,t} \sum_{\{f_i\}\subseteq F} \frac{1}{2}\Big\{ &\|\pi_\omega(t^{-1}(W(tf_i) - \mathbb{1}))\psi\|^2 \\ &+ \|\pi_\omega(t^{-1}(W(itf_i) - \mathbb{1}))\psi\|^2 - \|\psi\|^2 \Big\}\end{aligned}$$

and $D(n_\omega)$ is exactly the set of ψ for which the supremum is finite.

The proof relies on the fact that if $U(t) = e^{itH}$ is a continuous unitary group on a Hilbert space, then $\psi \in D(H)$ if, and only if,

$$\sup_t \|t^{-1}(U(t) - \mathbb{1})\psi\| < +\infty$$

by Proposition 3.1.23. Using the spectral representation of U one then finds that

$$\|H\psi\|^2 = \sup_t \|t^{-1}(U(t) - \mathbb{1})\psi\|^2 = \lim_{t\to 0} \|t^{-1}(U(t) - \mathbb{1})\psi\|^2 \ .$$

Now assume the supremum in the statement of the observation is finite. In particular

$$\sup_t \Big\{ \|t^{-1}(\pi_\omega(W(tf) - \mathbb{1}))\psi\|^2 + \|t^{-1}(\pi_\omega(W(itf) - \mathbb{1}))\psi\|^2 - \|\psi\|^2 \Big\} < +\infty$$

for each $f \in \mathfrak{h}$. Thus $\psi \in D(\Phi_\omega(f)) \cap D(\Phi_\omega(if)) = D(a_\omega(f)) = D(a_\omega^*(f))$ and

$$\begin{aligned}&\sup_t \Big\{ \|t^{-1}(\pi_\omega(W(tf) - \mathbb{1}))\psi\|^2 + \|t^{-1}(\pi_\omega(W(itf) - \mathbb{1}))\psi\|^2 - \|\psi\|^2 \Big\}\Big/2 \\ &\quad = \lim_{t\to 0} \Big\{ \|t^{-1}(\pi_\omega(W(tf) - \mathbb{1}))\psi\|^2 + \|t^{-1}(\pi_\omega(W(itf) - \mathbb{1}))\psi\|^2 - \|\psi\|^2 \Big\}\Big/2 \\ &\quad = (\|\Phi_\omega(f)\psi\|^2 + \|\Phi_\omega(if)\psi\|^2 - \|\psi\|^2)/2 = \|a_\omega(f)\psi\|^2\end{aligned}$$

whenever $\|f\| = 1$ where the last step uses Lemma 5.2.12. This identification shows that the form defined by the supremum is at least an extension of n_ω. But if, conversely, ψ is in the domain of n_ω, then $\psi \in D(\Phi_\omega(f)) \cap D(\Phi_\omega(if))$ for all $f \in \mathfrak{h}$ and the same argument identifies the two forms.

OBSERVATION 2

$$\pi_\omega(W(g))D(n_\omega) = D(n_\omega),$$
$$n_\omega(\pi_\omega(W(g))\psi) = n_\omega(\psi) + (\psi, \Phi_\omega(ig)\psi) + \|g\|^2\|\psi\|^2/2 \ .$$

This follows by first using the Weyl form of the commutation relations to establish that

$$\begin{aligned}
&\lim_{t\to 0}\|t^{-1}(\pi_\omega(W(tf) - \mathbb{1}))\pi_\omega(W(g))\psi\|^2 \\
&\quad = \lim_{t\to 0}\|t^{-1}(\pi_\omega(W(tf) - \mathbb{1}))\psi + t^{-1}(e^{-it\,\mathrm{Im}(f,g)} - \mathbb{1})\pi_\omega(W(tf))\psi\|^2 \\
&\quad = \|\Phi_\omega(f)\psi - \mathrm{Im}(f,g)\psi\|^2 \ .
\end{aligned}$$

Thus by Observation 1

$$\begin{aligned}
n_\omega(\pi_\omega(W(g))\psi) = n_\omega(\psi) + (\psi, \Phi_\omega(ig)\psi) + \|g\|^2\|\psi\|^2/2 \\
+ \lim_F(\psi, \Phi_\omega(i(g_F - g))\psi),
\end{aligned}$$

where

$$g_F = \sum_{\{f_i\}\subseteq F} f_i(f_i, g) \ .$$

But $\|\Phi_\omega(i(g_F - g))\psi\|^2 \leq (2n_\omega(\psi) + \|\psi\|^2)\|g_F - g\|^2 \to 0$ and the desired result follows immediately.

The implication (3) $\Rightarrow$ (2) is a consequence of Observation 2 and the linearity of $D(n_\omega)$. Thus if $\psi \in D(n_\omega)$ is cyclic, then $D(n_\omega)$ contains the dense set formed by finite linear combinations of $\pi_\omega(W(f))\psi, f \in \mathfrak{h}$.

OBSERVATION 3

$$a_\omega(f)D(N_\omega^{3/2}) \subseteq D(N_\omega)$$

and for $\psi \in D(N_\omega^{3/2})$

$$N_\omega a_\omega(f)\psi = a_\omega(f)(N_\omega - \mathbb{1})\psi \ .$$

Observation 2 implies that

$$\begin{aligned}
(N_\omega\varphi, W(tf)\psi) = (W(tf)^*\varphi, N_\omega\psi) + t(W(tf)^*\varphi, \Phi(if)\psi) \\
+t^2(W(tf)^*\varphi, \psi)\|f\|^2/2
\end{aligned}$$

for $\varphi \in D(N_\omega)$ and $\psi \in D(N_\omega^{3/2})$. Differentiation of this expression and a similar one with f replaced by if and the subsequent addition of the two results gives

$$(N_\omega\varphi, a_\omega(f)\psi) = (a_\omega^*(f)\varphi, (N_\omega - \mathbb{1})\psi)$$

because $D(N_\omega) \subseteq D(n_\omega) \subseteq \bigcap_f D(\Phi_\omega(f))$. But then $(N_\omega - \mathbb{1})\psi \in D(N_\omega^{1/2}) = D(n_\omega) \subseteq \bigcap_f D(a_\omega(f))$. Thus one has

$$(N_\omega\varphi, a_\omega(f)\psi) = (\varphi, a_\omega(f)(N_\omega - \mathbb{1})\psi)$$

for all $\varphi \in D(N_\omega)$ where we have used $a_\omega^*(f)^* \supseteq a_\omega(f)$. The result follows by continuity of the right-hand side in φ.

Now we are prepared to prove (2) $\Rightarrow$ (1) of the theorem.

Let E_ω denote the spectral family of N_ω and for simplicity set $P_\lambda = E_\omega(\langle -\infty, \lambda])$. For each $f \in \mathfrak{h}$ the operator $P_\mu a_\omega(f) P_\lambda$ is a bounded operator from $P_\lambda \mathfrak{H}_\omega$ to $P_\mu \mathfrak{H}_\omega$ because $\|a_\omega(f)\psi\| \leq \|N_\omega^{1/2}\psi\|$. But $P_\lambda N_\omega$ and $P_\mu N_\omega$ are bounded operators on $P_\lambda \mathfrak{H}_\omega$ and $P_\mu \mathfrak{H}_\omega$ and hence Observation 3 and functional analysis of bounded operators gives

$$F(N_\omega) P_\mu a_\omega(f) P_\lambda = P_\mu a_\omega(f) P_\lambda F(N_\omega - \mathbb{1})$$

for any bounded function F. In particular

$$P_{\lambda-1} a_\omega(f) P_\lambda = P_\mu a_\omega(f) P_\lambda$$

for all $\mu \geq \lambda$. Therefore,

$$P_{\lambda-1} a_\omega(f) P_\lambda = a_\omega(f) P_\lambda \ .$$

But N_ω is positive and hence if λ_0 denotes the greatest lower bound of its spectrum, one must have

$$a_\omega(f) P_{\lambda_0+1/2} = 0 \ .$$

Thus if ψ_0 is a unit vector in the range of $P_{\lambda_0+1/2}$,

$$a_\omega(f)\psi_0 = 0$$

for all $f \in \mathfrak{h}$.

Next let P_{ψ_0} be the projection onto the cyclic subspace generated by application of the operators $a_\omega^*(f)$ to ψ_0. It follows from $a_\omega(f)\psi_0 = 0$ that the subrepresentation $P_{\psi_0}\pi_\omega$ of π_ω is unitarily equivalent to the Fock representation. (The implementing unitary operator is given by

$$U a_\omega^*(f_1) \cdots a_\omega^*(f_n)\Omega_\omega = a^*(f_1) \cdots a^*(f_n)\Omega$$

where $\Omega = (1, 0, 0, \ldots) \in \mathfrak{F}_+(\mathfrak{h})$.) Now we repeat the same construction for the subrepresentation $\pi_\omega^0 = (\mathbb{1} - P_{\psi_0})\pi_\omega$ and $\mathfrak{H}_\omega^0 = (\mathbb{1} - P_{\psi_0})\mathfrak{H}_\omega$ to find a $\psi_1 \in \mathfrak{H}_\omega^0$ such that $P_{\psi_1}\mathfrak{H}_\omega^0$ is unitarily equivalent to the Fock representation. The proof is achieved by complete induction.

In the CAR case Observation 1 is irrelevant. Observations 2 and 3 are replaced by

$$n_\omega(a_\omega(f)\psi) + n_\omega(a_\omega^*(f)\psi) = n_\omega(\psi) - 2\|a_\omega(f)\psi\|^2 + \|f\|^2 \ ,$$

$$n_\omega(\varphi, a_\omega(f)\psi) = n_\omega(a_\omega^*(f)\varphi, \psi) - (\varphi, a_\omega(f)\psi)$$

which are computed before taking the limit in the definition of n_ω. The rest of the argument is identical to the CCR case.

The final statement of the theorem follows directly from Lemma 5.2.13.

One classic consequence of Theorem 5.2.14 is the following:

Corollary 5.2.15 (Stone–von Neumann uniqueness theorem). *Let $\mathfrak{A}(\mathfrak{h})$ be the CCR algebra over a finite-dimensional Hilbert space $\mathfrak{h}$.*

It follows that each regular state ω over $\mathfrak{A}(\mathfrak{h})$ is normal with respect to the Fock representation and hence any regular representation of $\mathfrak{A}(\mathfrak{h})$ is a multiple of the Fock representation.

PROOF. From Theorem 5.2.14 it suffices to show that the operators $\{a_\omega(f); f \in \mathfrak{h}\}$ have a common dense domain in $\mathfrak{H}_\omega$. But as $\mathfrak{h}$ is finite dimensional this follows from Lemma 5.2.12.

We can also use this result to complete the proof of Lemma 5.2.12, i.e., to show that $a_\omega(f)^* = a_\omega^*(f)$ for each regular ω and $f \in \mathfrak{h}$. The restriction of π_ω to the CCR algebra over $\mathbb{C}f$ is a multiple of the Fock representation of this algebra by Corollary 5.2.15. Hence it is enough to prove that $a(f)^* = a^*(f)$ in the Fock representation. Writing the Fock space $\mathfrak{F}_+$ as a direct sum of n-particle spaces

$$\mathfrak{F}_+ = \oplus \mathfrak{h}_+^n \ ,$$

we know that $\mathfrak{h}_+^n \subseteq D(a^*(f))$ for all n and the linear span of the $\mathfrak{h}_+^n$ is a core for $a^*(f)$, since it is a joint core for $\Phi(f)$ and $\Phi(if)$. We know already that $a^*(f) \subseteq a(f)^*$. To show the converse, assume that $\psi = \bigoplus_{n\geq 0} \psi^{(n)} \in D(a(f)^*)$. This means that the functional

$$\varphi \in D(a(f)) \to (\psi, a(f)\varphi)$$

is bounded. But if $\varphi = \bigoplus_{n\geq 0}\varphi^{(n)}$ is a finite-particle vector it follows from $a(f)\mathfrak{h}_+^n \subseteq \mathfrak{h}_+^{n-1}$ that

$$(\psi, a(f)\varphi) = \sum_{n\geq 1}(\psi^{(n-1)}, a(f)\varphi^{(n)}) = \sum_{n\geq 1}(a^*(f)\psi^{(n-1)}, \varphi^{(n)}) \ .$$

Hence the boundedness in φ implies that

$$\sum_{n\geq 0} \|a^*(f)\psi^{(n)}\|^2 < +\infty \ .$$

But as $a^*(f)$ is closed, this implies that $\psi = \bigoplus_{n\geq 0}\psi^{(n)} \in D(a^*(f))$ and

$$(a^*(f)\psi)^{(n)} = a^*(f)\psi^{(n-1)} \ .$$

Thus

$$a^*(f) = a(f)^* \ , \qquad a(f) = a^*(f)^* \ .$$

The proof we have given of the von Neumann uniqueness theorem is only one of several existing proofs. One can for example give another proof by employing the argument used to show the uniqueness of the CCRs in Theorem 5.2.8, but regarding $\mathfrak{h}$ as the locally compact abelian group $\mathbb{R}^{2n}$ in its usual topology rather than the discrete one, where n is the complex dimension of $\mathfrak{h}$.

Corollary 5.2.15 identifies the regular states on the CCR algebra $\mathfrak{A}(\mathfrak{h})$ over a general pre-Hilbert space $\mathfrak{h}$ with the states which are locally normal with respect to the quasi-local structure defined by the finite-dimensional complex subspaces of $\mathfrak{h}$. Thus, as far as regular states are concerned, one could define the CCR algebra as a closure of a union of algebras of the form $\mathscr{L}(\mathfrak{F}_+(M))$, where $\mathfrak{F}_+(M)$ is the symmetric Fock space over the finite-dimensional subspace M and $\mathscr{L}(\mathfrak{F}_+(M))$ is the weak closure of $\mathfrak{A}(M)$ in the Fock representation. This latter definition of the CCR algebra gives a larger algebra without the deficiencies mentioned in the introduction to this subsection, i.e., it contains all bounded Borel functions of the fields $\Phi(f)$.

Although the Fock representation is the unique irreducible regular representation of $\mathfrak{A}(\mathbb{C}^n)$, up to equivalence, it often appears in a seemingly different form, e.g., it occurs as the Schrödinger representation in quantum mechanics. The physical interpretation of this latter reformulation is rather different and it is of some interest to cast the representation in this form because it also immediately allows the construction of a nonregular irreducible representation.

EXAMPLE 5.2.16 (The Schrödinger representation). Let $\{f_j; j = 1, 2, \ldots, n\}$ be an orthonormal basis of the finite-dimensional Hilbert space $\mathfrak{h}$ and introduce $2n$ one-parameter groups U_j and V_j by

$$U_j(s_j) = W(s_j f_j) \ , \qquad V_j(t_j) = W(it_j f_j) \ ,$$

where the W are Weyl operators. These groups can be represented on $L^2(\mathbb{R}^n)$ by

$$(U_j(s_j)\psi)(x_1, \ldots, x_n) = e^{is_j x_j}\psi(x_1, \ldots, x_n) \ ,$$

$$(V_j(t_j)\psi)(x_1, \ldots, x_n) = \psi(x_1, \ldots, x_j - t_j, \ldots, x_n) \ .$$

Now if $f \in \mathfrak{h}$ has the decomposition

$$f = \sum_{j=1}^{n} (s_j + it_j) f_j \ ,$$

one obtains a representation of the Weyl algebra with

$$W(f) = \prod_{j=1}^{n} e^{is_j t_j/2} U_j(s_j) V_j(t_j) \ .$$

In particular

$$(\Phi(f_j)\psi)(x_1, \ldots, x_n) = x_j \psi(x_1, \ldots, x_n) \ ,$$
$$(\Phi(if_j)\psi)(x_1, \ldots, x_n) = -i \frac{\partial}{\partial x_j} \psi(x_1, \ldots, x_n)$$

and

$$a(f_j) = 2^{-1/2}\left(x_j + \frac{\partial}{\partial x_j}\right), \qquad a^*(f_j) = 2^{-1/2}\left(x_j - \frac{\partial}{\partial x_j}\right) \ .$$

Now the Fock vacuum, i.e., the vector $\Omega = (1, 0, 0, \ldots)$, is determined by the equation

$$a(f)\Omega = 0 \ ,$$

and hence its representative $\Omega(x_1, \ldots, x_n)$ in the Schrödinger representation is the unique (up to a phase factor) solution of

$$\left(x_j + \frac{\partial}{\partial x_j}\right)\Omega(x_1, \ldots, x_n) = 0 \ .$$

Thus

$$\Omega(x_1, x_2, \ldots, x_n) = \pi^{-n/2} \exp\left(-(x_1^2 + x_2^2 + \cdots + x_n^2)/2\right) \ ,$$

and the representatives of the multiparticle states are given by

$$a^*(f_{j_1})\cdots a^*(f_{j_m})\Omega = 2^{-m/2}\prod_{k=1}^{m}\left(x_{jk} - \frac{\partial}{\partial x_{jk}}\right)\Omega(x_1,\ldots,x_n\ )\ .$$

This identification determines the equivalence of the Fock and Schrödinger representation.

Physically one can interpret $L^2(\mathbb{R}^n)$ as the space of states of one-particle moving in n dimensions. The $\Phi(f_j)$ correspond to the position operators, or observables, and the $\Phi(if_j)$ correspond to the coordinates of momentum. The Fock number operator is given by the differential operator

$$N = \sum_{j=1}^{n}(-\partial^2/\partial x_j^2 + x_j^2 - 1)/2$$

and in the Schrödinger picture this is interpreted as the Hamiltonian of a harmonic oscillator. Thus from this point of view Ω is the ground state, the state of lowest energy, of the oscillator and the creation and annihilation operators create and annihilate quanta of energy.

EXAMPLE 5.2.17. Let $A(\mathbb{R}^n)$ be the almost periodic functions over $\mathbb{R}^n$ and let M denote the unique invariant mean over $A(\mathbb{R}^n)$ (see Section 4.3.4). The mean M defines a scalar product on $A(\mathbb{R}^n)$ by

$$(f,g) = M(\bar{f}g)$$

and the completion of $A(\mathbb{R}^n)$ with respect to the associated norm is a Hilbert space $\mathfrak{H}$. If $\mathfrak{h}$ is n dimensional, one can define a representation of the associated Weyl algebra on $A(\mathbb{R}^n)$ by exactly the same construction given in Example 5.2.16. Extension by continuity then gives a representation on $\mathfrak{H}$. This representation is not, however, regular. For example, if $f \neq 0$ and $\Omega(x_1,\ldots,x_n) = 1$, then

$$(\Omega, W(tf)\Omega) = \begin{cases} 1, & \text{if } t = 0 \\ 0, & \text{if } t \neq 0 \end{cases}\ .$$

Note that the Hilbert space $\mathfrak{H}$ is nonseparable, $\{\exp\{i\sum_{j=1}^{n}\lambda_j x_j\};\lambda_i \in \mathbb{R}\}$ forms an orthonormal basis of the space. A similar nonregular representation of the CCRs is given by R_b in the proof of Theorem 5.2.8.

We complete this discussion of normal states with a few comments on a special subclass, the finite-density states. Theorem 5.2.14 establishes that ω is normal if, and only if, $D(n_\omega)$ contains a cyclic vector. But there is a preferred cyclic vector Ω_ω associated with ω and we call ω a *finite-density state* if $\Omega_\omega \in D(n_\omega)$. Thus ω has finite density if, and only if, ω is normal with respect to the Fock representation and $\Omega_\omega \in D(N_\omega^{1/2})$. If ρ is the density matrix on Fock space which determines ω, then the latter property is equivalent to the positive selfadjoint operator $N^{1/2}\rho N^{1/2}$ having a finite trace. Note also that one can define a positive functional, the number functional, $\omega \in E_{\mathfrak{A}} \mapsto \widehat{N}(\omega) \in [0,\infty]$ by

$$\widehat{N}(\omega) = \sup_F \sum_{\{f_i\}\subseteq F} \omega(a^*(f_i)a(f_i))$$

if $\mathfrak{A}$ is the CAR algebra and

$$\widehat{N}(\omega) = \sup_{t,F} \sum_{\{f_i\} \subseteq F} \{t^{-2}\omega((W(tf_i) - \mathbb{1})^*(W(tf_i) - \mathbb{1}))$$
$$+t^{-2}\omega((W(itf_i) - \mathbb{1})^*(W(itf_i) - \mathbb{1})) - 1\}/2$$

for the Weyl algebra, and then ω has finite density if, and only if, $\widehat{N}(\omega) < +\infty$. In both formulae the suprema are over finite orthonormal subsets $\{f_i\}$ of $\mathfrak{h}$ and the assertion for the CCR algebra uses Observation 1 of the proof of Theorem 5.2.14.

Note also that in the CCR case it follows from the proof of Theorem 5.2.14 that $\widehat{N}(\omega) < +\infty$ implies that $\Omega_\omega \in D(a_\omega(f))$ for all f and

$$\widehat{N}(\omega) = \sup_F \sum_{\{f_i\} \subseteq F} \|a_\omega(f_i)\Omega_\omega\|^2$$

in analogy with the CAR case. Moreover, if $\widehat{N}(\omega) < +\infty$, then its value can be interpreted as the extension of ω to the number operator and one has the identifications

$$\widehat{N}(\omega) = \|N_\omega^{1/2}\Omega_\omega\|^2 = \mathrm{Tr}_{\widetilde{\mathfrak{H}}}(N^{1/2}\rho N^{1/2}) \ .$$

It is of some interest to remark that $\widehat{N}$ is affine, because the suprema are net limits, and lower semi-continuous in the weak* topology, because $\widehat{N}$ is the upper envelope of a family of weak*-continuous functionals. In particular $\widehat{N}$ respects barycentric decompositions, by Corollary 4.1.18 applied to $-\widehat{N}$, and the subsets of states with density below a fixed bound, i.e., the sets $\{\omega; \widehat{N}(\omega) \leq \lambda\}$, are weak*-closed by lower semicontinuity.

Next we examine more detailed properties of states with respect to the annihilation and creation operators and, in particular, the determination of a state by its values on these operators. Discussion of states over the CAR algebra is simpler because the algebra contains the annihilation and creation operators $a(f), a^*(g); f, g \in \mathfrak{h}$ and it follows easily that each ω is determined by the set of values $\omega(a^*(f_1)\cdots a^*(f_n)a(f_{n+1})\cdots a(f_{n+m})), n, m \geq 0, f_i \in \mathfrak{h}$. A similar result is also true for a subset of regular states over the Weyl algebra.

If ω is a regular state over the Weyl algebra $\mathfrak{A}(\mathfrak{h})$, then the infinitesimal generators $\Phi_\omega(f)$ of the Weyl groups $t \in \mathbb{R} \mapsto \pi_\omega(W(tf))$ are defined for all $f \in \mathfrak{h}$ and one can introduce the annihilation and creation operators $a_\omega(f)$ and $a_\omega^*(f)$. But, as we have mentioned above, the cyclic vector Ω_ω is not necessarily in the domain of these operators. Thus it is generally impossible to define analogues of the $\omega(a^*(f_1)a(f_2))$, etc. For this reason it is natural to introduce more stringent notions of regularity of states and their associated cyclic vectors.

A state ω over $\mathfrak{A}(\mathfrak{h})$ is defined to be in the class C^m if $t \mapsto \omega(W(tf))$ is m times differentiable for all $f \in \mathfrak{h}$. Similarly, $\psi \in C^m$ if $\pi_\omega(W(tf))\psi$ is m times strongly differentiable for all $f \in \mathfrak{h}$. This latter condition is equivalent to $\psi \in D(\Phi_\omega(f)^m)$ for all f, and it is not difficult to see that $\omega \in C^{2m}$ if, and only if, $\Omega_\omega \in C^m$. In particular the value of C^∞ states can be defined on all polynomials of the $\Phi_\omega(f)$, and we use the natural notation

$$\omega(\Phi_\omega(f_1)\cdots\Phi_\omega(f_n)) = (\Omega_\omega, \Phi_\omega(f_1)\cdots\Phi_\omega(f_n)\Omega_\omega) \ ,$$

$$\omega(A\Phi_\omega(f_1)\cdots\Phi_\omega(f_n)) = (\Omega_\omega, \pi_\omega(A)\Phi_\omega(f_1)\cdots\Phi_\omega(f_n)\Omega_\omega) \ ,$$

etc. Finally a C^∞ state ω is called *analytic* (*entire analytic*) whenever the functions $t \in \mathbb{R} \mapsto \omega(W(tf))$ are analytic in an open neighborhood of the origin (are entire analytic), for all $f \in \mathfrak{h}$. There are two interesting properties of analytic states.

First, a state ω is analytic if, and only if, Ω_ω is an analytic vector for all $\Phi_\omega(f)$. For example, if Ω_ω is analytic for $\Phi_\omega(f)$, then $t \mapsto \pi_\omega(W(tf))\Omega_\omega$ is strongly analytic and hence $t \mapsto \omega(W(tf))$ is analytic. Conversely, if ω is analytic, then Ω_ω is a C^∞ vector and

$$\omega(W(tf)) = \sum_{n \geq 0} \frac{i^n t^n}{n!} (\Omega_\omega, \Phi_\omega(f)^n \Omega_\omega) \ .$$

Therefore

$$t \in \mathbb{R} \mapsto \sum_{n \geq 0} (-1)^n \frac{t^{2n}}{(2n)!} \|\Phi_\omega(f)^n \Omega_\omega\|^2$$

is analytic and as $(2n)! \geq 2^{2(n-1)}(n-1)!^2$ one has

$$\sum_{n \geq 0} \left(\frac{|t|^n}{(n-1)!} \|\Phi_\omega(f)^n \Omega_\omega\| \right)^2 < +\infty$$

for all $|t| < t_0$ and for some $t_0 > 0$. Equivalently

$$\sum_{n \geq 0} \frac{|t|^n}{n!} \|\Phi_\omega(f)^n \Omega_\omega\| < +\infty$$

for $|t| < t_0$, i.e., Ω_ω is analytic for $\Phi_\omega(f)$.

Second, if ω is analytic, then each of the functions $t \in \mathbb{R} \mapsto \omega(W(tf))$ is actually analytic in an open strip around the real axis. This is because the W are unitary and hence one has estimates of the form

$$|(\Omega_\omega, \pi_\omega(W(tf))\Phi_\omega(f)^{2n}\Omega_\omega)| \leq |(\Omega_\omega, \Phi(f)^{2n}\Omega_\omega)| \ ,$$

$$|(\Omega_\omega, \pi_\omega(W(tf))\Phi_\omega(f)^{2n-1}\Omega_\omega)| \leq |(\Omega_\omega, \Phi_\omega(f)^{2n}\Omega_\omega)|^{1/2} |(\Omega_\omega, \Phi_\omega(f)^{2n-2}\Omega_\omega)|^{1/2} \ .$$

This second remark has an important consequence.

Each state ω over the Weyl algebra is determined by its values on the set of Weyl operators $\{W(f); f \in \mathfrak{h}\}$. But if ω is analytic, then $\omega(W(f))$ is determined by the derivatives of the function $t \mapsto \omega(W(tf))$ at the origin. Thus each analytic state is determined by the set of matrix elements, or expectation values, $\{\omega(\Phi_\omega(f)^n); f \in \mathfrak{h}, n \geq 1\}$. Alternatively ω is determined by the set $\{\omega(a_\omega^*(f)^n a_\omega(f)^m)\}$. Hence properties of the analytic states can, in principle, be completely reconstructed from knowledge of either of these sets.

The conclusion of these observations is that analytic states ω over the Weyl algebra are determined by the set of multilinear functionals $\{\omega(a_\omega^*(f_1)\cdots a_\omega^*(f_n)a_\omega(f_{n+1})\cdots a_\omega(f_{n+m})); n, m \geq 0, f_i \in \mathfrak{h}\}$. In this sense analytic states are analogous to states over the CAR algebra. Both are de-

termined by a family of functionals which are expressed in terms of operators with a clear physical interpretation.

It is often useful to consider other classes of multilinear functionals, the truncated functionals, whose values are directly related to correlations between physical events. These functionals are determined by recursion relations which are different for the CARs and CCRs and are combinatorically somewhat easier for the latter. Thus we first describe the definitions corresponding to the CCRs.

Let $\mathfrak{I}$ denote an arbitrary index set and F a function from the nonempty finite subsets of $\mathfrak{I}$ to the complex numbers. We associate with F the *truncated function* F_T by the recursion relations

$$F(I) = \sum_{\mathscr{P}_I} \prod_{J \in \mathscr{P}_I} F_T(J) \ ,$$

where the sum is over all partitions $\mathscr{P}_I$ of the finite set I into ordered subsets. Explicitly $\mathscr{P}_I = \{J_1, J_2, \ldots, J_n\}$ where $J_i \cap J_i = \varnothing$ if $i \neq j$, the union of the J_i is I, and the elements of each J_i retain the order of I. For example, one has

$$F(\alpha) = F_T(\alpha) \ , \qquad F(\alpha, \beta) = F_T(\alpha, \beta) + F_T(\alpha) F_T(\beta) \ , \qquad \text{etc.},$$

and these equations have the solutions

$$F_T(\alpha) = F(\alpha) \ , \qquad F_T(\alpha, \beta) = F(\alpha, \beta) - F(\alpha) F(\beta) \ , \qquad \text{etc.},$$

It is often useful to remark that

$$F(I) = \sum_{\alpha \in J \subseteq I} F_T(J) F(I \backslash J)$$

for any $I \ni \alpha$, where we take $F(\varnothing) = 1$. This follows directly from the recursion relations by noting that the coefficient of an arbitrary term $F_T(J)$ in these relations is given by

$$\sum_{\mathscr{P}_{I \backslash J}} \prod_{K \in \mathscr{P}_{I \backslash J}} F_T(K) = F(I \backslash J) \ .$$

These algorithms can now be used to associate truncated functionals with an analytic state ω over the Weyl algebra on $\mathfrak{h}$. Let $\mathfrak{I}$ consist of elements of $\mathfrak{h}$ and then the values $\omega(\Phi_\omega(f_1) \cdots \Phi_\omega(f_n))$ of ω on monomials of the $\Phi_\omega(f)$ define a complex function over the ordered finite subsets of $\mathfrak{I}$. The above procedure defines a truncation ω_T which satisfies

$$\omega_T(\Phi_\omega(f)) = \omega(\Phi_\omega(f)) \ ,$$
$$\omega_T(\Phi_\omega(f_1), \Phi_\omega(f_2)) = \omega(\Phi_\omega(f_1)\Phi_\omega(f_2)) - \omega(\Phi_\omega(f_1))\omega(\Phi_\omega(f_2)) \ , \ \text{etc.}$$

By linear combination, or reapplication of the same procedure, one also obtains truncations of the functions $\omega(a_\omega^*(f_1) \cdots a_\omega^*(f_n) a_\omega(g_1) \cdots a_\omega(g_m))$. It is evident that the truncated functionals inherit all the linearity and antilinearity properties of the nontruncated functionals and, moreover, that the state ω is determined by the truncated functionals.

The truncated functional $\omega_T(a_\omega^*(f), a_\omega(g))$ represents the correlation between the operations of annihilation of a particle with wavefunction g and the

creation of a particle with wave function f. The higher truncations represent multiple correlations. In Section 5.2.5 we demonstrate that the equilibrium states of a system of noninteracting bosons have the simple property that the higher-order correlations vanish identically and this property can be used to characterize a special class of states, the quasi-free states. Explicitly an analytic state ω is called *quasi-free* if

$$\omega_T(\Phi_\omega(f_1), \ldots, \Phi_\omega(f_n)) = 0$$

for all $n > 2$ and all $f_1, \ldots, f_n \in \mathfrak{h}$. Thus a quasi-free state is determined by two functionals $\omega_T(\Phi_\omega(f))$ and $\omega_T(\Phi_\omega(f_1), \Phi_\omega(f_2))$. Of course these functionals must satisfy certain positivity properties. In particular the conditions

$$\|\{\Phi_\omega(f_1) + i\Phi_\omega(f_2) - \omega(\Phi_\omega(f_1) + i\Phi_\omega(f_2))\mathbb{1}\}\Omega_\omega\|^2 \geq 0$$

can be reexpressed as

$$\omega_T(\Phi_\omega(f_1), \Phi_\omega(f_1)) + \omega_T(\Phi_\omega(f_2), \Phi_\omega(f_2)) - \mathrm{Im}(f_1, f_2) \geq 0 \ .$$

Therefore, these conditions are necessary for the truncated functionals to determine a state. What is less obvious is that this set of conditions, for all $f_1, f_2 \in \mathfrak{h}$, is also sufficient for the ω_T to determine a quasi-free state ω. The sufficiency can be proved by explicit construction of the representation $(\mathfrak{H}_\omega, \pi_\omega, \Omega_\omega)$ (see Notes and Remarks). In particular every analytic state ω determines a quasi-free state which is obtained by setting $\omega_T(\Phi_\omega\ (f_1), \ldots, \Phi_\omega(f_n)) = 0$ for all $n > 2$.

EXAMPLE 5.2.18. Let ω be a state on the CCR algebra over the pre-Hilbert space $\mathfrak{h}$ and assume that ω is invariant under the group of gauge transformations $\theta \in [0, 2\pi\rangle \to \tau_0(W(f)) = W(e^{i\theta}f)$. If ω is analytic, then this invariance can be expressed by

$$\omega(a^*_\omega(f_1) \cdots a^*_\omega(f_n) a_\omega(g_1) \cdots a_\omega(g_m)) = 0$$

if $n \neq m$. Hence a gauge-invariant quasi-free state is determined by a single sesquilinear form $\omega_T(a^*(f), a(g))$ and the positivity conditions reduce to the simple conditions

$$\omega_T(a^*(f), a(f)) \geq 0 \ .$$

Conversely assume that one has a positive sesquilinear form t over $\mathfrak{h}$ and for simplicity assume that it is given by a positive selfadjoint operator T on the completion $\bar{\mathfrak{h}}$, of $\mathfrak{h}$, i.e.,

$$t(g, f) = (T^{1/2}g,\ T^{1/2}f)$$

for all $f, g \in \mathfrak{h}$. Let $\mathfrak{H}_\omega = \mathfrak{F}_+(\mathfrak{h}) \otimes \mathfrak{F}_+\mathfrak{h}$ and $\Omega_\omega = \Omega \otimes \Omega$, where $\Omega = (1, 0, 0, \ldots)$ is the Fock vacuum. If J is an anti-linear involution satisfying $(Jf, Jg) = (g, f)$, then the operators

$$a_\omega(f) = a(\sqrt{1+T}f) \otimes \mathbb{1} + \mathbb{1} \otimes a^*(J\sqrt{T}f) \ ,$$

$$a^*_\omega(g) = a^*(\sqrt{1+T}g) \otimes \mathbb{1} + \mathbb{1} \otimes a(J\sqrt{T}g)$$

satisfy the CCRs on $\mathfrak{H}_\omega$. (The a and a^* denote the Fock annihilation and creation operators.) It follows easily that the state $\omega(A) = (\Omega_\omega, A\Omega_\omega)$ is a gauge-invariant quasi-free state and one has

$$\omega(a_\omega^*(f)a_\omega(g)) = (J\sqrt{T}f, J\sqrt{T}g) = (\sqrt{T}g, \sqrt{T}f) = t(g,f) \ .$$

On the CCR algebra itself this state is given by

$$\begin{aligned}\omega(W(f)) &= \exp\{-\omega(\varphi_\omega(f)^2)/2\} \\ &= \exp\{-\|f\|^2/4\} \exp\{-t(f,f)/2\} \ .\end{aligned}$$

The truncated functionals can be used to reexpress mixing properties of a state, with respect to groups of Bogoliubov transformations, in a particularly simple manner. This reformulation explicitly connects mixing properties and the lack of correlation between physical events. It is illustrated by the following example.

EXAMPLE 5.2.19. Let $\mathfrak{A}$ denote the CCR algebra over $L^2(\mathbb{R}^\nu)$, or the quasi-local C^*-subalgebra of $\mathfrak{A}$ defined in Example 5.2.11. The group $\mathbb{R}^\nu$ of space translations acts as *-automorphisms τ of $\mathfrak{A}$ via Bogoliubov transformations, e.g.,

$$\tau_x(W(f)) = W(U_x f) \ , \qquad (U_x f)(y) = f(y-x) \ .$$

Note that the CCRs give

$$\begin{aligned}\|[\tau_x(W(f)), W(g)]\| &= |2\sin(\mathrm{Im}(U_x f, g)/2)| \\ &\leq |(U_x f, g)|\end{aligned}$$

and hence

$$\lim_{|x|\to\infty} \|[\tau_x(W(f)), W(g)]\| = 0 \ .$$

It follows that $\mathfrak{A}$ is asymptotically abelian for space translations in the norm sense, i.e.,

$$\lim_{|x|\to\infty} \|[\tau_x(A), B]\| = 0$$

for all $A, B \in \mathfrak{A}$. Thus if ω is any state over $\mathfrak{A}$, the strong mixing property

$$\lim_{|x|\to\infty} |\omega(A\tau_x(B)) - \omega(A)\omega(\tau_x(B))| = 0$$

for all $A, B \in \mathfrak{A}$, is equivalent to the three-body cluster property

$$\lim_{|x|\to\infty} |\omega(A\tau_x(B)C) - \omega(AC)\omega(\tau_x(B))| = 0$$

for all $A, B, C \in \mathfrak{A}$. If, however, ω is $\mathbb{R}^\nu$-invariant and analytic the following are equivalent:

(1) ω is strongly mixing for space translations,

(2) $\lim_{|x|\to\infty} \omega_T(\Phi_\omega(f_1), \ldots, \Phi_\omega(f_n), \tau_x(\Phi_\omega(g_1)), \ldots, \tau_x(\Phi_\omega(g_m))) = 0$

for all $n, m \geq 1$ and all $f_1, \ldots f_n, g_1, \ldots, g_m \in L^2(\mathbb{R}^\nu)$, where $\tau_x(\Phi_\omega(f)) = \Phi_\omega(U_x\ f)$.

PROOF. (1) $\Rightarrow$ (2). For $g \in L^2(\mathbb{R}^\nu)$ and all $x \in \mathbb{R}^\nu$ the vector-valued functions

$$t \in \mathbb{R} \mapsto \pi_\omega(W(tU_x f))\Omega_\omega$$

have an analytic extension to a strip around the real axis whose width is independent of x. This follows from the $\mathbb{R}^\nu$-invariance and analyticity of ω. It then follows by power-series expansion and the density of the Weyl operators that condition (1) is equivalent to

$$(1') \qquad \lim_{|x|\to\infty} \omega(\Phi_\omega(f)^n \tau_x(\Phi_\omega(g))^m) = \omega(\Phi_\omega(f)^n)\omega(\Phi_\omega(g)^m)$$

for all $f, g \in L^2(\mathbb{R}^\nu)$ and all $n, m \geq 1$. But (1′) is equivalent to

$$(2') \qquad \lim_{|x|\to\infty} \omega_T\, \underbrace{(\Phi_\omega(f), \ldots, \Phi_\omega(f)}_{n\text{-factors}},\ \tau_x\, \underbrace{(\Phi_\omega(g)), \ldots, \tau_x(\Phi_\omega(g)))}_{m\text{-factors}} = 0$$

for all $f, g \in L^2(\mathbb{R}^\nu)$ and all $n, m \geq 1$. This is obvious for $n = m = 1$ but the general case follows by inductive reasoning from the formula

$$F(I) = \sum_{\alpha \in J \subseteq I} F_T(J) F(I \backslash J)$$

connecting a function and its truncations. Finally (2) and (2′) are equivalent by linearity and anti-linearity.

Note that the above properties all stem from the fact that $(U_x f, g) \to 0$ as $|x| \to \infty$ and hence they generalize easily to other Bogoliubov transformations. Moreover the various results are valid if the pointwise limits are replaced by mean values.

The notion of truncated function can be extended to the CAR algebra $\mathfrak{A}$ over $\mathfrak{h}$ but with two differences. First, there is a simplification because the $a(f)$ and $a^*(g)$ are elements of the algebra and thus there is no inherent restriction on the states. The second difference is a slight complication of the combinatorics of the truncation process which is necessary for consistency with the anti-commutation relations. This modification is only possible for even states, i.e., states which are invariant under the unique *-automorphism σ of $\mathfrak{A}$ for which $\sigma(a(f)) = -a(f), f \in \mathfrak{h}$. The appropriate definitions are as follows.

Let $\mathfrak{I}$ once again denote an index set and F a function from the nonempty ordered even subsets of $\mathfrak{I}$ to the complex numbers. The truncation F_T of F is now defined recursively by

$$F(I) = \sum_{\mathscr{P}_I} \varepsilon(\mathscr{P}_I) \prod_{J \in \mathscr{P}_I} F_T(J) \ ,$$

where the sum is over all partitions $\mathscr{P}_I$ of I into ordered even subsets, $\mathscr{P}_I = \{J_1, \ldots, J_n\}$ and $\varepsilon(\mathscr{P}_I)$ is $+1$ or -1 according to whether the permutation $I \mapsto (J_1, J_2, \ldots, J_n)$ is even or odd. Note that as the J_i are even their interchange does not affect the even or odd character of the permutation. The simplest examples are

$$F(\alpha, \beta) = F_T(\alpha, \beta) \ ,$$

$$\begin{aligned} F(\alpha, \beta, \gamma, \delta) = {} & F_T(\alpha, \beta, \gamma, \delta) + F_T(\alpha, \beta) F_T(\gamma, \delta) \\ & - F_T(\alpha, \gamma) F_T(\beta, \delta) + F_T(\alpha, \delta) F_T(\beta, \gamma) \end{aligned}$$

and by inversion one obtains F_T in terms of F. Again one has a simple inductive relation connecting the F and F_T,

$$F(I) = \sum_{\alpha \in J \subseteq I} \varepsilon(J, I\backslash J) F_T(J) F(I\backslash J)$$

for any $I \ni \alpha$ where $F(\emptyset) = 1$ and $\varepsilon(J, I\backslash J) = \pm 1$ according to whether $I \mapsto (J, I\backslash J)$ is an even or odd permutation of I.

If ω is an even state over the CAR algebra, then the above process can be used to define a truncation ω_T as a function over the monomials in the $a^*(f)$ and $a(g)$. For example, one has

$$\begin{aligned}
\omega_T(a^*(f), a^*(g)) &= \omega(a^*(f)a^*(g)) \ , \\
\omega_T(a^*(f), a(g)) &= \omega(a^*(f)a(g)) \ , \\
\omega_T(a^*(f_1), a^*(f_2), a(g_1), a(g_2)) &= \omega(a^*(f_1)a^*(f_2)a(g_1)a(g_2)) \\
&\quad - \omega(a^*(f_1)a^*(f_2))\omega(a(g_1)a(g_2)) \\
&\quad + \omega(a^*(f_1)a(g_1))\omega(a^*(f_2)a(g_2)) \\
&\quad - \omega(a^*(f_1)a(g_2))\omega(a^*(f_2)a(g_1)) \ ,
\end{aligned}$$

etc.

An even state ω over $\mathfrak{A}$ is called *quasi-free* if, and only if,

$$\omega_T(a^\#(f_1), a^\#(f_2), \ldots, a^\#(f_n)) = 0$$

for $n > 2$ and all $f_1, \ldots, f_n \in \mathfrak{h}$ where $a^\#$ is used to represent either a^* or a. Thus a quasi-free state is determined by two functionals $\omega_T(a^*(f), a(g))$ and $\omega_T(a^*(f), a^*(g))$ and conditions can be given on any two functionals with the correct linearity and anti-linearity conditions to ensure that they determine a quasi-free state ω. Necessary and sufficient conditions are

$$\omega_T(a(f), a^*(f)) + \omega_T(a^*(g), a(g)) + \omega_T(a(f), a(g)) + \omega_T(a^*(g), a^*(f)) \geq 0$$

which correspond to the conditions

$$\|\pi_\omega(a^*(f) + a(g))\Omega_\omega\|^2 \geq 0 \ .$$

EXAMPLE 5.2.20. A state ω over the CAR algebra on the Hilbert space $\mathfrak{h}$ is gauge-invariant if it is invariant under the group of Bogoliubov transformations $\tau_\theta(a(f)) = a(e^{i\theta} f), \theta \in [0, 2\pi\rangle$, the so-called gauge transformations. A gauge-invariant quasi-free state is determined by one truncated function and the positivity conditions reduce to the conditions

$$\|f\|^2 \geq \omega_T(a^*(f), a(f)) \geq 0 \ .$$

The functional ω_T automatically determines a selfadjoint operator T such that $1 \geq T \geq 0$ and

$$\omega_T(a^*(f), a(g)) = (g, Tf) \ .$$

If ω is the state determined by ω_T, then the corresponding representation is given by $\mathfrak{H}_\omega = \mathfrak{F}_-(\mathfrak{h}) \otimes \mathfrak{F}_-(\mathfrak{h}), \Omega_\omega = \Omega \otimes \Omega$, where $\Omega = (1, 0, 0, \ldots)$ is the Fock vacuum, and

$$a_\omega(f) = a((\mathbb{1} - T)^{1/2} f) \otimes \mathbb{1} + \theta \otimes a^*(JT^{1/2} f) \ ,$$
$$a^*_\omega(g) = a^*((\mathbb{1} - T)^{1/2} g) \otimes \mathbb{1} + \theta \otimes a(JT^{1/2} g) \ .$$

In these last equations a and a^* denote the Fock space representatives of the CARs, J is an anti-linear involution satisfying $(Jf, Jg) = (g, f)$, and θ is an operator which anti-commutes with the a and a^* and satisfies $\theta\Omega = \Omega$.

The truncated functionals are directly related to correlations in much the same way as for the CCRs. The following example is the analogue of Example 5.2.19.

EXAMPLE 5.2.21. Let $\mathfrak{A}$ be the CAR algebra over $L^2(\mathbb{R}^\nu)$. The group R^ν of space translations acts as a strongly continuous group of *-automorphism τ of $\mathfrak{A}$ whose action is such that

$$\tau_x(a(f)) = a(U_x f) \ , \qquad (U_x f)(y) = f(y - x) \ .$$

The CARs preclude that $\mathfrak{A}$ is an asymptotically abelian with respect to space translations but if ω is $\mathbb{R}^\nu$-invariant, then the pair $(\mathfrak{A}, \omega)$ is $\mathbb{R}^\nu$-abelian and ω is automatically even. The proof of these statements is essentially contained in the proof of Theorem 2.6.5. It proceeds as follows. Let E_ω denote the projection on the subspace of $U_\omega(\mathbb{R}^\nu)$-invariant vectors in $\mathfrak{H}_\omega$ and let $\mathfrak{A}_-$ and $\mathfrak{A}_+$ denote the odd and even elements of $\mathfrak{A}$. It follows from the CARs and a monomial approximation that

$$\lim_{|x|\to\infty} \|[\tau_x(A), B]\| = 0$$

if either A or B is even. Thus

$$\begin{aligned}[E_\omega \pi_\omega(A) E_\omega, E_\omega \pi_\omega(B) E_\omega] &= M_x(E_\omega \pi_\omega([\tau_x(A), B]) E_\omega) \\ &= 0\end{aligned}$$

by the mean ergodic theorem where M denotes an invariant mean over $\mathbb{R}^\nu$. If, however, A is odd, then a similar argument gives

$$\lim_{|x|\to\infty} \|\{\tau_x(A), A^*\}\| = 0$$

and hence

$$\{E_\omega \pi_\omega(A) E_\omega, E_\omega \pi_\omega(A^*) E_\omega\} = 0 \ .$$

Since both terms in the anti-commutator are positive, one concludes that $E_\omega \pi_\omega(A) E_\omega = 0$. Thus ω is even and $(\mathfrak{A}, \omega)$ is $\mathbb{R}^\nu$-abelian.

In fact the $\mathbb{R}^\nu$-abelianness coupled with the CARs implies that

$$M(\omega(A_1[\tau(B_1), B_2]A_2)) = 0$$

for all $\mathbb{R}^\nu$-invariant states ω and all $A_i, B_i \in \mathfrak{A}$. This follows by first considering even B_1 and then

$$\begin{aligned}M(\omega(A_1 \tau(B_1) B_2 A_2)) &= (\Omega_\omega, \pi_\omega(B_1) E_\omega \pi_\omega(A_1 B_2 A_2) \Omega_\omega) \\ &= M(\omega(A_1 B_2 \tau(B_1) A_2))\end{aligned}$$

by the above asymptotic commutation for even elements and $\mathbb{R}^\nu$-abelianness. But if B_1 is odd and A_i^-, A_i^+ denote the odd and even parts of A_i, then

$$M(\omega(A_1\tau(B_1)B_2A_2)) = (\Omega_\omega, \pi_\omega(B_1)E_\omega\pi_\omega((A_1^+ - A_1^-)B_2A_2)\Omega_\omega))$$
$$= 0$$

by the asymptotic commutation and anti-commutation, and $E_\omega\pi_\omega(B_1)E_\omega = 0$. Similarly for the second term of the commutator.

Finally, one concludes that the following conditions are equivalent.

(1) $\lim_{|x|\to\infty} \omega(A\tau_x(B)) = \omega(A)\omega(B)$ for all $A, B \in \mathfrak{A}$.
(2) $\lim_{|x|\to\infty} \omega(A\tau_x(B)C) = \omega(AC)\omega(B)$ for all $A, B, C \in \mathfrak{A}$.
(3) $\lim_{|x|\to\infty} \omega_T(B(f_1), \ldots, B(f_n), \tau_x(B(g_1)), \ldots, \tau_x(B(g_m))) = 0$ for all $f_1, \ldots f_n, g_1, \ldots, g_m$, where $B(f) = (a(f) + a^*(f))/2$.

Clearly (2) $\Rightarrow$ (1), but the converse follows by noting that if $B = B^- + B^+$ and $C = C^- + C^+$ are the decompositions of B and C into odd and even parts, then

$$\lim_{|x|\to\infty} \{\omega(A\tau_x(B)C) - \omega(AC\tau_x(B^+)) - \omega(AC^+\tau_x(B^-)) + \omega(AC^-\tau_x(B^-))\} = 0$$

by the asymptotic commutation relations cited above. But then condition (1) gives

$$\lim_{|x|\to\infty} \omega(A\tau_x(B)C) = \omega(AC)\omega(B^+) + \omega(AC^+)\omega(B^-) - \omega(AC^-)\omega(B^-)$$
$$= \omega(AC)\omega(B^+) = \omega(AC)\omega(B) \ ,$$

where the last steps follow because ω is even. The equivalence of (1) and (3) is proved as in Example 5.2.19.

Again it should be remarked that the above properties basically follow from the fact that $(U_x f, g) \to 0$ as $|x| \to \infty$ and hence easily generalize to other groups of Bogoliubov transformations.

5.2.4. The Ideal Fermi Gas

The foregoing discussion of the CAR algebra, the CCR algebra, their states, and their representations was motivated by the theory of systems of point particles. This algebraic apparatus provides a kinematical description of such systems and it remains to specify the dynamics. The simplest thermodynamically interesting models describe noninteracting particles confined to some bounded open set Λ of $\mathbb{R}^\nu$, the so-called *ideal gases*. Our immediate aim is to describe the equilibrium formalism for such systems in the Gibbs grand canonical ensemble and in this subsection we consider fermions. We begin with a general discussion of noninteracting systems and subsequently specialize to point particles in the configuration space.

Let $\mathfrak{F}_-(\mathfrak{h})$ be the anti-symmetric Fock space built over the one-particle Hilbert space $\mathfrak{h}$. The dynamics of a system with an arbitrary number of fermions moving independently is dictated by the Schrödinger equation

$$i\hbar\frac{d\psi_t}{dt} = d\Gamma(H)\psi_t$$

on $\mathfrak{F}_-(\mathfrak{h})$. In this equation H is a selfadjoint Hamiltonian operator on $\mathfrak{h}$, $d\Gamma(H)$ denotes the second quantization of H discussed in Section 5.2.1, and $\hbar$ is Planck's constant. The lack of interaction between the particles is reflected

by the direct sum and tensor product structure of $d\Gamma(H)$, e.g., the n-particle energy is the sum of the energies of the n individual particles. We will choose units such that $\hbar = 1$.

The solution of the Schrödinger equation gives the evolution

$$\psi \in \mathfrak{F}_-(\mathfrak{h}) \mapsto \psi_t = \exp\{-itd\Gamma(H)\}\psi = \Gamma(e^{-itH})\psi$$

and the evolution of any bounded observable, i.e., any bounded operator on $\mathfrak{F}_-(\mathfrak{h})$, is given by transposition as

$$A \in \mathscr{L}(\mathfrak{F}_-(\mathfrak{h})) \mapsto \tau_t(A) = \Gamma(e^{itH})A\Gamma(e^{-itH}) \ .$$

The action on the annihilation, and creation, operators is particularly simple. One finds

$$\tau_t(a(f)) = a(e^{itH}f), \qquad \tau_t(a^*(f)) = a^*(e^{itH}f) \ .$$

Thus, the evolution can be expressed as a one-parameter group of Bogoliubov transformations of the CAR algebra $\mathfrak{A}(\mathfrak{h})$. This group is strongly continuous because

$$\|\tau_t(a(f)) - a(f)\| = \|a(e^{itH}f - f)\| = \|e^{itH}f - f\| \ .$$

Next let us consider the Gibbs grand canonical equilibrium state of the particle system at inverse temperature $\beta \in \mathbb{R}$ and chemical potential $\mu \in \mathbb{R}$. If K_μ denotes the modified Hamiltonian

$$K_\mu = d\Gamma(H - \mu\mathbb{1}) = d\Gamma(H) - \mu N \ ,$$

then the Gibbs state is defined by

$$\omega(A) = \frac{\mathrm{Tr}(e^{-\beta K_\mu}A)}{\mathrm{Tr}(e^{-\beta K_\mu})} \ ,$$

where $A \in \mathfrak{A}(\mathfrak{h})$, the trace is over $\mathfrak{F}_-(\mathfrak{h})$, and it is implicitly assumed that $e^{-\beta K_\mu}$ is of trace-class. Typically the individual particle energy is lower semibounded and this last restriction requires at least that $\beta > 0$. It can be reformulated as a condition on the one-particle Hamiltonian.

Proposition 5.2.22. *Let H be a selfadjoint operator on the Hilbert space $\mathfrak{h}$ and let $\beta \in \mathbb{R}$. The following conditions are equivalent.*

(1) $\exp\{-\beta H\}$ *is trace-class on* $\mathfrak{h}$.
(2) $\exp\{-\beta\, d\Gamma(H - \mu\mathbb{1})\}$ *is trace-class on* $\mathfrak{F}_-(\mathfrak{h})$ *for all* $\mu \in \mathbb{R}$.

Proof. (1) $\Rightarrow$ (2). Let $\{\varepsilon_n\}_{n\geq 0}$ denote the eigenvalues of H in increasing (decreasing) order if $\beta \geq 0$ (if $\beta < 0$) repeated according to multiplicity. If $z = e^{\beta\mu}$, one has

$$\mathrm{Tr}_{\mathfrak{h}_-^m}(e^{-\beta K_\mu}) = z^m \sum_{0\leq n_1<n_2<\cdots<n_m} \exp\left\{-\beta \sum_{p=1}^{m} \varepsilon_{n_p}\right\}$$

because of anti-symmetrization and the definition of the second quantization process. Thus

$$\begin{aligned} 0 \leq \operatorname{Tr}(e^{-\beta K_\mu}) &= \sum_{m \geq 0} \operatorname{Tr}_{\mathfrak{h}_-^m}(e^{-\beta K_\mu}) \\ &= \prod_{m \geq 0} (1 + z e^{-\beta \varepsilon_m}) \\ &\leq \prod_{m \geq 0} \exp\{z e^{-\beta \varepsilon_m}\} = \exp\{z \operatorname{Tr}(e^{-\beta H})\} \ . \end{aligned}$$

(2) $\Rightarrow$ (1). The operator $\exp\{-\beta K_\mu\}$ leaves the one-particle subspace $\mathfrak{h}$ of $\mathfrak{F}_-(\mathfrak{h})$ invariant and, moreover,

$$\exp\{-\beta K_\mu\}|_{\mathfrak{h}} = z \exp\{-\beta H\} \ .$$

The variable z which occurs in the foregoing calculation is usually referred to as the *activity*. It often occurs in the sequel.

The Gibbs equilibrium state is particularly easy to calculate with the algorithm

$$e^{-\beta K_\mu} a^*(f) = z a^*(e^{-\beta H} f) e^{-\beta K_\mu} \ .$$

This algorithm combined with the CARs gives

$$\begin{aligned} \omega(a^*(f)a(g)) &= \frac{z \operatorname{Tr}(a^*(e^{-\beta H} f) e^{-\beta K_\mu} a(g))}{\operatorname{Tr}(e^{-\beta K_\mu})} \\ &= z\omega(a(g)a^*(e^{-\beta H} f)) \\ &= -z\omega(a^*(e^{-\beta H} f)a(g)) + z(g, e^{-\beta H} f) \ . \end{aligned}$$

But then one has

$$\omega(a^*((\mathbb{1} + z e^{-\beta H}) f) a(g)) = z(g, e^{-\beta H} f)$$

and hence

$$\omega(a^*(f)a(g)) = (g, z e^{-\beta H} (\mathbb{1} + z e^{-\beta H})^{-1} f) \ .$$

A similar calculation gives

$$\begin{aligned} \omega\left(\prod_{i=1}^n a^*(f_i) \prod_{j=1}^n a(g_j)\right) &= z\omega\left(\prod_{i=2}^n a^*(f_i) \prod_{j=1}^n a(g_j) a^*(e^{-\beta H} f_1)\right) \\ &= \sum_{p=1}^n (-1)^{n-p} z(g_p, e^{-\beta H} f_1) \omega\left(\prod_{i=2}^n a^*(f_i) \prod_{\substack{j=1 \\ j \neq p}}^n a(g_j)\right) \\ &\quad - z\omega\left(a^*(e^{-\beta H} f_1) \prod_{i=2}^n a^*(f_i) \prod_{j=1}^n a(g_j)\right) . \end{aligned}$$

Therefore, by linearity and the replacement of f_1 by $(\mathbb{1} + z e^{-\beta H})^{-1} f_1$ one finds

$$\omega\left(\prod_{i=1}^{n} a^*(f_i)\prod_{j=1}^{n} a(g_j)\right) = \sum_{p=1}^{n}(-1)^{n-p}\omega(a^*(f_1)a(g_p))\omega\left(\prod_{i=2}^{n} a^*(f_i)\prod_{\substack{j=1\\ j\neq p}}^{n} a(g_j)\right) .$$

Iteration of this identity expresses the value of ω on the product of the $a^*(f_i)$ and $a(g_i)$ as the sum of products of two-point functions $\omega(a^*(f_i)a(g_j))$. Note that if the number of $a^*(f_i)$ and $a(g_j)$ differ, then the corresponding value is zero because $\exp\{-\beta K_\mu\}$ leaves each of the subspaces $\mathfrak{h}_-^m$ invariant, i.e., ω is gauge-invariant (see Example 5.2.20). Thus, the Gibbs state is a quasi-free state over $\mathfrak{A}(\mathfrak{h})$.

Note that the above calculation is a direct application of the KMS condition, discussed in Chapter 1 and the introduction to this chapter, to the evolution determined by the generalized Hamiltonian K_μ, i.e., the group of Bogoliubov transformations such that

$$\hat{\tau}_t(a(f)) = e^{itK_\mu}a(f)e^{-itK_\mu} = e^{-it\mu}a(e^{itH}f) \ .$$

In particular we used the algorithm

$$\omega(a^*(f)A) = \omega(A\hat{\tau}_t(a^*(f)))|_{t=i\beta} \ .$$

The result of these calculations is summarized in the following.

Proposition 5.2.23. *Let H be a selfadjoint operator on the Hilbert space $\mathfrak{h}$ and assume that $\exp\{-\beta H\}$ is trace-class. Let*

$$\omega(A) = \frac{\mathrm{Tr}(e^{-\beta K_\mu}A)}{\mathrm{Tr}(e^{-\beta K_\mu})}$$

denote the Gibbs grand canonical equilibrium state over the CAR algebra $\mathfrak{A}(\mathfrak{h})$ and

$$A \in \mathfrak{A}(\mathfrak{h}) \mapsto \hat{\tau}_t(A) = e^{itK_\mu}Ae^{-itK_\mu} \in \mathfrak{A}(\mathfrak{h})$$

the evolution corresponding to the generalized Hamiltonian $K_\mu = d\Gamma(H) - \mu N$, where $\mu \in \mathbb{R}$.

It follows that ω is the unique $\hat{\tau}$-KMS state, at the value β, and that this state is the gauge-invariant quasi-free state with two-point function

$$\omega(a^*(f)a(g)) = (g, ze^{-\beta H}(\mathbb{1} + ze^{-\beta H})^{-1}f) \ ,$$

where $z = e^{\beta\mu}$.

This proposition identifies the Gibbs equilibrium states and the $\hat{\tau}$-KMS states with one small discrepancy. The Gibbs states are only defined if $\exp\{-\beta H\}$ is of trace-class or, equivalently, if $\exp\{-\beta K_\mu\}$ is of trace-class. These properties are unimportant, however, for the definition of the evolution $\hat{\tau}$ which exists whenever H is selfadjoint. Moreover, the notion of the KMS state can be directly defined in terms of $\hat{\tau}$ (this will be extensively discussed in Section 5.3) and the same combinatoric calculation given before the proposi-

tion establishes that the quasi-free state given in Proposition 5.2.23 is the unique $\hat{\tau}$-KMS state. Thus, the KMS states can exist when the Gibbs states are not defined. Nevertheless, one can establish that all the $\hat{\tau}$-KMS states can be obtained as weak*-limits of Gibbs states for dynamics $\hat{\tau}^{(n)}$ which approximate $\hat{\tau}$ in the sense that $\|\hat{\tau}_t^{(n)}(A) - \hat{\tau}_t(A)\| \to 0$ as $n \to \infty$ for all $A \in \mathfrak{A}(\mathfrak{h})$. This result is established by constructing H_n on $\mathfrak{h}$ such that (1) $\exp\{-\beta H_n\}$ is of trace-class, and (2) $\exp\{itH_n\}$ converges strongly to $\exp\{itH\}$. The groups $\tau^{(n)}$ are then defined by replacing H by H_n and the convergence of the corresponding Gibbs states follows from Lemma 5.2.25.

Now we examine the thermodynamic limit of Gibbs or, more generally, KMS states, of noninteracting Fermi systems. For the discussion we specialize to point particles in the configuration space $\mathbb{R}^\nu$. Thus we choose $f \in L^2(\Lambda)$ where Λ is a bounded open subset of $\mathbb{R}^\nu$ and specify the one-particle Hamiltonian as a selfadjoint extension of the Laplacian $-\nabla^2$. This latter operator will always be understood as defined on the infinitely often differentiable functions $C_0^\infty(\Lambda)$ with support in Λ. The conventional quantum-mechanical Hamiltonian for free particles of mass m is $-\hbar^2\nabla^2/2m$ but we now choose units such that $\hbar^2/2m = 1$.

There are many selfadjoint extensions of $-\nabla^2$ on $L^2(\Lambda)$, each corresponding to a choice of boundary conditions, i.e., a specification of the dynamical behavior of the particle on arrival at the boundary of the finite system. The number and nature of the possible extensions is partially governed by the smoothness properties of the boundary of Λ. We examine some specific cases below (see Example 5.2.26). If, however, Λ is replaced by $\mathbb{R}^\nu$, then there is no ambiguity introduced by the boundary and $-\nabla^2$ has a unique selfadjoint extension H whose action is given by

$$(Hf)(x) = (2\pi)^{-\nu/2} \int d^\nu p \hat{f}(p) p^2 e^{ipx} \ ,$$

where $\hat{f}$ denotes the Fourier transform of f. The domain of H is the set of $f \in L^2(\mathbb{R}^\nu)$ such that

$$\int d^\nu p p^4 |\hat{f}(p)|^2 < +\infty \ .$$

There are two basic quantities of interest in the thermodynamic limit, the dynamics and the equilibrium states. For these latter one can take either the Gibbs states or the KMS states. The following theorem describes the former but can easily be reformulated for the KMS states.

Theorem 5.2.24. *For each bounded open set $\Lambda \subset \mathbb{R}^\nu$ let H_Λ denote a selfadjoint extension, on $L^2(\Lambda)$, of the Laplacian $-\nabla^2$ and let H denote the unique selfadjoint extension on $L^2(\mathbb{R}^\nu)$ of $-\nabla^2$. Let $\mathfrak{A}_\Lambda$ denote the* CAR *algebra over $L^2(\Lambda)$, $\mathfrak{A}$ the* CAR *algebra over $L^2(\mathbb{R}^\nu)$, and τ^Λ and τ the groups of *-automorphisms of $\mathfrak{A}_\Lambda$ and $\mathfrak{A}$ such that $\tau_t^\Lambda(a(f)) = a(e^{itH_\Lambda} f)$ and $\tau_t(a(f)) = a(e^{itH} f)$. It follows that*

(1) $\lim_{\Lambda'\to\infty}\|\tau_t^{\Lambda'}(A) - \tau_t(A)\| = 0$, *for all* $A \in \mathfrak{A}_\Lambda$ *and all* $\Lambda \subseteq \mathbb{R}^\nu$, *uniformly for t in finite intervals of* $\mathbb{R}$, *where* $\Lambda' \to \infty$ *in the sense that* Λ' *eventually contains any given* $\Lambda \subseteq \mathbb{R}^\nu$.

(2) *If* ω_Λ *is the quasi-free state given by*

$$\omega_\Lambda(a^*(f)a(g)) = (g, ze^{-\beta H_\Lambda}(\mathbb{1} + ze^{-\beta H_\Lambda})^{-1} f) \ ,$$

then

$$\lim_{\Lambda'\to\infty} \omega_{\Lambda'}(A) = \omega(A)$$

for all $A \in \mathfrak{A}_\Lambda$ *and all* $\Lambda \subseteq \mathbb{R}^\nu$, *where the limit is in the sense of* (1) *and* ω *is the gauge-invariant quasi-free state over* $\mathfrak{A}$ *with two-point function*

$$\begin{aligned}\omega(a^*(f)a(g)) &= (g, ze^{-\beta H}(\mathbb{1} + ze^{-\beta H})^{-1} f) \\ &= \frac{1}{(2\pi)^\nu}\int d^\nu p\, \overline{\hat{g}(p)}\, \hat{f}(p) ze^{-\beta p^2}(1 + ze^{-\beta p^2})^{-1}\end{aligned}$$

where $\hat{f}$ *denotes the Fourier transform of f.*

PROOF. (1) In Example 3.1.29 we showed that

$$\lim_{\Lambda\to\infty} \|(e^{itH_\Lambda} - e^{itH})\psi\| = 0 \ .$$

The desired result then follows from the continuity condition

$$\|\tau_t^\Lambda(a(f)) - \tau_t(a(f))\| = \|(e^{itH_\Lambda} - e^{itH})f\|$$

and the fact that $\mathfrak{A}_\Lambda$ is uniformly generated by the a(f).

(2) It follows from Proposition 5.2.23 that $\omega_\Lambda(a^*(f)a(g))$ is the matrix element of a bounded function of H_Λ. Thus the convergence of $\omega_\Lambda(a^*(f)a(g))$ to $\omega(a^*(f)a(g))$ and hence the weak*-convergence of the quasi-free states ω_Λ to the quasi-free state ω is a consequence of the following lemma.

Lemma 5.2.25. *Let* U_α *and* U *be strongly continuous unitary groups, on the Hilbert space* $\mathfrak{H}$, *with generators* iH_α *and* iH. *Assume that the net* U_α *converges strongly, i.e.,*

$$\lim_{\alpha\to\infty} \|(U_{\alpha,t} - U_t)\psi\| = 0$$

for all $\psi \in \mathfrak{H}$, *uniformly for t in finite intervals of* $\mathbb{R}$.

It follows that

$$\lim_{\alpha\to\infty} \|(f(H_\alpha) - f(H))\psi\| = 0$$

for all $\psi \in \mathfrak{H}$, *and for all bounded continuous functions f on* $\mathbb{R}$.

PROOF. If the Fourier transform $\hat{f}$ of f is absolutely integrable, then the estimate

$$\|(f(H_\alpha) - f(H))\psi\| \leq \int dt\, |\hat{f}(t)|\, \|(e^{itH_\alpha} - e^{itH})\psi\| \ ,$$

which follows from spectral analysis, allows one to conclude that

$$f(H_\alpha)\psi \to f(H)\psi \ .$$

But these f are dense in $C_0(\mathbb{R})$ in supremum norm, and hence the convergence follows for all $f \in C_0(\mathbb{R})$.

Next let $g_m(t) = \exp\{-t^2/m\}$. One has $g_m(H)\psi \underset{m=\infty}{\longrightarrow} \psi$ and, by the foregoing, $g_m(H_\alpha)\psi \underset{\alpha=\infty}{\longrightarrow} g_m(H)\psi$. But

$$\|g_m(H_\alpha)\psi - \psi\| \leq \|(g_m(H_\alpha) - g_m(H))\psi\| + \|g_m(H)\psi - \psi\|$$

and hence for $\varepsilon > 0$ one can choose an m and a β such that

$$\|g_m(H_\alpha)\psi - \psi\| < \varepsilon/3, \ \|g_m(H)\psi - \psi\| < \varepsilon/3$$

for all $\alpha > \beta$. But $fg_m \in C_0(\mathbb{R})$ and hence there is a γ such that

$$\|f(H_\alpha)g_m(H_\alpha)\psi - f(H)g_m(H)\psi\| < \varepsilon\|f\|_\infty/3$$

for all $\alpha > \gamma$. Therefore,

$$\begin{aligned}\|f(H_\alpha)\psi - f(H)\psi\| &\leq \|f(H_\alpha)g_m(H_\alpha)\psi - f(H)g_m(H)\psi\| \\ &\quad + \|f(H_\alpha)\|\, \|g_m(H_\alpha)\psi - \psi\| + \|f(H)\|\, \|g_m(H)\psi - \psi\| \leq \varepsilon\|f\|_\infty\end{aligned}$$

for all $\alpha > \beta \vee \gamma$. Since ψ and ε were arbitrary, $f(H_\alpha)$ converges strongly to $f(H)$.

Theorem 5.2.24 demonstrates several points of interest. First, the dynamics of the infinite idealized Fermi gas are determined by a strongly continuous one-parameter group of *-automorphisms of the CAR algebra $\mathfrak{A}$ over $L^2(\mathbb{R}^\nu)$. Second, the thermodynamic limit of the finite-volume equilibrium states is uniquely defined and independent of the choice of boundary conditions, i.e., there is a unique thermodynamic phase. This latter point is valid for either of the possible definitions of the finite-volume states, the conventional Gibbs definition, or the definition as a KMS state.[1] Finally the theorem gives an explicit identification of the thermodynamic equilibrium state of the Fermi gas as a quasi-free state ω and this allows a detailed analysis of equilibrium phenomena. Let us examine some of the most relevant features.

First consider the dynamics. The group τ with generator $-\nabla^2$, or the related group with generator $-\nabla^2 - \mu\mathbb{1}$, is usually referred to as the *free evolution*. The Riemann–Lebesgue lemma implies the property

[1] $-\nabla^2$ may have selfadjoint extensions H_Λ on $L^2(\Lambda)$ which are not lower semibounded when $\nu \geq 2$. For all classical boundary conditions however, H_Λ is lower semibounded, and the operator $\exp\{-\beta H_\Lambda\}$ has a finite trace for $\beta > 0$. (See Example 5.2.26.) Hence the Gibbs definition is restricted to classical boundary conditions and positive values of the temperature β^{-1}. The KMS definition is, however, valid for positive or negative temperatures and any boundary condition, and negative temperature states can be interpreted as limits of Gibbs states for neighboring dynamics. This difference between the Gibbs description and the more general KMS condition could be of significance in more realistic models because certain phenomena of magnetism indicate the possibility of attaining negative temperature states (see Notes and Remarks).

$$\lim_{|t|\to\infty}(f, e^{itH}g) = \lim_{|t|\to\infty}\int d^\nu p\,\overline{\hat{f}(p)}\hat{g}(p)e^{itp^2} = 0 \ .$$

Hence the properties of $\mathbb{R}$-abelianness, asymptotic abelianness in mean, etc., derived for an $\mathbb{R}$-invariant state in Example 5.2.20 are applicable. In particular,

$$M(\omega(A_1[\tau(B_1), B_2]A_2)) = 0$$

for any $\mathbb{R}$-invariant state ω, any invariant mean M, and all $A_i, B_i \in \mathfrak{A}$. We will derive more detailed properties of the free evolution in Example 5.4.9.

Second, consider the equilibrium state ω. This state is invariant under the group τ of time translations and under the group $\mathbb{R}^\nu$ of space translations, i.e., the group of Bogoliubov transformations induced by the unitary transformations U; $(U_x f)(y) = f(y-x)$ of $L^2(\mathbb{R}^\nu)$. In fact the state is strongly mixing for both groups. This can easily be verified by application of the Riemann-Lebesgue lemma to the two-point function. The state ω also has finite particle density per unit volume $\rho(\beta, z)$ for $0 < \beta < \infty$.

Recall that in Section 5.2.3 we associated with each state ω over the CAR algebra a number functional $\hat{N}(\omega)$ which measures the number of particles in the state. Thus, by restricting ω to the local algebras $\mathfrak{A}_\Lambda$ one can define local number functionals $N_\Lambda(\omega)$. Then $N_\Lambda(\omega)/|\Lambda|$, where $|\Lambda|$ is the volume, i.e., Lebesgue measure, of Λ, is exactly the number of particles per unit volume in Λ. Since the equilibrium state is invariant under space translations, this number should be independent of Λ and indeed one easily computes the density as

$$\begin{aligned}\rho(\beta, z) &= |\Lambda|^{-1}\hat{N}_\Lambda(\omega)\\ &= |\Lambda|^{-1}\sum_{n\geq 0}\omega(a^*(f_n)a(f_n))\\ &= (2\pi)^\nu\int d^\nu p\, z e^{-\beta p^2}(1 + z e^{-\beta p^2})^{-1} < +\infty \ ,\end{aligned}$$

where $\{f_n\}_{n\geq 0}$ is an orthonormal basis of $L^2(\Lambda)$. Thus it follows from Theorem 5.2.14 that ω is locally normal, i.e., normal with respect to the Fock representation in restriction to each of the local CAR algebras. It is also possible to evaluate the local energy per unit volume, and hence the energy per unit particle, but for this it is first convenient to introduce an algorithm for the local Hamiltonians on Fock space.

Let $\{f_n\}_{n\geq 0}$ be an orthonormal basis of $L^2(\Lambda)$ formed of once-continuously differentiable functions and define a quadratic form t_Λ on the Fock space $\mathfrak{F}_-(\Lambda)$ over $L^2(\Lambda)$ by

$$t_\Lambda(\psi) = \sum_{n\geq 0}(\psi, a^*(\underline{\nabla} f_n)\cdot a(\underline{\nabla} f_n)\psi)$$

with the domain of t_Λ consisting of those ψ for which the sum is finite. It follows from Lemma 5.2.13 that t_Λ is a positive, closed quadratic form and an explicit calculation shows that $P_- g_1 \otimes g_2 \otimes \cdots \otimes g_m \in D(t_\Lambda)$ for all once-continuosly differentiable g_i and all $m \geq 1$. Thus t_Λ is densely defined. Hence, there exists a positive selfadjoint operator T_Λ on $\mathfrak{F}_-(\Lambda)$ such that

$$t_\Lambda(\psi) = (T_\Lambda^{1/2}\psi, T_\Lambda^{1/2}\psi)$$

for all $\psi \in D(t_\Lambda)$. Choosing ψ to be an infinitely-often differentiable one-particle vector with support in Λ, one calculates that

$$t_\Lambda(\psi) = -(\psi, \nabla^2\psi)$$

and hence T_Λ, in restriction to the one-particle space, is a selfadjoint extension of $-\nabla^2$ on $C_0^\infty(\Lambda)$. More generally one deduces by calculation with multiparticle vectors that T_Λ is a selfadjoint extension of the second quantization $\Gamma(-\nabla^2)$ of $-\nabla^2$. In fact, it follows from the classical theory of quadratic forms and differential operators that T_Λ corresponds to the second quantization of the selfadjoint extension of $-\nabla^2$ which satisfies Neumann boundary condition (see Example 5.2.26). This extension is very convenient for the calculation of the local energy per unit volume $\varepsilon(\beta, z)$ of the equilibrium state ω. One has

$$\begin{aligned}\varepsilon(\beta, z) &= |\Lambda|^{-1} \sum_{n \geq 0} \omega(a^*(\underline{\nabla} f_n) \cdot a(\underline{\nabla} f_n)) \\ &= (2\pi)^{-\nu} \int d^\nu p \; p^2 z e^{-\beta p^2} (1 + z e^{-\beta p^2})^{-1} \\ &= \left(\frac{\nu}{2\beta}\right)(2\pi)^{-\nu} \int d^\nu p \; \log(1 + z e^{-\beta p^2}) \; .\end{aligned}$$

(The last equality follows through integration by parts and expresses the classical equation of state

$$P(\beta, z) = \frac{2}{\nu}\varepsilon(\beta, z)$$

with the pressure $P(\beta, z)$ identified by

$$P(\beta, z) = \beta^{-1}(2\pi)^{-\nu} \int d^\nu p \; \log(1 + z e^{-\beta p^2}) \; .$$

The temperature dependence of ρ, ε, and P is particularly simple. For example,

$$\rho(\beta, z) = \lambda^{-\nu} I(z), \quad \varepsilon(\beta, z) = \beta^{-1}\lambda^{-\nu} J(z) \; ,$$

where

$$\begin{aligned} I(z) &= \pi^{-\nu/2} \int d^\nu x \; z e^{-x^2} (1 + z e^{-x^2})^{-1} \; , \\ J(z) &= \pi^{-\nu/2} \int d^\nu x \; z x^2 e^{-x^2} (1 + z e^{-x^2})^{-1} \end{aligned}$$

are independent of β and $\lambda = (4\pi\beta)^{1/2}$ corresponds to the thermal wavelength of the individual particles, i.e., λ is a measure of the "effective" size of the fermions.

Quantum mechanically the Fourier variable p conjugate to x is interpreted as particle momentum and the formulas for ρ and ε indicate that

$$(2\pi)^{-\nu} z e^{-\beta p^2} (1 + z e^{-\beta p^2})^{-1} d^\nu p$$

should be interpreted as the momentum distribution per unit volume. In the high-temperature-low-density region, $\lambda^{\nu/2}\rho \ll 1$, one must have $z \ll 1$ and

$$\rho(\beta, z) \simeq (2\pi)^{-\nu} z \int d^\nu p \; e^{-\beta p^2}, \quad \varepsilon(\beta, z) = (2\pi)^{-\nu} z \int d^\nu p \; p^2 e^{-\beta p^2} \; .$$

Thus the momentum distribution takes the Maxwellian form $(2\pi)^{-\nu} z e^{-\beta p^2} d^\nu p$ and by use of the equation of state one can derive Boyle's law

$$\frac{P(\beta, \mu)}{\rho(\beta, \mu)} = \frac{2\varepsilon(\beta, \mu)}{\nu\rho(\beta, \mu)} = \beta^{-1} \; .$$

In fact, this is the ultimate justification of β as the inverse temperature, in suitable units. The low-temperature–high-density region, $\lambda^{\nu/2}\rho \gg 1$ is best illustrated by examining the idealization of zero temperature, i.e., by taking the limit $\beta \to \infty$. One then has

$$\begin{aligned} \lim_{\beta \to \infty} z e^{-\beta p^2}(1 + z e^{-\beta p^2})^{-1} &= \lim_{\beta \to \infty} e^{-\beta(p^2 - \mu)}(1 + e^{-\beta(p^2 - \mu)})^{-1} \\ &= \begin{cases} 1, & \text{if } p^2 < \mu \\ 0, & \text{if } p^2 > \mu \; . \end{cases} \end{aligned}$$

Thus only particles with energy (= momentum^2) less than or equal to μ occur. This situation is often described as the *Fermi sea*. All states with particle energy less than μ are occupied and all states with energy greater than μ are empty. The critical values of p, the surface $p^2 = \mu$, are called the *Fermi surface*.

One can also conclude that the weak*- limit of the equilibrium states as $\beta \to \infty$ exists and is the gauge-invariant quasi-free state ω_0 with two-point function given by

$$\omega_0(a^*(f)a(g)) = (2\pi)^{-\nu} \int_{p^2 \le \mu} d^\nu p \; \overline{\hat{g}(p)} \hat{f}(p) \; .$$

The zero-temperature states are usually called ground states and can be independently defined by the requirement of minimal energy per unit volume at fixed density. The general definition of ground states will be examined in Section 5.3. Note that the energy ε and density ρ are easily calculated in the ground state of the Fermi gas and one has $\varepsilon \sim \rho^{1 + 2/\nu}$, in contrast to the linear behavior at low densities and high temperatures.

To complete the thermodynamic description one should also prove that the local density, energy, pressure, etc., are equal to the thermodynamic limit of their finite-volume counterparts. These limits are seemingly more sensitive, however, to the manner in which $\Lambda \to \infty$ and the boundary conditions vary. In the simplest situations one can, of course, calculate explicitly the limit and for the classical boundary conditions various techniques of convexity, monotonicity, subadditivity, etc., have been developed which apply even to interacting systems. These methods are mostly based upon the characterization of selfadjoint extensions of $-\nabla^2$ by quadratic forms.

EXAMPLE 5.2.26 (The classical boundary conditions). Let D denote the Laplacian operator $-\nabla^2$ defined on all twice-continuously differentiable functions in $L^2(\Lambda)$ where Λ is assumed to have a piecewise differentiable boundary $\partial\Lambda$. Green's formula

$$(D\psi,\ \varphi) - (\psi,\ D\varphi) = \int dS \left\{ \frac{\partial\bar{\psi}}{\partial n}\varphi - \bar{\psi}\frac{\partial\varphi}{\partial n} \right\}$$

demonstrates that a restriction H of D to a domain $D(H)$ is symmetric if

$$\bar{\psi}\frac{\partial\varphi}{\partial n} = \frac{\partial\bar{\psi}}{\partial n}\varphi$$

on the boundary $\partial\Lambda$ of Λ for all $\varphi, \psi \in D(H)$. Here we have used $\partial/\partial n$ to denote the inward normal derivative. The simplest and most basic examples of the boundary conditions are (1) *Dirichlet conditions,* $\psi = 0$ on $\partial\Lambda$. and (2) *Neumann conditions,* $\partial\psi/\partial n = 0$ on $\partial\psi$ where $\sigma \in C^1(\partial\Lambda)$ is a real differentiable function over $\partial\Lambda$ (Dirichlet conditions formally correspond to $\sigma = +\infty$). These conditions determine a family of selfadjoint extensions H^σ of $-\nabla^2$ which are best described through quadratic forms.

Let h^0 denote the quadratic form defined by $D(h^0) = C^1(\Lambda)$ and

$$h^0(\psi) = \|\underline{\nabla}\psi\|^2 \ .$$

This form is densely defined, positive, and closable ($\underline{\nabla}$ is closable on $C^1(\Lambda)$). The closure of h^0, which we also denote by h^0, determines a selfadjoint extension H^0 of $-\nabla^2$ by

$$h^0(\psi) = \|\sqrt{H^0}\psi\|^2$$

and this operator corresponds to Neumann boundary conditions. The closure h^∞ of the restriction of h^0 to $C_0^1(\Lambda)$ determines the Dirichlet extension H^∞ in the same manner. Moreover, the quadratic forms h^σ defined by $D(h^\sigma) = D(h^0)$ and

$$h^\sigma(\psi) = h^0(\psi) \ + \ \int dS\ \sigma|\psi|^2$$

determine the $\partial\psi = \sigma\psi$ extensions. These latter forms are closed because for $b < 1$ there is an $a > 0$ such that

$$\left| \int dS\ \sigma|\psi|^2 \right| \leq a\|\psi\|^2 \ + \ bh^0(\psi) \ .$$

Note that if $0 \leq \sigma_1 \leq \sigma_2$, then

$$h^0 \leq h^{\sigma_1} \leq h^{\sigma_2} \leq h^\infty$$

in the sense of quadratic forms. It follows from the mini-max principle that if $\{\varepsilon_n^\sigma\}_{n\geq 1}$ denotes the eigenvalues of H^σ arranged in increasing order, repeated according to multiplicity, then

$$\varepsilon_n^0 \ \leq \ \varepsilon_n^{\sigma_1} \ \leq \ \varepsilon_n^{\sigma_2} \ \leq \ \varepsilon_n^\infty$$

for all $n \geq 1$.

If Λ is a parallelepiped, $-\nabla^2$ also has a selfadjoint extension H^{per} corresponding to *periodic boundary conditions.* This extension is determined by the restriction h^{per} of h^0 to the periodic functions in $D(h^0)$ and hence one also has

$$h^0 \leq h^{\text{per}} \leq h^\infty$$

and the corresponding order for the eigenvalues.

Finally let h^∞_Λ, $\{\varepsilon^\infty_n(\Lambda)\}_{n\geq 1}$, etc., denote the forms and eigenvalues and consider a variation in Λ. If $\Lambda_1 \subseteq \Lambda_2$ one has $h^\infty_{\Lambda_1} \geq h^\infty_{\Lambda_2}$ and hence

$$\varepsilon^\infty_n(\Lambda_1) \geq \varepsilon^\infty_n(\Lambda_2)$$

for all n. This property is often useful. For example, one can compute that $\exp\{-H^\infty_\Lambda\}$ is trace-class for all parallelepipeds and hence, by monotonicity, it is trace-class for all Λ.

We will not consider the limit of the thermodynamic functions in any detail but content ourselves by noting that if Λ_L is a parallelepiped, with edges of length $L_1, L_2, \ldots, L_v$, the density with Dirichlet boundary conditions is given by

$$\begin{aligned}\rho_{\Lambda_L}(\beta, z) &= |\Lambda_L|^{-1}\,\mathrm{Tr}(ze^{-\beta H_{\Lambda_L}}(1 + ze^{-\beta H_{\Lambda_L}})^{-1}) \\ &= (L_1 L_2 \cdots L_v)^{-1} \sum_{n_1,\ldots,n_v\geq 1} ze^{-\beta\varepsilon_{\underline{n}}(\Lambda)}(1 + ze^{-\beta\varepsilon_{\underline{n}}(\Lambda)})^{-1} ,\end{aligned}$$

where the eigenvalues are given by

$$\varepsilon_{\underline{n}}(\Lambda) = \sum_{i=1}^{v}\left(\frac{n_i\pi}{L_i}\right)^2 .$$

An identical expression is valid for Neumann boundary conditions but the value $n_i = 0$ is also allowed. But the sum is just a Riemann approximation to the local density and hence $\rho_{\Lambda_L}(\beta, z)$ tends to $\rho(\beta, z)$ for Dirichlet or Neumann conditions. Thus the same conclusion is valid for the $\partial\psi = \sigma\psi$ conditions with any $\sigma \geq 0$ by monotonicity. Note that as

$$\begin{aligned}\int_{n-1}^{n} dx\, ze^{-ax^2}(1 + ze^{-ax^2})^{-1} &\geq ze^{-an^2}(1 + ze^{-an^2}) \\ &\geq \int_{n}^{n+1} dx\, ze^{-ax^2}(1 + ze^{-ax^2})^{-1} ,\end{aligned}$$

one can conclude that $\rho_{\Lambda_L} \leq \rho$ for the Dirichlet boundary condition and obtain an upper bound on the difference $\rho - \rho_{\Lambda_L}$. An explicit calculation gives

$$\rho(\beta, z) - \rho_{\Lambda_L}(\beta, z) \leq \frac{12z}{1 + z}\frac{1}{\lambda^3}\left(\frac{\lambda}{L}\right) ,$$

where $\lambda = (4\pi\beta)^{1/2}$ is the thermal wavelength. One also easily obtains the estimate

$$\frac{z}{1 + z}\frac{1}{\lambda^3} \leq \rho(\beta, z) .$$

Combination of these inequalities gives a bound on the error occurring when one replaces ρ_{Λ_L} by its thermodynamic limit,

$$0 \leq 1 - \frac{\rho_{\Lambda_L}(\beta, z)}{\rho(\beta, z)} \leq 12 \frac{\lambda}{L} .$$

Explicitly one has $\lambda \sim 2 \times 10^{-8}$ cm for helium at room temperature and hence if $L = 1$ cm the error is about 2 parts in 10^7. At lower temperatures for example 3°K, the error would be about 2 in 10^6 because λ is proportional to the inverse root of the temperature, but for heavier atoms the accuracy improves. Hence, the infinite-volume limit provides an excellent approximation even for systems whose diameter is as small as 1 cm.

5.2.5. The Ideal Bose Gas

We begin the description of the ideal Bose gas with a general discussion which parallels that of the previous section. Subsequently we specialize to particles in $\mathbb{R}^\nu$.

Let $\mathfrak{F}_+(\mathfrak{h})$ be the symmetric Fock space over the one-particle Hilbert space $\mathfrak{h}$. The dynamics of the noninteracting system is again defined in terms of the second quantization $d\Gamma(H)$ of the one-particle Hamiltonian H on $\mathfrak{h}$.
One has the evolution

$$\psi \in \mathfrak{F}_+(\mathfrak{h}) \mapsto \psi_t = \Gamma(e^{-itH})\psi$$

for the wave functions and

$$A \in \mathscr{L}(\mathfrak{F}_+(\mathfrak{h})) \mapsto \tau_t(A) = \Gamma(e^{itH})A\Gamma(e^{-itH})$$

for the observables. In particular, the dynamics yield a one-parameter group of *-automorphisms τ of the CCR algebra $\mathfrak{A}(\mathfrak{h})$ and

$$\tau_t(W(f)) = W(e^{itH}f)$$

for the Weyl operators $W(f)$. In contrast to the Fermi gas this group of Bogoliubov transformations is not strongly continuous because of Theorem 5.2.8.

The Gibbs grand canonical equilibrium state is defined in terms of the generalized Hamiltonian $K_\mu = d\Gamma(H - \mu\mathbb{1}) = d\Gamma(H) - \mu N$ whenever

$$\exp\{-\beta K_\mu\}$$

is trace-class. This latter property places a constraint on the possible values of μ.

Proposition 5.2.27. *Let H be a selfadjoint operator on the Hilbert space $\mathfrak{h}$ and let $\beta, \mu \in \mathbb{R}$. The following conditions are equivalent.*

(1) $\exp\{-\beta H\}$ *is trace-class on* $\mathfrak{h}$ *and* $\beta(H - \mu\mathbb{1}) > 0$,
(2) $\exp\{-\beta d\Gamma(H - \mu\mathbb{1})\}$ *is trace-class on* $\mathfrak{F}_+(\mathfrak{h})$.

PROOF. (1) $\Rightarrow$ (2). Let $\{\varepsilon_n\}_{n \geq 0}$ denote the eigenvalues of H in increasing (decreasing) order if $\beta > 0$ (if $\beta < 0$) repeated according to multiplicity. If $z = e^{\beta\mu}$ one has

$$\mathrm{Tr}_{\mathfrak{h}_+^m}(e^{-\beta K_\mu}) \leq z^m \sum_{n_1, n_2, \ldots, n_m \geq 0} \exp\left\{ -\beta \sum_{p=1}^{m} \varepsilon_{n_p} \right\}$$

and hence

$$\begin{aligned} 0 \leq \mathrm{Tr}(e^{-\beta K_\mu}) &= \sum_{m \geq 0} \mathrm{Tr}_{\mathfrak{h}_+^m}(e^{-\beta K_\mu}) \\ &\leq \prod_{m \geq 0} (1 - ze^{-\beta \varepsilon_m})^{-1} \\ &= \prod_{m \geq 0} (1 + ze^{-\beta \varepsilon_m}(1 - ze^{-\beta \varepsilon_m})^{-1}) \\ &\leq \exp\left\{ \sum_{m \geq 0} ze^{-\beta \varepsilon_m}(1 - ze^{-\beta \varepsilon_m})^{-1} \right\} \\ &\leq \exp\{z(1 - ze^{-\beta \varepsilon_0})^{-1} \mathrm{Tr}(e^{-\beta H})\} \ , \end{aligned}$$

where the second relation uses the assumption $\beta(\varepsilon_m - \mu) > 0$.

(2) $\Rightarrow$ (1). The restriction of K_μ to the one-particle space is $H - \mu\mathbb{1}$ and hence $\exp\{-\beta(H - \mu\mathbb{1})\}$ must be of trace-class. But then it follows from the above identification of the trace of $\exp\{-\beta K_\mu\}$ that $\beta(\varepsilon_m - \mu) > 0$ for all m, i.e., $\beta(H - \mu\mathbb{1}) > 0$.

Let us now assume that $\exp\{-\beta K_\mu\}$ is of trace-class and then calculate the Gibbs equilibrium state

$$\omega(A) = \frac{\mathrm{Tr}(e^{-\beta K_\mu} A)}{\mathrm{Tr}(e^{-\beta K_\mu})} \ .$$

This is most easily accomplished by extending ω to the annihilation and creation operators. For this we first note that if $\psi \in \mathfrak{h}_+^m$, one has

$$\|a(f_1)a(f_2)\cdots a(f_n)\psi\| \leq m^{n/2}\|\psi\| \ \|f_1\| \cdots \|f_n\| \ .$$

Moreover $\exp\{-\beta K_\mu\}\mathfrak{h}_+^m \subseteq \mathfrak{h}_+^m$ and hence

$$\begin{aligned} &\mathrm{Tr}_{\mathfrak{h}_+^m}(e^{-\beta K_\mu/2} a^*(f_n) \cdots a^*(f_1) a(f_1) \cdots a(f_n) e^{-\beta K_\mu/2}) \\ &\quad \leq m^n \mathrm{Tr}_{\mathfrak{h}_+^m}(e^{-\beta K_\mu})\|f_1\|^2 \cdots \|f_n\|^2 \\ &\quad = \left(z\frac{d}{dz}\right)^n \mathrm{Tr}_{\mathfrak{h}_+^m}(e^{-\beta K_\mu})\|f_1\|^2 \cdots \|f_n\|^2 \ . \end{aligned}$$

A simple extension of the estimates used in the proof of Proposition 5.2.27 establishes that the operators

$$A_f = a(f_1) \cdots a(f_n) e^{-\beta K_\mu/2}$$

have a bounded closure $\bar{A}_f$ and both $\bar{A}_f^* \bar{A}_f$ and $\bar{A}_f \bar{A}_f^*$ are of trace-class. Thus one can extend ω to monomials or polynomials in the $a(f)$ and $a^*(g)$. Moreover, this extension is continuous in the sense that

$$|\omega(a^*(f_1)\cdots a^*(f_n)a(g_1)\cdots a(g_m))| \leq C\prod_{i=1}^{n}\|f_i\|\prod_{j=1}^{m}\|g_j\|$$

for a suitable constant C. Now one can use the algorithm

$$e^{-\beta K_\mu/2}a^*(f) = a^*(e^{-\beta(H-\mu\mathbb{1})/2}f)e^{-\beta K_\mu/2}$$

to calculate ω in a manner similar to that used to evaluate the Fermi equilibrium state prior to Proposition 5.2.23. In particular,

$$\begin{aligned}\omega(a^*(f)a(g)) &= \mathrm{Tr}(a^*(e^{-\beta(H-\mu\mathbb{1})/2}f)e^{-\beta K_\mu}a(e^{-\beta(H-\mu\mathbb{1})/2}g))/\mathrm{Tr}(e^{-\beta K_\mu})\\ &= \omega(a(e^{-\beta(H-\mu\mathbb{1})/2}g)a^*(e^{-\beta(H-\mu\mathbb{1})/2}f))\\ &= \omega(a^*(e^{-\beta(H-\mu\mathbb{1})/2}f)a(e^{-\beta(H-\mu\mathbb{1})/2}g))\\ &\quad + (g, e^{-\beta(H-\mu\mathbb{1})}f)\ ,\end{aligned}$$

where the last step uses the CCRs. Iteration of this identity gives

$$\begin{aligned}\omega(a^*(f)a(g)) &= \omega(a^*(e^{-n\beta(H-\mu\mathbb{1})/2}f)a(e^{-n\beta(H-\mu\mathbb{1})/2}g))\\ &\quad + \sum_{m=1}^{n}(g, e^{-m\beta(H-\mu\mathbb{1})/2}f)\ .\end{aligned}$$

But $\beta(H - \mu\mathbb{1}) > 0$ and hence

$$\lim_{n\to\infty}\|e^{-n\beta(H-\mu\mathbb{1})/2}f\| = 0\ .$$

Moreover, $f, g \mapsto \omega(a^*(f)a(g))$ is continuous by the previous observations. Therefore, in the limit that $n \to \infty$ the above identity gives

$$\omega(a^*(f)a(g)) = (g, ze^{-\beta H}(\mathbb{1} - ze^{-\beta H})^{-1}f)\ .$$

Repetition of this method establishes that the value of ω on monomials of the a and a^* are determined by sums of products of the above two-point function. Thus ω is a gauge-invariant quasi-free state over the CCR algebra $\mathfrak{A}(\mathfrak{h})$. The value of ω on the Weyl operators $W(f)$ is then easily calculated. The quasi-free structure gives

$$\omega(W(f)) = \exp\{-\omega(\Phi_\omega(f)^2)/2\}$$

and one has

$$\begin{aligned}\omega(\Phi_\omega(f)^2) &= \omega(a(f)a^*(f) + a^*(f)a(f))/2\\ &= (f, (\mathbb{1} + ze^{-\beta H})(\mathbb{1} - ze^{-\beta H})^{-1}f)/2\ .\end{aligned}$$

The foregoing calculation of ω was based once again on the combinatoric relation provided by the KMS condition but expressed on the unbounded operators $a(f)$ and $a^*(g)$. It can be verified from the value of $\omega(W(f))$ that the state ω also satisfies the KMS condition on the CCR algebra but care has to be taken in phrasing the necessary continuity and analyticity properties because

the evolution is not strongly continuous. We postpone the detailed discussion of this point to Section 5.3.

The following proposition summarizes the above results.

Proposition 5.2.28. *Let H be a selfadjoint operator on the Hilbert space $\mathfrak{h}$ and let $\beta, \mu \in \mathbb{R}$. Assume that* $\exp\{-\beta H\}$ *is of trace-class, $\beta(H - \mu\mathbb{1}) > 0$, and let*

$$\omega(A) = \frac{\mathrm{Tr}(e^{-\beta K_\mu} A)}{\mathrm{Tr}(e^{-\beta K_\mu})}$$

denote the Gibbs grand canonical equilibrium state over the CCR *algebra $\mathfrak{A}(\mathfrak{h})$, where $K_\mu = d\Gamma(H - \mu\mathbb{1})$.*

It follows that ω is the gauge-invariant quasi-free state with two-point function

$$\omega(a^*(f)a(g)) = (g, ze^{-\beta H}(\mathbb{1} - ze^{-\beta H})^{-1} f)$$

and therefore

$$\omega(W(f)) = \exp\{-(f, (\mathbb{1} + ze^{-\beta H}(\mathbb{1} - ze^{-\beta H})^{-1} f)/4\} \ .$$

Once again we remark that the quasi-free state occurring in the proposition exists whenever $H \geq \mu\mathbb{1}, \beta > 0$, and μ is not a discrete eigenvalue for H. Example 5.2.18 shows that if $ze^{-\beta H}(\mathbb{1} - ze^{-\beta H})^{-1}$ is a positive selfadjoint operator, then the associated sesquilinear form determines a quasi-free state. It is not necessary that the operator is bounded or that it has discrete spectrum. One can demonstrate that this wider class of states can be constructed as weak* -limits of Gibbs states ω_n corresponding to dynamics $\tau^{(n)}$ which approximate the dynamics τ defined by H in the sense that $\omega_n(A\tau_t^{(n)}(B)C) \to \omega(A\tau_t(B)C)$ for all $A, B, C \in \mathfrak{A}(\mathfrak{h})$ and $t \in \mathbb{R}$.

The infinitely extended ideal Bose gas is more interesting than the Fermi gas from the point of view of phase structure because it describes a phase transition at low temperatures. We first describe the properties of the thermodynamic limit of the equilibrium states and the dynamics in the single-phase region. Subsequently, we examine the details of the two-phase region. We adopt the notation used for point particles in Section 5.2.4.

Proposition 5.2.29. *Let H_Λ denote a selfadjoint extension of the Laplacian $-\nabla^2$ on $L^2(\Lambda)$ corresponding to a classical boundary condition, and let H denote the unique selfadjoint extension of $-\nabla^2$, on $L^2(\mathbb{R}^\nu)$. Further let $\mathfrak{A}_\Lambda$ denote the CCR algebra over $L^2(\Lambda)$ and $\mathfrak{A}$ the CCR algebra over the subspace $\mathfrak{h}$ of $L^2(\mathbb{R}^\nu)$ formed by the union of the $L^2(\Lambda)$. Finally let τ^Λ be the group of *-automorphisms of $\mathfrak{A}_\Lambda$ and $\mathfrak{A}$, such that $\tau_t^\Lambda(W(f)) = W(e^{itH_\Lambda} f)$. Let $\beta > 0$. If follows that:*

(1) *If ω_Λ is the Gibbs grand canonical state corresponding to (H_Λ, β, μ) and if there is a $C > 0$ such that $H_\Lambda - \mu\mathbb{1} \geq C\mathbb{1}$ for all Λ, then*

$$\lim_{\Lambda' \to \infty} \omega_{\Lambda'}(A) = \omega(A)$$

for all $A \in \mathfrak{A}_\Lambda$ and all $\Lambda \subseteq \mathbb{R}^\nu$. The limit is in the sense that Λ' eventually contains any given $\Lambda \subseteq \mathbb{R}^\nu$ and ω is the gauge-invariant quasi-free state over $\mathfrak{A}$ with the two-point function

$$\begin{aligned}\omega(a_\omega^*(f)a_\omega(g)) &= (g, ze^{-\beta H}(\mathbb{1} - ze^{-\beta H})^{-1} f) \\ &= \frac{1}{(2\pi)^\nu} \int d^\nu p\, \overline{\hat{g}(p)}\, \hat{f}(p) ze^{-\beta p^2}(1 - ze^{-\beta p^2})^{-1}\end{aligned}$$

and hence

$$\omega(W(f)) = \exp\{-(f, (\mathbb{1} + ze^{-\beta H})(\mathbb{1} - ze^{-\beta H})^{-1} f)/4)\} \ .$$

(2) *If $(\mathfrak{H}_\omega, \pi_\omega, \Omega_\omega)$ is the cyclic representation corresponding to ω, then $\pi_\omega(\mathfrak{A})''$ contains a representation of the CCR algebra over $L^2(\mathbb{R}^\nu)$ by a family of unitary Weyl operators $\{W_\omega(f); f \in L^2(\mathbb{R}^\nu)\}$ such that*

(a) $\|(W_\omega(f) - W_\omega(g))W_\omega(h)\Omega_\omega\| \leq C_h\|f - g\|(\|f\| + \|g\|)$, *for all f, g, $h \in L^2(\mathbb{R}^\nu)$.*

(b) $W_\omega(f) = s\lim_{n\to\infty} \pi_\omega(W(f_n))$, *if $f_n \in \mathfrak{h}$ and $\|f_n - f\| \to 0$.*

(3) *There exists a strongly continuous one-parameter group of unitary operators U_ω on $\mathfrak{H}_\omega$ such that*

$$U_\omega(t)\Omega_\omega = \Omega_\omega \ , \quad U_\omega(t)W_\omega(f)U_\omega(t)^{-1} = W_\omega(e^{iHt}f) \ .$$

The U_ω implement a σ-weakly continuous group of *-automorphisms τ of $\pi_\omega(\mathfrak{A})''$ such that $\tau_t(A) = U_\omega(t)AU_\omega(t)^{-1}$ and one has

$$\begin{aligned}\lim_{\Lambda' \to \infty} \omega_{\Lambda'}(A\tau_t^{\Lambda'}(B)C) &= (\Omega_\omega, \pi_\omega(A)\tau_t(\pi_\omega(B))\pi_\omega(C)\Omega_\omega) \\ &= \lim_{\Lambda' \to \infty} \omega(A\tau_t^{\Lambda'}(B)C)\end{aligned}$$

for all $A, B, C \in \mathfrak{A}$.

Proof. (1) All the operators H_Λ are automatically lower semi-bounded and the Gibbs state is defined only for $\beta > 0$ by Example 5.2.26 and Proposition 5.2.28. The condition $H_\Lambda - \mu\mathbb{1} \geq C\mathbb{1}$ then ensures that

$$0 \leq \frac{\mathbb{1} + ze^{-\beta H_\Lambda}}{\mathbb{1} - ze^{-\beta H_\Lambda}} \leq \mathbb{1} \coth(\beta C/2) \ .$$

Now it follows from Example 3.1.29, Lemma 5.2.25, and Proposition 5.2.28 that $\omega_{\Lambda'}(W(f))$ converges to $\omega(W(f))$ for all $f \in \mathfrak{h}$ and hence $\omega_{\Lambda'}$ converges to ω in the weak* topology.

(2) Using the CCRs one can successively estimate that

$$\|\pi_\omega(W(f)-W(g))\pi_\omega(W(h))\Omega_\omega\| \le |e^{-i\mathrm{Im}(f-g,h)}-1| + \|\pi_\omega(W(f)-W(g))\Omega_\omega\|$$

and

$$\|\pi_\omega(W(f)-W(g))\Omega_\omega\| \le |e^{-i\mathrm{Im}(f,g)/2}-1| + \|\pi_\omega(W(f-g)-\mathbb{1})\Omega_\omega\| \ .$$

But one has

$$|e^{-i\mathrm{Im}(f-g,h)}-1| \le \|f-g\|\,\|h\|, \qquad |e^{-i\mathrm{Im}(f,g)/2}-1| \le \|f-g\|\,\|f\|/2 \ .$$

Moreover,

$$\begin{aligned}\|\pi_\omega(W(f-g)-\mathbb{1})\Omega_\omega\|^2 &= (1-\omega(W(f-g))) + (1-\omega(W(g-f)))\\ &\le 2\omega(\Phi_\omega(f-g)^2/2)\\ &\le \coth(\beta C/2)\|f-g\|^2/2 \ .\end{aligned}$$

The last step uses the obvious bound on the two-point function following from the assumption $\beta(H-\mu\mathbb{1}) \ge \beta C\mathbb{1}$. Collecting these estimates gives the desired continuity.

Finally, as Ω_ω is cyclic and $\|W_\omega(g)\| \le 1$ for all $g \in \mathfrak{h}$ one can define $W_\omega(f)$ for $f \in L^2(\mathbb{R}^\nu)$ by continuity, i.e., if $f_n \in \mathfrak{h}$ and $f_n \to f$, then $W_\omega(f)$ is defined as the strong limit of $\pi_\omega(W(f_n))$. This establishes the existence of the $W_\omega(f)$ and property (b) is automatically satisfied.

(3) Define U_ω on $\{W_\omega(f)\Omega_\omega; f \in L^2(\mathbb{R}^\nu)\}$ by

$$U_\omega(t)W_\omega(f)\Omega_\omega = W_\omega(e^{itH}f)\Omega_\omega \ .$$

It follows from the CCRs and the explicit form of $\omega(W_\omega(g))$ that the U_ω are isometric and extend to unitary operators. The strong continuity follows from (2a), e.g.,

$$\|U_\omega(t)W_\omega(f)\Omega_\omega - W_\omega(f)\Omega_\omega\| \le 2C_0\|e^{itH}f-f\|\|f\| \ .$$

The invariance of Ω_ω and the automorphism property follow by the definition of U_ω. Finally, it suffices to establish the last properties with A, B, and C chosen to be Weyl operators. But then $\omega_{\Lambda'}(A\tau_t^{\Lambda'}(B)C)$ can be explicitly calculated and its limit determined by use of Lemma 5.2.25. A straightforward calculation gives the first identification. The second follows from the continuity of $f \in L^2(\mathbb{R}^\nu) \mapsto W_\omega(f)$ and the definition of τ^Λ and τ.

Remark. (1) Statement (3) can be extended. By the same calculational procedure one deduces that

$$\begin{aligned}&\lim_{\Lambda'\to\infty} \omega_{\Lambda'}(A_0\,\tau_{t_1}^{\Lambda'}(A_1)\cdots\tau_{t_n}^{\Lambda'}(A_n))\\ &\quad=(\Omega_\omega,\ \pi_\omega(A_0)\tau_{t_1}(\pi_\omega(A_1))\cdots\tau_{t_n}(\pi_\omega(A_n))\Omega_\omega)\\ &\quad= \lim_{\Lambda'_1,\ldots,\Lambda'_n\to\infty} \omega(A_0\,\tau_{t_1}^{\Lambda'_1}(A_1)\cdots\tau_{t_n}^{\Lambda'_n}(A_n))\end{aligned}$$

for all $A_i \in \mathfrak{A}$ and $t_i \in \mathbb{R}$.

(2) It can also be shown that ω satisfies a KMS condition with respect to τ. We will return to this point in Section 5.3.

Under the restrictions imposed the above proposition gives a satisfactory description of the thermodynamic limit. This limit can be taken in a very

general form and the equilibrium state ω is explicitly identified. Moreover, the dynamics is constructed in a natural manner as a group of automorphisms of $\pi_\omega(\mathfrak{A})''$ which appears as a limit of the finite-volume dynamics. It is readily verifiable that ω is invariant not only under time translations but also under the group $\mathbb{R}^\nu$ of space translations. Moreover, it is strongly mixing for both these groups. Furthermore, ω has finite density per unit volume and hence is a locally normal state over the quasi-local algebra generated by the $\mathfrak{A}_\Lambda$. The momentum distribution of the particles is now given by

$$(2\pi)^{-\nu} z e^{-\beta p^2}(1 - z e^{-\beta p^2})^{-1} d^\nu p$$

and in the high-temperature–low-density region, which again coincides with $z \ll 1$, this distribution is approximately Maxwellian and agrees with the Fermi-Dirac distribution.

Let us next examine the shortcomings due to the conditions $H - \mu\mathbb{1} \geq C\mathbb{1}$.

Since all the selfadjoint extensions H_Λ of $-\nabla^2$ corresponding to classical boundary conditions are lower semi-bounded, the conditions $H - \mu\mathbb{1} \geq C\mathbb{1}$ state that $\mu < \mu_0$ for some μ_0 which depends on the boundary conditions used for the H_Λ. In the simplest case of $\partial\psi = \sigma\psi$ boundary conditions with $\sigma \geq 0$ or periodic boundary conditions, one has $\mu_0 = 0$ and hence $\mu < 0$ or $z < 1$. But an explicit calculation of the density $\rho(\beta, z)$ gives

$$\begin{aligned}\rho(\beta, z) &= (2\pi)^{-\nu} \int d^\nu p \; z e^{-\beta p^2}(1 - z e^{-\beta p^2})^{-1} \\ &\leq \lambda^{-\nu} \pi^{-\nu/2} \int d^\nu x \; e^{-x^2}(1 - e^{-x^2})^{-1} \;,\end{aligned}$$

where $\lambda = (4\pi\beta)^{1/2}$ is once again the thermal wavelength. If $\nu \geq 3$ the last integral is finite and one concludes that the density at fixed temperature is a bounded function of the activity. (The same conclusion is valid for all ν if $\mu_0 < 0$.) But this boundedness does not faithfully reflect the properties of large but finite systems. The density of a finite system Λ is given from Proposition 5.2.28 by

$$\begin{aligned}\rho_\Lambda(\beta, z) &= |\Lambda|^{-1} \mathrm{Tr}(z e^{-\beta H_\Lambda}(1 - z e^{-\beta H_\Lambda})^{-1}) \\ &= |\Lambda|^{-1} \sum_{n \geq 0} z e^{-\beta \varepsilon_n(\Lambda)}(1 - z e^{-\beta \varepsilon_n(\Lambda)})^{-1} \;,\end{aligned}$$

where $\varepsilon_n(\Lambda)$ are the eigenvalues of H_Λ. Thus for β and Λ fixed, the density may be made arbitrarily large by choosing z close to $\exp\{\beta\varepsilon_0(\Lambda)\}$. In this case the first term in the above sum contributes a significant proportion to $\rho_\Lambda(\beta, z)$. The drawback of Proposition 5.2.29 is that it does not take account of this latter phenomenon which is known as *Bose–Einstein condensation*.

In order to understand the basic effect of Bose–Einstein condensation on the high-density regime of the Bose gas we examine the thermodynamic limit of the Gibbs states at fixed density, but variable activity. This discussion demands more detailed analysis than was previously necessary. A complete description of all possibilities, e.g., all possible boundary conditions, etc., would lead us

too far astray and hence we examine the simplest case, Dirichlet boundary conditions, and mostly consider parallelepipeds Λ_L with edges of length $L_1, L_2, \ldots, L_\nu$. Thus the local density ρ_{Λ_L} is given by

$$\rho_{\Lambda_L}(\beta, z) = (L_1 L_2 \cdots L_\nu)^{-1} \sum_{n_1,\ldots,n_\nu \geq 1} z e^{-\beta\varepsilon_{\underline{n}}(L)}(1 - z e^{-\beta\varepsilon_{\underline{n}}(L)})^{-1}$$

where

$$\varepsilon_{\underline{n}}(L) = \sum_{i=1}^{\nu} \left(\frac{\pi n_i}{L_i}\right)^2 .$$

A Riemann approximation argument establishes that $\rho_{\Lambda_L}(\beta, z) \leq \rho(\beta, z)$, a bound that we frequently use, and

$$\lim_{\Lambda_L \to \infty} \rho_{\Lambda_L}(\beta, z) = (2\pi)^{-\nu} \int d^\nu p \, z e^{-\beta p^2}(1 - z e^{-\beta p^2})^{-1} = \rho(\beta, z)$$

for all $\beta > 0$ and all $0 < z \leq 1$. In particular the limiting value $z = 1$ is allowed but then $\rho(\beta, 1)$ is infinite if $\nu = 1$ or $\nu = 2$. Note that $z \mapsto \rho_{\Lambda_L}(\beta, z)$ and $z \mapsto \rho(\beta, z)$ are both strictly increasing. Now we begin the examination of the thermodynamic limit at fixed density by considering the variation of the activity. The following result is crucial for the understanding of Bose-Einstein condensation of thermodynamic systems.

Theorem 5.2.30. *Assume $\nu \geq 3$. Let $\rho_{\Lambda_L}(\beta, z)$ be the particle density of the Gibbs state with Dirichlet boundary conditions for a parallelepiped Λ_L and $\rho(\beta, z)$ the thermodynamic limit of $\rho_{\Lambda_L}(\beta, z)$. Define $\rho_c(\beta) = \rho(\beta, 1)$ and for each $\bar{\rho} > 0$ choose z_L as the unique root of*

$$\rho_{\Lambda_L}(\beta, z_L) = \bar{\rho} .$$

It follows that:

(1) *If $\bar{\rho} \leq \rho_c(\beta)$ and $\bar{z}$ is that unique root of $\rho(\beta, \bar{z}) = \bar{\rho}$ then*

$$\lim_{\Lambda_L \to \infty} z_L = \bar{z}$$

where $\Lambda_L \to \infty$ indicates that $L_1, \ldots, L_\nu \to \infty$.

(2) *If $\bar{\rho} > \rho_c(\beta)$ then $\lim_{\Lambda_L \to \infty} z_L = 1$ and if $(\sup_{1 \leq j \leq \nu} L_j)/(\inf_{1 \leq j \leq \nu} L_j)$ remains bounded as $\Lambda_L \to \infty$ then*

$$\lim_{\Lambda_L \to \infty} |\Lambda_L|^{-1} z_L e^{-\beta\varepsilon_0(\Lambda_L)}(1 - z_L e^{-\beta\varepsilon_0(\Lambda_L)})^{-1} = \bar{\rho} - \rho_c(\beta) ,$$

where $\varepsilon_0(\Lambda_L) = \varepsilon_{\underline{1}}(\Lambda_L)$, with $\underline{1} = (1, \ldots, 1)$, is the smallest eigenvalue of the Dirichlet Hamiltonian H_{Λ_L}.

PROOF. The proof is based upon convexity and growth properties of the density. For example, if $z_1 > z_2$, then convexity of $z \mapsto \rho_\Lambda(\beta, z)$ implies that

$$\frac{\partial \rho_\Lambda}{\partial z}(\beta, z_2) \leq \frac{\rho_\Lambda(\beta, z_1) - \rho_\Lambda(\beta, z_2)}{z_1 - z_2} \leq \frac{\partial \rho_\Lambda}{\partial z}(\beta, z_1) \ .$$

But

$$\frac{\partial \rho_\Lambda}{\partial z}(\beta, z) = |\Lambda|^{-1} \sum_{\underline{n}} e^{-\beta \varepsilon_{\underline{n}}(\Lambda)} (1 - e^{-\beta \varepsilon_{\underline{n}}(\Lambda)})^{-2} \ ,$$

where $\varepsilon_{\underline{n}}(\Lambda)$ are the eigenvalues of H_Λ. Therefore,

$$\frac{\rho_\Lambda(\beta, z)}{z} \leq \frac{\partial \rho_\Lambda(\beta, z)}{\partial z} \leq \frac{\rho_\Lambda(\beta, z)}{z(1 - ze^{-\beta \varepsilon_0(\Lambda)})} \ .$$

Combining these inequalities gives

$$\frac{\rho_\Lambda(\beta, z_2)}{z_2} \leq \frac{\rho_\Lambda(\beta, z_1) - \rho_\Lambda(\beta, z_2)}{z_1 - z_2} \leq \frac{\rho_\Lambda(\beta, z_1)}{z_1(1 - z_1 e^{-\beta \varepsilon_0(\Lambda)})} \ .$$

These bounds will be used throughout the remainder of the proof.

(1) As $\rho_{\Lambda_L}(\beta, z) \leq \rho(\beta, z)$ and both functions are increasing in z one must have $z_L \geq \bar{z}$. Thus choosing $z_1 = z_L$ and $z_2 = \bar{z}$ in the above inequality one finds

$$0 \leq z_L - \bar{z} \leq \frac{\bar{z}(\bar{\rho} - \rho_{\Lambda_L}(\beta, \bar{z}))}{\rho_{\Lambda_L}(\beta, \bar{z})}$$

and hence

$$\lim_{\Lambda_L \to \infty} z_L = \bar{z} \ .$$

(2) Assume $\rho_c(\beta) < \bar{\rho}$. If $z_L \leq 1$ then $\rho_c(\beta) < \rho_{\Lambda_L}(\beta, z_L) \leq \rho(\beta, z_L) \leq \rho_c(\beta)$ and one has a contradiction. Hence $z_L > 1$. But $z_L < e^{\beta \varepsilon_0(\Lambda_L)}$ so $\lim_{\Lambda_L \to \infty} z_L = 1$.

Next define $\overline{\rho_0}$ and $\rho_{\Lambda_L}^{(\underline{m})}$ by

$$\overline{\rho_0} = \limsup_{\Lambda_L \to \infty} |\Lambda_L|^{-1} z_L e^{-\beta \varepsilon_0(\Lambda_L)} (1 - z_L e^{-\beta \varepsilon_0(\Lambda_L)})^{-1}$$

and

$$\rho_{\Lambda_L}^{(\underline{m})}(\beta, z) = |\Lambda_L|^{-1} \sum_{\underline{n} > \underline{m}} z e^{-\beta \varepsilon_{\underline{n}}(\Lambda_L)} (1 - z e^{-\beta \varepsilon_{\underline{n}}(\Lambda_L)})^{-1}$$

where $\underline{n} > \underline{m}$ indicates $n_i > m_i$ for at least one $i = 1, \ldots, \nu$. Thus $\rho_{\Lambda_L}^{(\underline{m})}$ is obtained from ρ_{Λ_L} by omitting a finite number of terms and the $\rho_{\Lambda_L}^{(\underline{m})}$ retain the monotonicity and convexity properties of the ρ_{Λ_L}.

Since $z_L > 1$ one has $\rho_{\Lambda_L}^{(\underline{m})}(\beta, z_L) \geq \rho_{\Lambda_L}^{(\underline{m})}(\beta, 1)$. Hence

$$\rho_{\Lambda_L}^{(\underline{1})}(\beta, z_L) \geq \rho_{\Lambda_L}^{(\underline{1})}(\beta, 1) \geq \rho_{\Lambda_L}(\beta, 1) - (\beta |\Lambda_L| \varepsilon_{\underline{1}}(\Lambda_L))^{-1}$$

as the $\varepsilon_{\underline{1}}(\Lambda_L)$ term is the only one omitted in the sum for $\underline{m} = \underline{1}$. But, by assumption there is a $\lambda \geq 1$ such that $(\sup_{1 \leq j \leq \nu} L_j) \leq \lambda (\inf_{1 \leq j \leq \nu} L_j)$ as $\Lambda_L \to \infty$. Therefore $|\Lambda_L| \varepsilon_{\underline{1}}(\Lambda_L) \geq \pi^2 \lambda^{-2} |\Lambda_L| / (\inf_{1 \leq j \leq \nu} L_j)^2 \to \infty$ as $\Lambda_L \to \infty$. Consequently

$$\begin{aligned}\rho_c(\beta) &\le \liminf_{\Lambda_L\to\infty} \rho^{(\underline{1})}_{\Lambda_L}(\beta, z_L)\\ &= \liminf_{\Lambda_L\to\infty}\left(\overline{\rho} - |\Lambda_L|^{-1} z_L e^{-\beta\varepsilon_{\underline{1}}(\Lambda_L)}(1 - z_L e^{-\beta\varepsilon_{\underline{1}}(\Lambda_L)})^{-1}\right) = \overline{\rho} - \overline{\rho_0}\end{aligned}$$

because $\varepsilon_{\underline{1}}(\Lambda_L) = \varepsilon_0(\Lambda_L)$. Hence $\overline{\rho_0} \le \overline{\rho} - \rho_c(\beta)$.

Next define $\underline{\rho_0}$ by

$$\underline{\rho_0} = \liminf_{\Lambda_L\to\infty} |\Lambda_L|^{-1} z_L e^{-\beta\varepsilon_0(\Lambda_L)}(1 - z_L e^{-\beta\varepsilon_0(\Lambda_L)})^{-1} \ .$$

It suffices to prove $\underline{\rho_0} \ge \overline{\rho} - \rho_c(\beta)$ because this implies that $\overline{\rho_0} = \underline{\rho_0} = \overline{\rho} - \rho_c(\beta)$. But $z_L < e^{\beta\varepsilon_{\underline{1}}(\Lambda_L)}$ and consequently

$$\begin{aligned}&|\Lambda_L|^{-1} z_L e^{-\beta\varepsilon_{\underline{n}}(\Lambda_L)}(1 - z_L e^{-\beta\varepsilon_{\underline{n}}(\Lambda_L)})^{-1}\\ &\qquad\le |\Lambda_L|^{-1} e^{-\beta(\varepsilon_{\underline{n}}(\Lambda_L) - \varepsilon_{\underline{1}}(\Lambda_L))}(1 - e^{-\beta(\varepsilon_{\underline{n}}(\Lambda_L) - \varepsilon_{\underline{1}}(\Lambda_L))})^{-1}\\ &\qquad\le (\beta|\Lambda_L|(\varepsilon_{\underline{n}}(\Lambda_L) - \varepsilon_{\underline{1}}(\Lambda_L)))^{-1} \ .\end{aligned}$$

Moreover $|\Lambda_L|(\varepsilon_{\underline{n}}(\Lambda_L) - \varepsilon_{\underline{1}}(\Lambda_L)) \to \infty$ as $\Lambda_L \to \infty$ for $\underline{n} \ne \underline{1}$. Thus one concludes that

$$\lim_{\Lambda_L\to\infty} |\Lambda_L|^{-1} z_L e^{-\beta\varepsilon_{\underline{n}}(\Lambda_L)}(1 - z_L e^{-\beta\varepsilon_{\underline{n}}(\Lambda_L)})^{-1} = 0$$

for $\underline{n} \ne \underline{1}$, i.e., only the state of lowest energy provides a non-zero contribution to the density. Therefore

$$\underline{\rho_0} = \liminf_{\Lambda_L\to\infty}\left(\overline{\rho} - \rho^{(\underline{1})}_{\Lambda_L}(\beta, z_L)\right) = \overline{\rho} - \limsup_{\Lambda_L\to\infty} \rho^{(\underline{m})}_{\Lambda_L}(\beta, z_L)$$

for all $\underline{m} > \underline{1}$. The $\rho^{(\underline{m})}_{\Lambda_L}$ have, however, convexity properties similar to the ρ_{Λ_L} and hence

$$\rho^{(\underline{m})}_{\Lambda_L}(\beta, z_L) - \rho^{(\underline{m})}_{\Lambda_L}(\beta, 1) \le \frac{(z_L - 1)\rho^{(\underline{m})}_{\Lambda_L}(\beta, z_L)}{z_L(1 - z_L e^{-\beta\varepsilon_m(\Lambda_L)})}$$

where $\varepsilon_m(\Lambda_L)$ denotes the smallest eigenvalue occurring in the series for $\rho^{(\underline{m})}_{\Lambda_L}$. Now we use the homogeneity assumption, $(\sup_{1\le j\le \nu} L_j) \le \lambda(\inf_{1\le j\le \nu} L_j)$ as $\Lambda_L \to \infty$, to estimate that

$$\varepsilon_{\underline{1}}(\Lambda_L) \le \pi^2 \nu\left(\inf_{1\le j\le \nu} L_j\right)^{-2} \le \pi^2 \nu\lambda^2\left(\sup_{1\le j\le \nu} L_j\right)^{-2} < (\nu\lambda^2/m^2)\varepsilon_m(\Lambda_L) \ .$$

Hence $2\varepsilon_{\underline{1}}(\Lambda_L)/\varepsilon_m(\Lambda_L) < 1$ for all $m \ge (2\nu)^{1/2}\lambda$. Then for this range of m one has $z_L^2 e^{-\beta\varepsilon_m(\Lambda_L)} < e^{-\beta(\varepsilon_m(\Lambda_L) - 2\varepsilon_{\underline{1}}(\Lambda_L))} < 1$ and one may rearrange the convexity inequality to obtain

$$\rho^{(\underline{m})}_{\Lambda_L}(\beta, z_L) \le \rho_{\Lambda_L}(\beta, 1) z_L(1 - z_L e^{-\beta\varepsilon_m(\Lambda_L)})(1 - z_L^2 e^{-\beta\varepsilon_m(\Lambda_L)})^{-1} \ .$$

But $1 < z_L < e^{\beta\varepsilon_{\underline{1}}(\Lambda_L)}$ and one concludes that

$$\begin{aligned}\limsup_{\Lambda_L\to\infty}\rho^{(\underline{m})}_{\Lambda_L}(\beta, z_L) &\le \rho_c(\beta)\limsup_{\Lambda_L\to\infty}\frac{(z_L^{-1}-e^{-\beta\varepsilon_m(\Lambda_L)})}{(z_L^{-2}-e^{-\beta\varepsilon_m(\Lambda_L)})}\\ &\le \rho_c(\beta)\limsup_{\Lambda_L\to\infty}\left(1-2\varepsilon_{\underline{1}}(\Lambda_L)/\varepsilon_m(\Lambda_L)\right)^{-1}\\ &\le \rho_c(\beta)(1-2\nu\lambda^2/m^2)^{-1}\ .\end{aligned}$$

Hence for all large m

$$\limsup_{\Lambda_L\to\infty}\rho^{(\underline{m})}_{\Lambda_L}(\beta, z_L) \le \rho_c(\beta)(1-2\nu\lambda^2/m^2)^{-1}$$

and consequently

$$\underline{\rho_0} \ge \bar{\rho} - \rho_c(\beta)(1-2\nu\lambda^2/m^2)^{-1}\ .$$

As the left hand side is independent of m one concludes that $\underline{\rho_0} \ge \bar{\rho} - \rho_c(\beta)$ by taking the limit $m \to \infty$.

Although Theorem 5.2.30 is formulated for Dirichlet boundary conditions a similar result is true for Neumann conditions or the intermediate conditions $\partial\psi = \sigma\psi$ with $\sigma \ge 0$ (see Example 5.2.26). The spectrum $\varepsilon_{\underline{n}}(\Lambda_L) = \sum_{i=1}^{\nu}(\pi n_i/L_i)^2$, $n_i = 0, 1, \ldots$, of the Neumann Hamiltonian contains the Dirichlet spectrum together with additional modes for which some, or all, $n_i = 0$. Hence the Neumann density $\tilde{\rho}_\Lambda$ has a decomposition

$$\tilde{\rho}_\Lambda(\beta, z) = |\Lambda|^{-1}z(1-z)^{-1} + \rho_\Lambda(\beta, z) + r_\Lambda(\beta, z)$$

where $|\Lambda|^{-1}z(1-z)^{-1}$ is the contribution from the zero-energy ground state, $\rho_\Lambda(\beta,z)$ is the Dirichlet density and the remainder $r_\Lambda(\beta,z)$ is the contribution from the eigenvalues with some, but not all, $n_i = 0$. Consequently, r_Λ satisfies an estimate

$$0 \le r_\Lambda(\beta, z) \le \sum_{\mu=1}^{\nu-1} c_\mu(L)(2\pi)^{-\mu}\int d^\mu p\ ze^{-\beta p^2}(1-ze^{-\beta p^2})^{-1}$$

where $c_\mu(L)$ is the coefficient of x^μ in the product $\prod_{i=1}^{\nu}(1+x/L_i)$. Now fix $\tilde{z}_L$ such that $\bar{\rho} = \tilde{\rho}_{\Lambda_L}(\beta, \tilde{z}_L)$. Then $\tilde{z}_L(1-\tilde{z}_L)^{-1} \le \bar{\rho}\,|\Lambda_L|$ and hence $\tilde{z}_L \le 1 - (\bar{\rho}\,|\Lambda_L|)^{-1}$. These bounds in combination with the foregoing bounds on r_Λ suffice to deduce that $\lim_{\Lambda_L\to\infty} r_{\Lambda_L}(\beta, \tilde{z}_L) = 0$. (Care has to be taken with the $\mu = 1, 2$ terms as the integrals in the bounds diverge as $z \to 1$. But the bound on $\tilde{z}_L$ suffices to control the divergence.) Therefore

$$\bar{\rho} \ \le\ \liminf_{\Lambda_L\to\infty}|\Lambda_L|^{-1}\tilde{z}_L(1-\tilde{z}_L)^{-1} + \rho_c(\beta)\ .$$

Hence if $\bar{\rho} > \rho_c(\beta)$ then $\tilde{z}_L(1-\tilde{z}_L)^{-1} \ge (\bar{\rho} - \rho_c(\beta))|\Lambda_L|$ for all sufficiently large L_i. Thus $0 \le 1 - \tilde{z}_L \le ((\bar{\rho} - \rho_c(\beta))|\Lambda_L|)^{-1}$ and $\lim_{\Lambda_L\to\infty}\tilde{z}_L = 1$. Moreover,

$$\lim_{\Lambda_L\to\infty}|\Lambda_L|^{-1}\tilde{z}_L(1-\tilde{z}_L)^{-1} = \bar{\rho} - \lim_{\Lambda_L\to\infty}\tilde{\rho}_{\Lambda_L}(\beta, \tilde{z}_L) = \bar{\rho} - \rho_c(\beta)\ .$$

If, however, $\bar{\rho} < \rho_c(\beta) = \rho(\beta, \bar{z})$ then $\bar{z} < 1$. But a Riemann approximation argument establishes that $\tilde{\rho}_{\Lambda_L}(\beta, \bar{z}) \ge \rho(\beta, \bar{z})$ and $\lim_{\Lambda_L\to\infty}\tilde{\rho}_{\Lambda_L}(\beta, \bar{z})$

$= \rho(\beta, \bar{z}) = \bar{\rho}$. Therefore $\tilde{z}_L \leq \bar{z} < 1$ and the convexity argument used in the proof of Thoerem 5.2.30 implies that

$$0 \leq \bar{z} - \tilde{z}_L \leq \bar{z}(\tilde{\rho}_{\Lambda_L}(\beta, \bar{z})/\bar{\rho} - 1) \ .$$

Hence $\lim_{\Lambda_L \to \infty} \tilde{z}_L = \tilde{z}$. Finally, the spectrum of the Hamiltonian corresponding to boundary conditions $\partial\psi = \sigma\psi$ with $\sigma \geq 0$ is sandwiched between the Dirichlet and Neumann spectra (see Example 5.2.26). Thus the density at fixed activity lies between the Dirichlet and Neumann densities. Therefore the activity z_L^σ corresponding to a fixed density $\bar{\rho}$ is intermediate to the activities z_L and $\tilde{z}_L$ for Dirichlet and Neumann conditions. Consequently z_L^σ converges to the common limit of z_L and $\tilde{z}_L$ as $\Lambda_L \to \infty$. The thermodynamic limit is to this extent insensitive to the boundary conditions.

The discussion of the thermodynamic limit of the Gibbs states at fixed density follows a very similar pattern. It is convenient, however, to first examine the limit at the critical value of z, namely, $z = 1$ with variable density. This is particularly easy for Dirichlet boundary conditions and the result is shape independent.

Proposition 5.2.31. *Let ω_Λ denote the Gibbs grand canonical state, over $\mathfrak{A}_\Lambda$, corresponding to H_Λ, β, and z where H_Λ is the Dirichlet extension of $-\nabla^2$, on $L^2(\Lambda)$, and $\mathfrak{A}_\Lambda$ is the CCR algebra over $L^2(\Lambda)$.*

It follows that the weak-limits*

$$\omega(A) = \lim_{\Lambda' \to \infty} \omega_{\Lambda'}(A)$$

exist for $z = 1$ and each $\beta > 0$, $A \in \overline{\bigcup_\Lambda \mathfrak{A}_\Lambda}$ when $\Lambda' \to \infty$ in the sense that Λ' eventually contains any $\Lambda \subseteq \mathbb{R}^\nu$. The limit state ω is the gauge-invariant quasi-free state such that

$$\begin{aligned}\omega(W(f)) &= \exp\left\{ -(f, (\mathbb{1} + e^{-\beta H})/(\mathbb{1} - e^{-\beta H})f)/4 \right\} \\ &= e^{-\|f\|^2/4} \exp\left\{ -(2\pi)^{-\nu} \int d^\nu p |\hat{f}(p)|^2 e^{-\beta p^2} (1 - e^{-\beta p^2})^{-1} \right\}\end{aligned}$$

for all $f \in \bigcup_\Lambda L^2(\Lambda)$, where H is the unique selfadjoint extension of $-\nabla^2$ on $L^2(\mathbb{R}^\nu)$. In particular, $\omega(W(f)) = 0$ if $\nu = 1, 2$ and $\int d^\nu x f(x) \neq 0$, and $\omega(W(f)) > 0$ in all other cases.

Proof. The proof relies upon a simple but rather surprising property of the operators $\exp\{-\beta H_\Lambda\}$, which we derive in Chapter 6; see Corollary 6.3.13. This property states that for each $\beta > 0$ and $f \in L^2(\Lambda)$ the function

$$\Lambda' \mapsto (f, \exp\{-\beta H_{\Lambda'}\} f)$$

is increasing and

$$\lim_{\Lambda' \to \infty} (f, e^{-\beta H_{\Lambda'}} f) = \sup_{\Lambda'} (f, e^{-\beta H_{\Lambda'}} f) = (f, e^{-\beta H} f) \ .$$

These results rely heavily on the choice of Dirichlet boundary conditions. If we accept them, then the proof of the proposition is simple.

One has from Proposition 5.2.28 that

$$\omega_\Lambda(W(f)) = e^{-\|f\|^2/4} \exp\left\{ -\sum_{n=1}^{\infty} (f, e^{-n\beta H_\Lambda} f) \right\}$$

and therefore

$$\begin{aligned}\lim_{\Lambda' \to \infty} \omega_{\Lambda'}(W(f)) &= e^{-\|f\|^2/4} \exp\left\{ -\sup_{\Lambda'} \sup_{z<1} \sum_{n=1}^{\infty} z^n (f, e^{-n\beta H_{\Lambda'}} f) \right\} \\ &= e^{-\|f\|^2/4} \exp\{-(f, e^{-\beta H}(\mathbb{1} - e^{-\beta H})^{-1} f)\} \\ &= e^{-\|f\|^2/4} \exp\left\{ -(2\pi)^{-\nu} \int d^\nu p |\hat{f}(p)|^2 e^{-\beta p^2} (1 - e^{-\beta p^2})^{-1} \right\} .\end{aligned}$$

But for $f \in L^2(\Lambda)$, $\hat{f}(0) \neq 0$, the integral in the exponent diverges for $\nu = 1$ or 2. It is, however, finite if $\hat{f}(0) = 0$ since $\hat{f}$ is analytic, and it is finite for general f when $\nu \leq 3$.

Now we can determine the thermodynamic behavior for the Gibbs equilibrium states at fixed density.

Theorem 5.2.32. *Let ω_{Λ_L} be the Gibbs grand canonical state corresponding to H_{Λ_L}, β and z_L for the parallelepiped $\Lambda_L = \{x \in \mathbb{R}^\nu; -L_i/2 < x_i < L_i/2\}$, where H_{Λ_L} is the Dirichlet extension of $-\nabla^2$ on $L^2(\Lambda_L)$ and z_L is chosen such that ω_{Λ_L} has particle density $\bar{\rho}$.*

It follows that the weak-limits*

$$\omega(A) = \lim_{\Lambda_L \to \infty} \omega_{\Lambda_L}(A)$$

exist for each $\beta > 0, \bar{\rho} > 0$, and $A \in \overline{\bigcup_\Lambda \mathfrak{A}_\Lambda}$, where $\Lambda_L \to \infty$ in the sense that $L_1, \ldots, L_\nu \to \infty$ and $(\sup_{1 \leq i \leq \nu} L_i)/(\inf_{1 \leq i \leq \nu} L_i)$ remains bounded when $\bar{\rho} \geq \rho_c(\beta)$. The ω are gauge-invariant quasi-free states.

Let $\rho(\beta, z)$ denote the thermodynamic density and set

$$\omega(W(f)) = \exp\{-\rho_\omega(f, f)/4\} .$$

The two-point function $\rho_\omega(f, f)$ is then determined as follows:

(A) *If $\bar{\rho} \leq \rho_c(\beta) = \rho(\beta, 1)$ then*

$$\rho_\omega(f, f) = (f, (\mathbb{1} + \bar{z} e^{-\beta H})(\mathbb{1} - \bar{z} e^{-\beta H})^{-1} f) ,$$

where H is the selfadjoint extension of $-\nabla^2$ on $L^2(\mathbb{R}^\nu)$ and $\bar{z}$ is the unique root of $\bar{\rho} = \rho(\beta, \bar{z})$.

(B) *If $\bar{\rho} > \rho_c(\beta)$ then*

$$\rho_\omega(f, f) = 2^{\nu+1} \rho_0(\beta) \left| \int d^\nu x f(x) \right|^2 + (f, (\mathbb{1} + e^{-\beta H})(\mathbb{1} - e^{-\beta H})^{-1} f) ,$$

where $\rho_0(\beta) = \bar{\rho} - \rho_c(\beta)$.

PROOF. (A) Let $\bar{\rho} < \rho_c(\beta)$. As $\rho_{\Lambda_L}(\beta, z) < \rho(\beta, z)$ one must have $\bar{z} < z_L$. Moreover, there must exist $\hat{L}_i$ and $\hat{z} < 1$ such that $z_L \leq \hat{z}$ for all $L_i > \hat{L}_i$. Therefore,

$$\begin{aligned} 0 &\leq (f, (\mathbb{1} + \bar{z}e^{-\beta H_{\Lambda_L}})(\mathbb{1} - \bar{z}e^{-\beta H_{\Lambda_L}})^{-1} f) \\ &\quad - (f, (\mathbb{1} + z_L e^{-\beta H_{\Lambda_L}})(\mathbb{1} - z_L e^{-\beta H_{\Lambda_L}})^{-1} f) \leq 2\|f\|^2 (1 - \hat{z})^{-2} (z_L - \bar{z}) \ . \end{aligned}$$

The convergence of ω_{Λ_L} to the correct state then follows from Proposition 5.2.28 and Theorem 5.2.30. The case $\bar{\rho} = \rho_c(\beta)$ will be covered by the proof of (B).
(B) Let $\varepsilon_{\underline{n}}(\Lambda_L)$ and $E_{\underline{n}}(\Lambda_L)$ denote the eigenvalues and eigenprojectors of H_{Λ_L}. The state ω_{Λ_L} is quasi-free and $\omega_{\Lambda_L}(W(f)) = \exp\{-\rho_{\omega_{\Lambda_L}}(f, f)/4\}$ where

$$\rho_{\omega_{\Lambda_L}}(f, f) = \sum_{\underline{n}} (1 + z_L e^{-\beta\varepsilon_{\underline{n}}(\Lambda_L)})(1 - z_L e^{-\beta\varepsilon_{\underline{n}}(\Lambda_L)})^{-1} (f, E_{\underline{n}}(\Lambda_L) f) \ .$$

Now the first term in this sum is a product of two factors each of which has a limit as $\Lambda_L \to \infty$. First,

$$\lim_{\Lambda_L \to \infty} |\Lambda_L|^{-1} (1 + z_L e^{-\beta\varepsilon_0(\Lambda_L)})(1 - z_L e^{-\beta\varepsilon_0(\Lambda_L)})^{-1} = 2(\bar{\rho} - \rho_c(\beta))$$

by Theorem 5.2.30; and second,

$$\begin{aligned} \lim_{\Lambda_L \to \infty} |\Lambda_L| (f, E_0(\Lambda_L) f) &= \lim_{\Lambda_L \to \infty} 2^\nu \left| \int d^\nu x f(x) \prod_{i=1}^{\nu} \cos\left(\frac{\pi x_i}{L_i}\right) \right|^2 \\ &= 2^\nu \left| \int d^\nu x f(x) \right|^2 , \end{aligned}$$

where we have used the fact that the normalized eigenfunction corresponding to the lowest eigenvalue is

$$\psi_0(x) = \frac{2^{\nu/2}}{|\Lambda_L|^{1/2}} \prod_{i=1}^{\nu} \sin\left(\frac{\pi}{L_i}\left(x_i - \frac{L_i}{2}\right)\right) = \frac{2^{\nu/2}}{|\Lambda_L|^{1/2}} \prod_{i=1}^{\nu} \cos\left(\frac{\pi x_i}{L_i}\right) \ .$$

But for the higher terms

$$|\Lambda_L| (f, E_{\underline{n}}(\Lambda_L) f) \leq 2^\nu \left(\int d^\nu x |f(x)| \right)^2$$

and

$$\lim_{\Lambda_L \to \infty} |\Lambda_L|^{-1} (1 + z_L e^{-\beta\varepsilon_{\underline{n}}(\Lambda_L)})(1 - z_L e^{-\beta\varepsilon_{\underline{n}}(\Lambda_L)})^{-1} = 0 \ .$$

The first statement follows by explicit calculation and the second by the estimates used to prove the second half of Theorem 5.2.30. (This again reflects the fact that only the lowest energy state gives a nonzero contribution to the density.) Thus for each $\underline{m} > \underline{1}$ one has

$$\lim_{\Lambda_L \to \infty} (\rho_{\omega_{\Lambda_L}}(f, f) - \rho^{(\underline{m})}_{\omega_{\Lambda_L}}(f, f)) = 2^{\nu+1} (\bar{\rho} - \rho_c(\beta)) \left| \int d^\nu x f(x) \right|^2 ,$$

where

$$\rho^{(\underline{m})}_{\omega_{\Lambda_L}}(f, f) = \sum_{\underline{n} > \underline{m}} (1 + z_L e^{-\beta\varepsilon_{\underline{n}}(\Lambda_L)})(1 - z_L e^{-\beta\varepsilon_{\underline{n}}(\Lambda_L)})^{-1} (f, E_{\underline{n}}(\Lambda_L) f) \ .$$

Finally, one may prove that

$$\lim_{m\to\infty} \lim_{\Lambda_L\to\infty} \{(\rho^{(\underline{m})}_{\omega_{\Lambda_L}}(f,f) - (f,(\mathbb{1}+e^{-\beta H})(\mathbb{1}-e^{-\beta H})^{-1}f)\} = 0$$

by repetition of the argument used to prove the second part of Theorem 5.2.30. First, one uses monotonicity of $\rho^{(\underline{m})}_{\Lambda_L}$ in z to obtain an estimate

$$\rho^{(\underline{m})}_{\omega_{\Lambda_L}}(f,f) \geq (f,(\mathbb{1}+e^{-\beta H_{\Lambda_L}})(\mathbb{1}-e^{-\beta H_{\Lambda_L}})^{-1}f) - \|f\|^2 \sum_{\underline{n}\leq\underline{m}} (\beta|\Lambda_L|\varepsilon_{\underline{n}}(\Lambda_L))^{-1}$$

and, second, one uses convexity in z to find

$$\rho^{(\underline{m})}_{\omega_{\Lambda_L}}(f,f) \leq (f,(\mathbb{1}+e^{-\beta H_{\Lambda_L}})(\mathbb{1}-e^{-\beta H_{\Lambda_L}})^{-1}f)\frac{(1-z_L e^{-\beta\varepsilon_{\underline{m}}(\Lambda_L)})}{(1-z_L^2 e^{-\beta\varepsilon_{\underline{m}}(\Lambda_L)})} \ .$$

The argument is then completed as in Theorem 5.2.30.

Theorem 5.2.32 establishes that there are two distinct regimes for the Bose gas. First, there is a high-temperature–low-density regime described by Proposition 5.2.29 and corresponding to $z<1$ for Dirichlet boundary conditions. Second, there is a low-temperature–high-density regime in which $z=1$ and Bose–Einstein condensation takes place, i.e., a finite proportion of the particles occupy the lowest energy state. In this second regime the system has a multitude of possible equilibrium states each of which has the same temperature and activity. The states differ by their particle densities and all densities $\rho\in[\rho_c(\beta),\infty)$ are possible. The two-point functions of the equilibrium states ω in the condensation region are given by

$$\begin{aligned}\omega(a^*_\omega(f)a_\omega(g)) &= 2^\nu\rho_0(\beta)\int d^\nu x\,\overline{g(x)}\int d^\nu x f(x)\\ &\quad + (2\pi)^{-\nu}\int d^\nu p\,\overline{\hat{g}(p)}\hat{f}(p)e^{-\beta p^2}(1-e^{-\beta p^2})^{-1}\end{aligned}$$

and the local density by

$$\rho(\beta) = 2^\nu\rho_0(\beta)+\rho_c(\beta) \ ,$$

where $\rho_0(\beta)=\bar{\rho}-\rho_c(\beta)$ and $\bar{\rho}\in[\rho_c(\beta),\infty)$. The term $\rho_0(\beta)$ measures the density of the condensate, i.e., the particles in the lowest, zero, energy state, and the coefficient 2^ν indicates the relative proportion of the condensate at the origin. This coefficient can be identified from our estimates as the thermodynamic limit of $|\Lambda_L|\,|\psi^L_0(0)|^2$ where ψ^L_0 is the lowest-energy eigenfunction of the Dirichlet Hamiltonian H_{Λ_L}. If one replaces Dirichlet boundary conditions by the elastic conditions $\partial\psi/\partial n=\sigma\psi$, then a slight modification of the foregoing arguments establishes the existence of the corresponding equilibrium state. The only noticeable difference is that the coefficient 2^ν is replaced by a positive constant c_σ,

$$c_\sigma = \lim_{\Lambda_L\to\infty}|\Lambda_L|\,|\psi^{\sigma,L}_0(0)|^2 \ ,$$

where $\psi^{\sigma,L}_0$ is now the lowest-energy eigenfunction with the new boundary conditions. One can check that c_σ is a decreasing function of σ and $c_\sigma\to 1$ as $\sigma\to 0$, i.e., $c_\sigma=1$ for Neumann conditions. In the Neumann case the condensate is

distributed evenly throughout the system and the local density takes the value $\bar{\rho}$ used in the limit. Thus the thermodynamic equilibrium state is sensitive to the choice of boundary conditions and each choice gives, in principle, a different state in the condensation region although accidental degeneracy is possible.

The phenomenon of condensation corresponds to a phase transition of the system and the equilibrium states have less ergodic properties than the states in the single phase ($z < 1$) region. Although the states occurring in Theorem 5.2.32(B) are invariant under the action τ of the group $\mathbb{R}^\nu$ of space translations, they are no longer $\mathbb{R}^\nu$-ergodic. This is most easily seen by calculating that

$$\lim_{|x|\to\infty} \omega(W(f)\tau_x(W(g))) = \omega(W(f))\omega(W(g)) \times \exp\left\{ -c_\sigma \rho_0(\beta) 2\,\mathrm{Re} \int d^\nu x \bar{f}(x) \int d^\nu x\, g(x) \right\} .$$

Thus ω is strongly mixing and $\mathbb{R}^\nu$-ergodic, if, and only if, $\rho_0(\beta) = 0$. The decomposition of ω into $\mathbb{R}^\nu$-ergodic states can be explicitly computed and one finds the following result[2]

$$\omega(A) = (2\pi)^{-1} \int_0^\infty d\rho\, K(\rho, \rho_0) \int_0^{2\pi} d\alpha\, \omega_{\rho,\alpha}(A) ,$$

where $K(\rho, \rho_0) = \rho_0(\beta)^{-1} \exp\{-\rho/\rho_0(\beta)\}$ and the states $\omega_{\rho,\alpha}$ are determined by

$$\omega_{\rho,\alpha}(W(f)) = \exp\left\{ i c_\sigma^{1/2} \rho^{1/2} \left(e^{i\alpha} \int d^\nu x f(x) + e^{-i\alpha} \int d^\nu x \overline{f(x)} \right) \right\} \times \exp\left\{ -(f, (\mathbb{1} + e^{-\beta H})(\mathbb{1} - e^{-\beta H})^{-1} f)/4 \right\}.$$

In particular the $\mathbb{R}^\nu$-ergodic states $\omega_{\rho,\alpha}$ are no longer gauge-invariant. The two-point functions of the states $\omega_{\rho,\alpha}$ are given by

$$\omega_{\rho,\alpha}(a_\omega^*(f) a_\omega(g)) = c_\sigma \rho \int d^\nu x f(x) \int d^\nu x\, \overline{g(x)} + (2\pi)^{-\nu} \int d^\nu p\, \overline{\hat{g}(p)} \hat{f}(p) e^{-\beta p^2} (1 - e^{-\beta p^2})^{-1}$$

and the local densities by

$$\rho_{\omega_{\rho,\alpha}}(\beta) = c_\sigma \rho + \rho_c(\beta) .$$

[2]This decomposition is readily verified with the aid of the two formulas

$$(2\pi)^{-1} \int_0^{2\pi} d\alpha\, e^{i(a \cos\alpha + b \sin\alpha)} = J_0((a^2 + b^2)^{1/2}) ,$$

$$\int_0^\infty dx\, e^{-x} J_0((2cx)^{-1/2}) = e^{-c/2} ,$$

where J_0 is the usual Bessel function, $a, b \in \mathbb{R}$ and $c \geq 0$.

Thus the variable ρ occurring in the integral decomposition measures the density of the condensate and the probability measure $d\rho\, K(\rho, \bar{\rho})$ determines the distribution of the various possible condensate densities.

It remains to describe the thermodynamic limit of the dynamics in the condensation region. This can be discussed from the same point of view adopted in Proposition 5.2.29 but various changes occur. Most noticeably the equilibrium states do not extend to states over the CCR algebra on $L^2(\mathbb{R}^\nu)$. If $(\mathfrak{H}_\omega, \pi_\omega, \Omega_\omega)$ is the cyclic representation corresponding to the equilibrium state ω obtained by the fixed-density thermodynamic limit with $\bar{\rho} \geq \rho_c(\beta)$, then $\pi_\omega(\mathfrak{A})''$ contains a representation of the CCR algebra over the subspace $\mathscr{S}(\mathbb{R}^\nu) \subseteq L^2(\mathbb{R}^\nu)$. This follows because any element in $\mathscr{S}(\mathbb{R}^\nu)$ can be approximated by elements in $\bigcup_\Lambda L^2(\Lambda)$ in the norm

$$\|f\|_{\mathscr{K}} = |\hat{f}(0)|^2 + \int d^\nu p\, |\hat{f}(p)|^2 (1 - e^{-p^2})^{-1}$$

and the unitary Weyl operators satisfy estimates of the form

$$\|(W_\omega(f) - W_\omega(g)) W_\omega(h)\Omega_\omega\| \leq c_h \|f - g\|_{\mathscr{K}} (\|f\| + \|g\|)$$

for $f, g \in \bigcup_\Lambda L^2(\Lambda)$. (Recall that $\nu \geq 3$ when $\rho_c(\beta) < +\infty$.) Note that the unitary group $U_t = \exp\{itH\}$ generated by the Laplacian on $L^2(\mathbb{R}^\nu)$ maps $\mathscr{S}(\mathbb{R}^\nu)$ on $\mathscr{S}(\mathbb{R}^\nu)$, because $\mathscr{S}(\mathbb{R}^\nu)$ is equal to its Fourier transform. Hence U implements a one-parameter group of Bogoliubov transformations on the CCR algebra over $\mathscr{S}(\mathbb{R}^\nu)$. Since any element in $\bigcup_\Lambda L^2(\Lambda)$ can be approximated by elements $\mathscr{S}(\mathbb{R}^\nu)$ in the norm $\| \quad \|_{\mathscr{K}}$, it follows that this group extends by strong continuity to a one-parameter group τ of *-automorphisms of $\pi_\omega(\mathfrak{A})''$ as in Proposition 5.2.29. If τ^Λ is the one-parameter group of Bogoliubov transformations of the CCR algebra over $L^2(\Lambda)$ implemented by the Dirichlet Laplacian H_Λ, one can then establish that

$$\lim_{\Lambda_L \to \infty} \omega_{\Lambda_L}(A \tau_t^{\Lambda_L}(B) C) = (\Omega_\omega,\ \pi_\omega(A) \tau_t(\pi_\omega(B)) \pi_\omega(C) \Omega_\omega)$$

for Weyl operators A, B, and C over $\mathscr{D}(\mathbb{R}^\nu)$, where Λ_L tends to infinity in the sense of Theorem 5.2.32. To explain the nature of this argument it is preferable to first examine the analogous problem in the setting of Proposition 5.2.31 for $\nu \geq 3$. Choosing A, B, and C as Weyl operators and using the CCRs one readily reduces the problem to the proof that

$$\lim_{\Lambda \to \infty} (f, X_\Lambda e^{itH_\Lambda} g) = (X^{1/2} f, X^{1/2} e^{itH} g) \ ,$$

where

$$X_\Lambda = (\mathbb{1} + e^{-\beta H_\Lambda})(\mathbb{1} - e^{-\beta H_\Lambda})^{-1}$$

and

$$X = (\mathbb{1} + e^{-\beta H})(\mathbb{1} - e^{-\beta H})^{-1} \ .$$

But if x_Λ and x are the positive quadratic forms canonically associated with the bounded positive operators X_Λ and the positive selfadjoint operator X, respectively, then the proof of Proposition 5.2.31 is based upon the fact that the

net x_Λ is monotonically increasing and its limit, in the sense of Lemma 5.2.13, is exactly x. But in the proof of Lemma 5.2.13 we established that

$$\lim_{\Lambda\to\infty} \|(X_\Lambda + \mathbb{1})^{1/2}(X+\mathbb{1})^{-1/2}\psi - \psi\| = 0$$

for all $\psi \in L^2(\mathbb{R}^\nu)$. Hence, if $\psi \in D(X^{1/2})$ one has

$$\lim_{\Lambda\to\infty} \|(X_\Lambda + \mathbb{1})^{1/2}\psi - (X+\mathbb{1})^{1/2}\psi\| = 0 \ .$$

Therefore, the desired result follows from the estimate

$$\begin{aligned}
&|(f, X_\Lambda e^{itH_\Lambda} g) - (X^{1/2} f, X^{1/2} e^{itH} g)| \\
&\quad \le |((X_\Lambda + \mathbb{1})^{1/2} f, e^{itH_\Lambda}((X_\Lambda + \mathbb{1})^{1/2} - (X+\mathbb{1})^{1/2})g)| \\
&\quad + |((X_\Lambda + \mathbb{1})^{1/2} f, (e^{itH_\Lambda} - e^{itH})(X+\mathbb{1})^{1/2} g)| \\
&\quad + |(((X_\Lambda + \mathbb{1})^{1/2} - (X+\mathbb{1})^{1/2}) f, e^{itH}(X+\mathbb{1})^{1/2} g)| \\
&\quad + |(f, (e^{itH} - e^{itH_\Lambda})g)| \ .
\end{aligned}$$

This result can now be used to establish the analogous fixed-density result by retracing the estimates used to prove Theorems 5.2.30 and 5.2.32. In particular one uses the last two estimates given in the proof of Theorem 5.2.32. We omit the details.

Finally, we emphasize that the quantitative properties of Bose–Einstein condensation are quite sensitive to changes of boundary conditions although the qualitative features remain unchanged. If one uses $\partial\psi/\partial n = \sigma\psi$ boundary conditions with $\sigma < 0$, then condensation occurs in all dimensions at a value of the activity $z_\sigma < 1$ and the condensate is principally located near the surface of the system. Thus, in the thermodynamic limit at fixed density the equilibrium state, which characterizes the properties of the system near the origin, shows no trace of the condensate.

EXAMPLE 5.2.33. Let $\mathfrak{H} = L^2(-L/2, L/2)$ and let H_L be the selfadjoint extension of $-d^2/dx^2$ which satisfies

$$\left[\frac{d\psi(x)}{dx} - \sigma\psi(x)\right]_{x=L/2} = 0 = \left[\frac{d\psi(x)}{dx} + \sigma\psi(x)\right]_{x=-L/2}$$

for all $\psi \in D(H_L)$, where $\sigma > 0$. The lowest eigenvalue $\lambda_0(L)$ of H_L is negative and is given by $\lambda_0(L) = -\lambda^2$, where λ is the unique solution of

$$\lambda \tanh(\lambda L/2) = \sigma \ .$$

This eigenvalue has the property that it increases with L to the asymptotic value $-\sigma^2$. The corresponding normalized eigenfunction ψ_0^L can be chosen as

$$\psi_0^L(x) = (2/L)^{1/2}\left\{1 + (\lambda L)^{-1}\sinh(\lambda L)\right\}^{-1/2} \cosh(\lambda x) \ .$$

(In fact, if L is large enough there is a second negative eigenvalue $\lambda_1(L)$ which decreases to $-\sigma^2$ and whose eigenfunction can be chosen to be anti-symmetric.) Thus, the Gibbs states are only defined for $\mu < \lambda_0(L) < -\sigma^2$, and condensation takes place for

$$z = z_\sigma = \exp\{-\beta\sigma^2\} < 1 \ .$$

The critical density $\rho(\beta, z_\sigma)$ is now given by

$$\rho(\beta, z_\sigma) = (2\pi)^{-1} \int dp\, z_\sigma e^{-\beta p^2} (1 - z_\sigma e^{-\beta p^2})^{-1}$$

and as $L|\psi_0^L(0)|^2 \to 0$ in the limit $L \to \infty$ the thermodynamic limit state ω at fixed density $\bar{\rho}$ satisfies

$$\omega(W(f)) = \exp\Big\{ -(f, (\mathbb{1} + ze^{-\beta H})/(\mathbb{1} - ze^{-\beta H})f)/4 \Big\}$$

for $\bar{\rho} \leq \rho(\beta, z_\sigma)$ and

$$\omega(W(f)) = \exp\Big\{ -(f, (\mathbb{1} + z_\sigma e^{-\beta H})/(\mathbb{1} - z_\sigma e^{-\beta H})f)/4 \Big\}$$

for $\bar{\rho} > \rho(\beta, z_\sigma)$. Similar conclusions are valid for $v > 1$.

5.3. KMS-States

5.3.1. The KMS Condition

In the previous section we analyzed two C^*-algebras which describe the kinematics of particle systems and also analyzed the simplest examples of equilibrium states. Now we discontinue this specific analysis and describe instead various general characterizations of equilibrium phenomena. Principally, we investigate the Kubo–Martin–Schwinger, or KMS, condition briefly outlined in the Introduction and used in the calculation of the Gibbs states of the ideal Fermi and Bose gases. Our description of this condition was, hitherto, rather sketchy and this will be corrected in the sequel. Recall that if $\mathfrak{A} = \mathscr{L}\mathscr{C}(\mathfrak{H})$, H is a selfadjoint operator on $\mathfrak{H}, \beta \in \mathbb{R}$, and $\exp\{-\beta H\}$ is of trace-class, then the Gibbs equilibrium state

$$\omega(A) = \frac{\mathrm{Tr}_{\mathfrak{H}}(e^{-\beta H}A)}{\mathrm{Tr}_{\mathfrak{H}}(e^{-\beta H})}$$

formally satisfies the condition

$$\omega(A\tau_t(B))|_{t=i\beta} = \omega(BA)$$

with respect to the automorphism group

$$\tau_t(A) = e^{itH}Ae^{-itH} \quad .$$

This is a particular example of the KMS condition and it basically involves two elements:

(1) The analyticity of the functions $t \mapsto \omega(A\tau_t(B))$ in a strip, the strip $0 < \mathrm{Im}\, t < \beta$ if $\beta > 0$, and,

(2) The approximate commutation of each pair A, and B, within the state ω.

We will choose a precise definition of the KMS condition which emphasizes the latter, algebraic, property and partially deemphasizes the analyticity property. Subsequently it will be necessary to extend the properties of analyticity.

Throughout most of the rest of this chapter we consider a C^*-dynamical system $(\mathfrak{A}, \mathbb{R}, \tau)$ based on the group $\mathbb{R}$ and for brevity we denote such systems by $(\mathfrak{A}, \tau)$. Moreover, we let $\mathfrak{A}_\tau$ denote the set of entire analytic elements for τ, Definition 2.5.20. Recall that $\mathfrak{A}_\tau$ is a norm dense *-subalgebra of $\mathfrak{A}$, Proposition 2.5.22, and it is clearly τ-invariant, i.e., if $A \in \mathfrak{A}_\tau$, then $\tau_t(A) \in \mathfrak{A}_\tau$ for all

$t \in \mathbb{R}$. We also consider a W^*-dynamical system $(\mathfrak{M}, \tau)$, where $\mathfrak{M}$ is a von Neumann algebra and τ a σ-weakly continuous one-parameter group of *-automorphisms of $\mathfrak{M}$. The set $\mathfrak{M}_\tau$ of entire analytic elements for τ is no longer norm dense in $\mathfrak{M}$ but nevertheless it is dense in the σ-weak topology and τ-invariant.

We now adopt a definition of KMS states phrased in terms of dense sets of analytic elements which has the advantage that it is often easy to corroborate.

Definition 5.3.1. Let $(\mathfrak{A}, \tau)$ be a C^*-dynamical system. The state ω over $\mathfrak{A}$ is defined to be a τ-KMS state at value $\beta \in \mathbb{R}$, or a (τ, β)-KMS state, if

$$\omega(A\tau_{i\beta}(B)) = \omega(BA)$$

for all A, B in a norm dense, τ-invariant *-subalgebra of $\mathfrak{A}_\tau$.

If $(\mathfrak{M}, \tau)$ is a W^*-dynamical system, a state ω over $\mathfrak{M}$ is defined to be a (τ, β)-KMS state, for $\beta \in \mathbb{R}$, if ω is normal and the above identity is valid for all A and B in a σ-weakly dense τ-invariant *-subalgebra of $\mathfrak{M}_\tau$.

A τ-KMS state at value $\beta = -1$ is called a τ-KMS state.

This definition has several immediate consequences.

The value $\beta = 0$ is distinct from the other values. In this case Definition 5.3.1 states that ω is a trace-state,

$$\omega(AB) = \omega(BA)$$

for all $A, B \in \mathfrak{A}$. Conversely, a trace-state is a $(\tau, 0)$-KMS state. If $\beta \neq 0$ and ω is a (τ, β)-KMS state the definition indicates that τ measures the deviation of ω from being a trace. This idea will be clarified later.

Another immediate consequence is that if $t \mapsto \tau_t = \iota$ is the trivial group of automorphisms, then ω is a (τ, β)-KMS state if, and only if, it is a trace-state.

Next note that ω is a (τ_t, β)-KMS state if, and only if, it is a $(\tau_{-\beta t}, -1)$-KMS state. If $\beta \neq 0$, this statement is evident but if $\beta = 0$ both sets of states are the trace-states. Thus by rescaling the group one can eliminate β. Hence, for many general purposes it suffices to consider τ-KMS states. This also shows that the choice $\beta = -1$ in the definition of these latter states has no particular significance. (The value -1 coincides with a convention adopted in the modular theory of Tomita-Takesaki). We emphasize, however, that despite these rescaling properties there is no simple prescription for connecting the (τ, β)-KMS states for different β (see Theorem 5.3.35).

EXAMPLE 5.3.2. Let $\mathfrak{A}(\mathfrak{h})$ be the CAR algebra over the Hilbert space $\mathfrak{h}$ and τ a one-parameter group of Bogoliubov transformations such that $\tau_t(a(f)) = a(e^{itH}f)$, etc. Let f be an analytic element for H, then the τ-KMS condition states that

$$\begin{aligned}\omega(a^*(f)a(g)) &= \omega(a(g)a^*(e^{-\beta H}f)) \\ &= (g, e^{-\beta H}f) - \omega(a^*(e^{-\beta H}f)a(g)) \ .\end{aligned}$$

Therefore

$$\omega(a^*(f)a(g)) = (g, e^{-\beta H}(\mathbb{1} + e^{-\beta H})^{-1} f) \ .$$

Iteration of this calculation in the manner preceding Proposition 5.2.23 shows that the gauge-invariant quasi-free state with the preceding two-point function is the unique (τ, β)-KMS state. Note that the polynomials in $a(f)$ and $a^*(g)$, with f and g analytic for H, are norm dense in $\mathfrak{A}$. In particular the limit Gibbs state constructed in Theorem 5.2.24 is the unique (τ, β)-KMS state for the limit dynamics.

Alternatively, let $\mathfrak{A}$ be the CCR algebra over a pre-Hilbert space $\mathfrak{h}$, H a positive selfadjoint operator defined on $\mathfrak{h}$ not having zero as its eigenvalue, and such that $e^{itH}\mathfrak{h} \subseteq \mathfrak{h}$ for all $t \in \mathbb{R}$, and $\mathfrak{h} \subseteq D(e^{-\beta H}(\mathbb{1} - e^{-\beta H})^{-1})$ for $\beta > 0$. Let ω be the gauge invariant quasi-free state with the two-point function

$$\omega(a_\omega^*(f)a_\omega(g)) \ = \ (g, \ e^{-\beta H}(\mathbb{1} - e^{-\beta H})^{-1} f)$$

and τ the σ-weakly-continuous group of *-automorphisms of $\pi_\omega(\mathfrak{A})''$ obtained by strong continuity from the Bogoliubov transformations determined by e^{itH}. It follows from the calculation preceding Proposition 5.2.28 that ω is a (τ, β)-KMS state over the von Neumann algebra $\pi_\omega(\mathfrak{A})''$. But if s is any positive sesquilinear form on $\mathfrak{h} \times \mathfrak{h}$ with the invariance property

$$s(g, f) = s(g, e^{itH} f)$$

for all $g, f \in \mathfrak{h}$ and all $t \in \mathbb{R}$, then the gauge-invariant quasi-free state with two-point function

$$\omega(a_\omega^*(f)a_\omega(g)) = (g, e^{-\beta H}(\mathbb{1} - e^{-\beta H})^{-1} f) + s(g, f)$$

is also a (τ, β)-KMS state over $\pi_\omega(\mathfrak{A})''$. Thus, one has a possibility of a nonunique (τ, β)-KMS state in this case. An example is the Bose-Einstein condensation extensively studied in Section 5.2.5. Here $\mathfrak{h} = \mathscr{S}(\mathbb{R}^\nu)$ with $\nu \geq 3$, $H = -\nabla^2$ is the Laplacian and

$$s(g, f) = \rho \int d^\nu x \, \overline{g(x)} \int d^\nu x \, f(x) \ ,$$

where $\rho > 0$.

It follows immediately from the commutation relations

$$W(f)W(g) = e^{-i\,\mathrm{Im}(f,g)} W(g)W(f)$$

that the CCR algebra over $\mathfrak{h}$ has a unique trace-state ω, given by

$$\omega(W(f)) = \begin{cases} 1, & \text{if } f = 0 \\ 0, & \text{if } f \neq 0 \ . \end{cases}$$

This state is invariant under all Bogoliubov transformations, and thus the group of automorphisms determined by e^{itH} extends to a one-parameter group τ of *-automorphisms of $\pi_\omega(\mathfrak{A})''$. However, this group is not σ-weakly-continuous and hence ω is not a $(\tau, 0)$-KMS state on $\pi_\omega(\mathfrak{A})''$ in the sense of Definition 5.3.1.

When $\beta < 0$, there exists no (τ, β)-KMS states over the CCRs in the von Neumann sense.

We begin the analysis of KMS states by proving that they satisfy the crudest characteristic of equilibrium, τ-invariance.

Propositions 5.3.3. *Let ω be a (τ, β)-KMS state over the C^*-algebra $\mathfrak{A}$ (or the W^*-algebra $\mathfrak{M}$) with $\beta \in \mathbb{R}\backslash\{0\}$.*

It follows that ω is τ- invariant, i.e.,

$$\omega(\tau_t(A)) = \omega(A)$$

for all $A \in \mathfrak{A}$ (for all $A \in \mathfrak{M}$) and all $t \in \mathbb{R}$.

Moreover the following conditions are equivalent for an arbitrary state ω over $\mathfrak{A}$ (which is assumed normal in the W^*-case):

(1) *ω is a (τ, β)-KMS state with $\beta \in \mathbb{R}$.*

(2) *$\omega(\tau_{-i\beta/2}(A)\tau_{i\beta/2}(B)) = \omega(BA)$, for all A, B in a norm-dense τ-invariant *-subalgebra of $\mathfrak{A}_\tau$.*

Proof. The proof of the two cases C^*, and W^*, is identical. We consider the former.

First note that by rescaling we may assume $\beta = -1$. Next let B be an element out of the norm-dense τ-invariant *-subalgebra $\mathfrak{B}_\tau \subseteq \mathfrak{A}_\tau$ for which the KMS condition holds and define the analytic function F by

$$F(z) = \omega(\tau_z(B)) \ .$$

Then F is an entire analytic function which is bounded on the strip

$$\bar{\mathfrak{D}} = \{z;\, z \in \mathbb{C}, -1 \leq \operatorname{Im} z \leq 0\}$$

by

$$M = \sup\{\, \|\tau_{i\gamma}(B)\| \,;\, \gamma \in [-1, 0]\} \ .$$

This follows because

$$|F(z)| \leq \|\tau_z(B)\| = \|\tau_{\operatorname{Re} z}(\tau_{i \operatorname{Im} z}(B))\| = \|\tau_{i \operatorname{Im} z}(B)\| \ .$$

But if $\mathfrak{A}$ has an identity $\mathbb{1}$ it follows directly from the τ-KMS condition that

$$F(z - i) = \omega(\mathbb{1}\tau_{-i}(\tau_z(B))) = \omega(\tau_z(B)\mathbb{1}) = F(z) \ .$$

Hence F is periodic with period $-i$. If $\mathfrak{A}$ does not have an identity, the same conclusion is easily reached by use of an approximate identity. But the periodicity now implies that

$$|F(z)| \leq M$$

for all $z \in \mathbb{C}$. Hence F is constant by Liouville's theorem. As $\mathfrak{B}_\tau$ is dense in $\mathfrak{A}$ it follows than ω is τ-invariant.

If condition (2) of Proposition 5.3.3 is valid, a similar argument shows that ω is τ-invariant if $\beta \in \mathbb{R}\backslash\{0\}$. But then

$$\omega(A\tau_{i\beta}(B)) = \omega(\tau_{i\beta/2}(\tau_{-i\beta/2}(A)\tau_{i\beta/2}(B))) = \omega(\tau_{-i\beta/2}(A)\tau_{i\beta/2}(B)) \ .$$

If $\beta = 0$, this relation is trivially fulfilled. Hence $1 \Leftrightarrow 2$.

It should be emphasized that the value $\beta = 0$, which is excluded in Proposition 5.3.3, is exceptional. If, for example, $\mathfrak{A}$ is abelian, then all states are $(\tau, 0)$-KMS states but if τ is not trivial there are certainly states which are not τ-invariant.

One immediate corollary of τ-invariance is that each KMS state of a C^*-dynamical system extends in a canonical fashion to a KMS state of an associated W^*-system.

Corollary 5.3.4. *Let ω be a (τ, β)-KMS state of the C^*-dynamical system $(\mathfrak{A}, \tau)$ with $\beta \in \mathbb{R}\backslash\{0\}$ and let $\hat{\omega}$ be the normal extension of ω to the weak closure $\mathfrak{M}_\omega = \pi_\omega(\mathfrak{A})''$ of $\mathfrak{A}$ in the cyclic representation $(\mathfrak{H}_\omega, \pi_\omega, \Omega_\omega)$.*

It follows that there exists a unique σ-weakly-continuous group $t \mapsto \hat{\tau}_t$ of *-automorphisms of $\mathfrak{M}_\omega$ such that

$$\hat{\tau}_t(\pi_\omega(A)) = \pi_\omega(\tau_t(A))$$

for all $A \in \mathfrak{A}$ and $t \in \mathbb{R}$. Moreover, $\hat{\omega}$ is $(\hat{\tau}, \beta)$-KMS on $\mathfrak{M}_\omega$.

Proof. Proposition 5.3.3 implies that ω is τ-invariant and hence there exists a unitary representation U_ω, of $\mathbb{R}$ on $\mathfrak{H}_\omega$, such that

$$\pi_\omega(\tau_t(A)) = U_\omega(t)\pi_\omega(A)U_\omega(t)^{-1}$$

for all $A \in \mathfrak{A}$ and $t \in \mathbb{R}$ by Corollary 2.3.17. Therefore,

$$\hat{\tau}_t(B) = U_\omega(t)BU_\omega(t)^{-1}$$

exists for each $t \in \mathbb{R}$ and $B \in \mathfrak{M}_\omega$. As U_ω is defined by

$$U_\omega(t)\pi_\omega(A)\Omega_\omega = \pi_\omega(\tau_t(A))\Omega_\omega$$

and $t \mapsto \tau_t$ is strongly continuous, it follows that $t \mapsto U_\omega(t)$ is strongly continuous on $\pi_\omega(\mathfrak{A})\Omega_\omega$, and hence on $\mathfrak{H}_\omega$. Therefore, $t \mapsto \hat{\tau}_t$ is σ-weakly-continuous on $\mathfrak{M}_\omega$. But any norm-dense τ-invariant *-subalgebra of $\pi_\omega(\mathfrak{A})$ is a σ-weakly-dense $\hat{\tau}$-invariant *-subalgebra of $\mathfrak{M}_\omega$. Thus, the $\hat{\tau}$-KMS condition follows directly from the τ-KMS condition.

Although for purposes of verification it is very practical to define τ-KMS states with dense subsets of analytic elements, it is mathematically somewhat unnatural. Thus our next purpose is to extend the KMS condition to a larger more natural class of elements. For this one needs a version of the maximum modulus principle which is often referred to as the three-line theorem.

Proposition 5.3.5 (Phragmen–Lindelöf). *Let $\mathfrak{D}$ be the open strip in $\mathbb{C}$ defined by*

$$\mathfrak{D} = \{z\,;\, z \in \mathbb{C},\, a < \operatorname{Im} z < b\}$$

and $\bar{\mathfrak{D}}$ the closure of $\mathfrak{D}$. Let f be a complex function which is analytic on $\mathfrak{D}$, and bounded and continuous on $\bar{\mathfrak{D}}$.

It follows that the function

$$y \in [a, b] \mapsto g(y) = \log\left(\sup_{x \in \mathbb{R}} |f(x + iy)|\right)$$

is convex. In particular,

$$\sup_{z \in \bar{\mathfrak{D}}} |f(z)| = \max\left\{\sup_{x \in \mathbb{R}} |f(x + ia)|,\ \sup_{x \in \mathbb{R}} |f(x + ib)|\right\}.$$

It should be emphasized that this result is not a straightforward extension of the maximum modulus principle because there exist entire analytic functions

which are bounded on the boundary $\{z; \operatorname{Im} z \in \{a, b\}\}$ of the strip $\bar{\mathfrak{D}}$ but, nevertheless, are unbounded on $\bar{\mathfrak{D}}$ itself. (For a reference to the three-line theorem, see Notes and Remarks).

We also need a version of the so-called edge of the wedge theorem. This theorem was originally motivated by problems of quantum field theory and it has many important applications in this latter domain (see Notes and Remarks). The general theorem concerns functions of several complex variables, but the following proposition is only stated for one variable, and in this form it is an immediate consequence of the Schwarz reflection principle.

Proposition 5.3.6. *Let $\mathcal{O} \subseteq \mathbb{C}$ be an open connected set such that $\mathcal{V} \equiv \mathcal{O} \cap \mathbb{R} \neq \emptyset$ and define*

$$\mathfrak{D} = \{z; z = x + iy \in \mathbb{C},\ y > 0\} \cap \mathcal{O} .$$

Let F be a complex function which is holomorphic on $\mathfrak{D}$ and continuous on $\mathfrak{D} \cup \mathcal{V}$. Suppose furthermore that $F(x) = 0$ for $x \in \mathcal{V}$.

It follows that $F(z) = 0$ for all $z \in \mathfrak{D}$.

After these function theoretic preliminaries we are now ready to derive the first set of alternative characterizations of KMS states.

Proposition 5.3.7. *Let $(\mathfrak{A}, \tau)$ be a C^*-dynamical system, or a W^*-dynamical system, ω a state over $\mathfrak{A}$ which is assumed to be normal in the W^*-case, and $\beta \in \mathbb{R}$. Define*

$$\mathfrak{D}_\beta = \{z; z \in \mathbb{C},\ 0 < \operatorname{Im} z < \beta\}$$

if $\beta \geq 0$ and

$$\mathfrak{D}_\beta = \{z; z \in \mathbb{C},\ \beta < \operatorname{Im} z < 0\}$$

if $\beta \leq 0$, and let $\bar{\mathfrak{D}}_\beta$ be the closure of $\mathfrak{D}_\beta$ if $\beta \neq 0$ and $\bar{\mathfrak{D}}_\beta = \mathbb{R}$ if $\beta = 0$.

The following conditions are equivalent:

(1) *ω is a τ-KMS state at value β.*

(2) *For any pair $A, B \in \mathfrak{A}$, there exists a complex function $F_{A,B}$ which is analytic on $\mathfrak{D}_\beta$, and bounded and continuous on $\bar{\mathfrak{D}}_\beta$, such that*

$$F_{A,B}(t) = \omega(A\tau_t(B)) ,$$

$$F_{A,B}(t + i\beta) = \omega(\tau_t(B)A)$$

for all $t \in \mathbb{R}$.

(3) *For any pair $A, B \in \mathfrak{A}$, there exists a complex function $F_{A,B}$ which is analytic on $\mathfrak{D}_\beta$, and continuous on $\bar{\mathfrak{D}}_\beta$, such that*

$$F_{A,B}(t) = \omega(A\tau_t(B)) ,$$

$$F_{A,B}(t + i\beta) = \omega(\tau_t(B)A)$$

for all $t \in \mathbb{R}$.

Furthermore if these conditions are satisfied, then the function $F_{A,B}$ *in conditions* (2) *and* (3) *satisfies the bound*

$$\sup_{z \in \bar{\mathfrak{D}}_\beta} |F_{A,B}(z)| \leq \|A\| \, \|B\|$$

and for $A \in \mathfrak{A}$, $B \in \mathfrak{A}_\tau$, *the function identifies with the restriction to* $\bar{\mathfrak{D}}$ *of the entire analytic function* $z \mapsto \omega(A\tau_z(B))$.

PROOF. (1) $\Rightarrow$ (2) Let $\mathfrak{B}_\tau$ denote the *-subalgebra of $\mathfrak{A}_\tau$ occuring in Definition 5.3.1. For $A, B \in \mathfrak{B}_\tau$, define $F_{A,B}$ by

$$F_{A,B}(z) = \omega(A\tau_z(B))$$

for all $z \in \mathbb{C}$. Then $F_{A,B}$ is entire analytic,

$$F_{A,B}(t) = \omega(A\tau_t(B))$$

for $t \in \mathbb{R}$, and

$$F_{A,B}(t + i\beta) = \omega(A\tau_{i\beta}(\tau_t(B))) = \omega(\tau_t(B)A) \; .$$

As $z \mapsto \tau_z(B)$ is strongly analytic, Proposition 2.5.21, it follows that $\gamma \in [0, \beta] \mapsto \|\tau_{i\gamma}(B)\|$ is continuous, and hence bounded. Define M by

$$M = \sup\{ \|\tau_{i\gamma}(B)\|; \; \gamma \in [0, \beta]\} \; .$$

Thus

$$|F_{A,B}(t + i\gamma)| \leq \|A\| \, \|\tau_{i\gamma}(B)\| \leq M \, \|A\|$$

for $t + i\gamma \in \bar{\mathfrak{D}}$, and (2) holds for $A, B \in \mathfrak{B}_\tau$. For general $A, B \in \mathfrak{A}$ choose sequences $\{A_n\}_{n \geq 1}$, $\{B_n\}_{n \geq 1}$, in $\mathfrak{B}_\tau$ such that $\|A_n\| \leq \|A\|$, $\|B_n\| \leq \|B\|$, and $\pi_\omega(A_n)\Omega_\omega \to \pi_\omega(A)\Omega_\omega$, $\pi_\omega(A_n^*)\Omega_\omega \to \pi_\omega(A^*)\Omega_\omega$, and $\pi_\omega(B_n)\Omega_\omega \to \pi_\omega(B)\Omega_\omega$, and $\pi_\omega(B_n^*)\Omega_\omega \to \pi_\omega(B^*)\Omega_\omega$. (In the C^*-case this approximation can be made in the norm topology. If $\mathfrak{A}$ is a W^*-algebra, the approximation is possible because of Theorem 2.4.16.)

Now define F_n by

$$F_n(z) = F_{A_n, B_n}(z)$$

for $z \in \bar{\mathfrak{D}}$. The three-line theorem, Proposition 5.3.3, implies that $|F_n(z) - F_m(z)|$ assumes its maximum value on the boundary of $\bar{\mathfrak{D}}$ and for z on this boundary one has

$$\begin{aligned} |F_n(z) - F_m(z)| \leq \max\Big\{ & \sup_{t \in \mathbb{R}} |\omega(A_n\tau_t(B_n)) - \omega(A_m\tau_t(B_m))| \; , \\ & \sup_{t \in \mathbb{R}} |\omega(\tau_t(B_n)A_n) - \omega(\tau_t(B_m)A_m)| \Big\} \\ \leq \; & \|B\| \{ \|\pi_\omega(A_n^* - A_m^*)\Omega_\omega\| + \|\pi_\omega(A_n - A_m)\Omega_\omega\| \} \\ & + \|A\| \{ \|\pi_\omega(B_n^* - B_m^*)\Omega_\omega\| + \|\pi_\omega(B_n - B_m)\Omega_\omega\| \} \; . \end{aligned}$$

The last estimate is valid for the sum of the terms in the maximum and follows from τ-invariance of ω established in Proposition 5.3.3 and the Cauchy-Schwarz inequality. Hence F_n is a Cauchy sequence uniformly on $\bar{\mathfrak{D}}$. The limit function is therefore continuous and bounded on $\bar{\mathfrak{D}}$, and analytic in $\mathfrak{D}$. Also

$$F_{A,B}(t) = \lim_{n\to\infty} \omega(A_n\tau_t(B_n)) = \omega(A\tau_t(B)) ,$$
$$F_{A,B}(t+i\beta) = \lim_{n\to\infty} F_{A_n,B_n}(t+i\beta)$$
$$= \lim_{n\to\infty} \omega(\tau_t(B_n)A_n) = \omega(\tau_t(B)A) .$$

(2) $\Rightarrow$ (3): This is trivial

(3) $\Rightarrow$ (1): If $A, B \in \mathfrak{A}_\tau$, define

$$G_{A,B}(z) = \omega(A\tau_z(B))$$

for all $z \in \mathbb{C}$. Then $G_{A,B}$ is an entire analytic function and

$$G_{A,B}(t) = F_{A,B}(t)$$

for $t \in \mathbb{R}$. It follows from the edge of the wedge theorem, Proposition 5.3.6, that $G_{A,B}(z) = F_{A,B}(z)$ for all $z \in \bar{\mathfrak{D}}$, i.e.,

$$F_{A,B}(z) = \omega(A\tau_z(B))$$

for all $z \in \bar{\mathfrak{D}}$. But then, by condition (3)

$$\omega(A\tau_{i\beta}(B)) = F_{A,B}(i\beta) = \omega(BA)$$

for all $A, B \in \mathfrak{A}_\tau$, i.e., ω is (τ, β)-KMS.

The last statement of the proposition was established during the proof of (1) $\Rightarrow$ (2) and (3) $\Rightarrow$ (1).

The same line of reasoning allows the explicit extension of a (τ, β)-KMS state ω over a C^*-dynamical system to a $(\hat{\tau}, \beta)$-KMS state over the associated von Neumann algebra $\mathfrak{M}_\omega = \pi_\omega(\mathfrak{A})''$ as described in Corollary 5.3.4. We next prove that the KMS condition implies that Ω_ω is separating for $\mathfrak{M}_\omega$, but for later purposes we isolate the following lemma.

Lemma 5.3.8. *Let $\mathfrak{M}$ be a C^*-algebra on a Hilbert space $\mathfrak{H}$, Ω a cyclic unit vector, and ω the corresponding state. If $\omega(A^*A) = 0$ implies that $\omega(AA^*) = 0$ for all $A \in \mathfrak{A}$, then it follows that Ω is separating for $\mathfrak{M}$.*

Proof. Assume that $A\Omega = 0$. Then $BA\Omega = 0$ for all $B \in \mathfrak{M}$, and hence by hypothesis $A^*B^*\Omega = (BA)^*\Omega = 0$. As Ω is cyclic it follows that $A^* = 0$ and hence $A = 0$.

Corollary 5.3.9. *Let $(\mathfrak{A}, \tau)$ be a C^*-dynamical system, ω a τ-KMS state on $\mathfrak{A}$ at value $\beta \in \mathbb{R}$, and $(\mathfrak{H}_\omega, \pi_\omega, \Omega_\omega)$ the corresponding cyclic representation. It follows that Ω_ω is separating for $\pi_\omega(\mathfrak{A})''$.*

Proof. If $\beta \neq 0$, it follows by Corollary 5.3.4 that the state $\hat{\omega}$ on $\mathfrak{M}_\omega = \pi_\omega(\mathfrak{A})''$ defined by

$$\hat{\omega}(A) = (\Omega_\omega, A\Omega_\omega)$$

satisfies the $(\hat{\tau}, \beta)$-KMS condition for a group $t \mapsto \hat{\tau}_t$ of *-automorphisms of $\mathfrak{M}_\omega$. Let $A \in \mathfrak{M}_\omega$ be an element such that $\hat{\omega}(A^*A) = 0$, i.e., such that $A\Omega_\omega = 0$. Let $F_{A^*,A}(z)$ be the function corresponding to A^*, A, as in Proposition 5.3.7. Then

$$F_{A^*,A}(t) = \hat{\omega}(A^*\tau_t(A)) = (A\Omega_\omega, U_\omega(t)A\Omega_\omega) = 0$$

for $t \in \mathbb{R}$. It follows from the edge of the wedge theorem, Proposition 5.3.6, that $F_{A^*,A}(z) = 0$ for all z with Im z between 0 and β. But then

$$\hat{\omega}(AA^*) = F_{A^*,A}(i\beta) = 0 .$$

Hence Ω_ω is separating for $\mathfrak{M}_\omega$ by Lemma 5.3.8.

If $\beta = 0$, then $\hat{\omega}$ is a trace-state on $\pi_\omega(\mathfrak{A})''$ and Lemma 5.3.8 is again applicable.

The separating property of Ω_ω for $\pi_\omega(\mathfrak{A})''$ provides the principal link between the modular theory of Tomita-Takesaki and the theory of KMS states.

Assume that ω is a τ-KMS state over a von Neumann algebra $\mathfrak{M}$ for some σ-weakly-continuous group τ of *-automorphisms. Thus by Corollary 5.3.9, ω is faithful on $\pi_\omega(\mathfrak{M})$. But the kernel of π_ω is a σ-weakly-closed two-sided ideal $\mathfrak{I} \subseteq \mathfrak{M}$ and by Proposition 2.4.22 there exists a projection $E \in \mathfrak{M} \cap \mathfrak{M}'$ such that $\mathfrak{I} = \mathfrak{M}(\mathbb{1} - E)$. It follows that $\omega(\mathbb{1} - E) = 0$, and ω is faithful on $\mathfrak{M}E$ because π_ω restricts to an isomorphism between $\mathfrak{M}E$ and $\pi_\omega(\mathfrak{M})$, and

$$\omega(AE) = \omega(A) = (\Omega_\omega, \pi_\omega(A)\Omega_\omega) .$$

The remarkable consequence of the Tomita–Takesaki modular theory is that this condition is also sufficient for ω to be a τ-KMS state for some group τ. This unexpected result follows basically from the identity of the modular condition, described after Definition 2.5.15, and the KMS condition expressed for the modular group.

Theorem 5.3.10 (Takesaki). *Let $\mathfrak{M}$ be a von Neumann algebra, and ω a normal state on $\mathfrak{M}$.*

The following conditions are equivalent:

(1) *ω is faithful as a state on $\pi_\omega(\mathfrak{M})$, i.e., there exists a projection $E \in \mathfrak{M} \cap \mathfrak{M}'$ such that $\omega(\mathbb{1} - E) = 0$ and $\omega|_{\mathfrak{M}E}$ is faithful.*

(2) *There exists a σ-weakly-continuous one-parameter group τ of *-automorphisms of $\mathfrak{M}$ such that ω is a τ-KMS state.*

Furthermore, if these conditions are fulfilled, the automorphism group τ leaves E fixed,

$$\tau_t(E) = E$$

for all $t \in \mathbb{R}$, and the restriction of τ to $\mathfrak{M}E$ is uniquely determined by ω. This restriction is the modular automorphism group of $\mathfrak{M}E$ associated with ω .

Proof. We have already remarked before the theorem that (2) $\Rightarrow$ (1) is a consequence of Corollary 5.3.9. As the definition of τ on $\mathfrak{M}(\mathbb{1} - E)$ has no influence on the KMS property, we may assume that $E = \mathbb{1}$, i.e., we may assume that ω is faithful on $\mathfrak{M}$, when proving (1) $\Rightarrow$ (2). Thus passing to the cyclic representation associated with ω, we may assume that ω is given by a separating and cyclic vector. Let Δ be the modular operator associated with the pair $(\mathfrak{M}, \Omega)$, Definition 2.5.10, and let $\sigma_t(A) = \Delta^{it} A \Delta^{-it}$ be the corresponding modular automorphism group, Definition 2.5.15. Then, for $A, B \in \mathfrak{M}_\tau$,

$$\begin{aligned}\omega(AB) &= (A^*\Omega, B\Omega)\\ &= (\Delta^{1/2}B^*\Omega,\ \Delta^{1/2}A\Omega)\\ &= (\Omega,\ B\Delta A\Delta^{-1}\Omega) = \omega(B\sigma_{-i}(A))\ .\end{aligned}$$

Hence ω is a τ-KMS state in the sense of Definition 5.3.1.

This ends the proof of (1) $\Rightarrow$ (2), and the property $\tau_t(E) = E$ is a consequence of the fact that ω is τ-invariant, i.e., τ lifts to the representation π_ω as described in Corollary 5.3.4. To show uniqueness of the restriction of τ to $\mathfrak{M}E$, we may again assume that ω is faithful and given by a separating and cyclic vector Ω. If $U(t) = e^{itH}$ is the unitary group on $\mathfrak{H}$ corresponding to τ, and $A, B \in \mathfrak{M}_\tau$, we have

$$\omega(AB) = \omega(\tau_i(B)A)$$

and hence

$$\begin{aligned}(\Delta^{1/2}B^*\Omega,\ \Delta^{1/2}A\Omega) &= (\Omega,\ AB\Omega)\\ &= (\Omega,\ Be^HA\Omega) = (B^*\Omega,\ e^HA\Omega)\ .\end{aligned}$$

As $\mathfrak{M}_\tau$ is strong*-dense in $\mathfrak{M}$, it follows that $\mathfrak{M}_\tau\Omega$ is a core for $\Delta^{1/2}$, and the above relation implies that $\Delta^{1/2}A\Omega \in D(\Delta^{1/2*}) = D(\Delta^{1/2})$ and

$$\Delta A\Omega = e^HA\Omega$$

for all $A \in \mathfrak{M}_\tau$. Now let $\mathfrak{M}_0$ be the *-subalgebra of $\mathfrak{M}_\tau$ consisting of elements with compact spectrum relative to τ. Then $\mathfrak{M}_0$ is dense in $\mathfrak{M}$ by Lemma 3.2.39 and since $\tau_{-i}(\mathfrak{M}_0) = \mathfrak{M}_0$ it follows that $e^H\mathfrak{M}_0\Omega \subseteq \mathfrak{M}_0\Omega$. But as any element in $\mathfrak{M}_0\Omega$ is contained in a spectral projection of H corresponding to a compact spectral interval, it follows that $\mathfrak{M}_0\Omega$ consists of entire analytic elements for e^H. Hence $\mathfrak{M}_0\Omega$ is a core for e^H, by application of Corollary 3.1.20 with $S = e^H$. Thus Δ is an extension of e^H. As Δ and e^H are selfadjoint it follows that $\Delta = e^H$, and hence τ is the modular automorphism group.

Combining 5.3.3, 5.3.9, and 5.3.10 one sees that a given state ω on a C^*-algebra $\mathfrak{A}$ is a KMS state for a one-parameter group τ of *-automorphisms of $\pi_\omega(\mathfrak{A})''$ if, and only if, the normal extension $\hat{\omega}$ of ω to $\pi_\omega(\mathfrak{A})''$ is faithful, and in this case the group τ is unique. The converse problem of constructing KMS states when τ is given is much more complicated and only has a positive solution for special classes of $\mathfrak{A}$ and τ. We will partially analyze this problem at the end of this subsection and in the following one.

The principal aim in the rest of this subsection is the derivation of alternative formulations and characterizations of the KMS condition. The analysis is essentially identical for C^*- or W^*-systems, and, for simplicity, we present all results in the C^*-case and omit the analogous W^*-statements. The first reformulation expresses the analytic properties in a way which is often useful for applications to the thermodynamic limit. For this we need some properties of analytic functions.

Recall that if $\mathscr{D} = \mathscr{D}(\mathbb{R})$ denotes the set of infinitely differentiable functions with compact support and if $\hat{f} \in \mathscr{D}$ the inverse Fourier transform

$$f(z) = (2\pi)^{-1/2} \int_{-\infty}^{\infty} dp\ e^{ipz} \hat{f}(p)$$

is an entire analytic function. Moreover, in restriction to $\mathbb{R}$ one has $f \in \mathscr{S} = \mathscr{S}(\mathbb{R})$, i.e., f is infinitely often differentiable, and $x \in \mathbb{R} \mapsto x^n\, d^m f(x)/d^m x$ is uniformly bounded for all $n, m \in \mathbb{N}$. More precisely one has the following:

Proposition 5.3.11 (Paley-Wiener). *A function f is the inverse Fourier transform of a function $\hat{f} \in \mathscr{D}$ with support in $[-R, R]$ if, and only if, f is entire analytic and for each integer n there exists a constant C_n such that*

$$|f(z)| \leq C_n(1 + |z|)^{-n} \exp(R|\mathrm{Im}\ z|)\ .$$

We only need the "only if" statement of this proposition. This is easily established (see Notes and Remarks).

Now we are prepared for the first reformulation of the KMS condition.

Proposition 5.3.12. *Let $(\mathfrak{A}, \tau)$ be a C^*-dynamical system, and ω a state over $\mathfrak{A}$. The following conditions are equivalent:*

(1) *ω satisfies the (τ, β)-KMS condition.*

(2) *The relation*

$$\int_{-\infty}^{\infty} dt\, f(t)\omega(A\tau_t(B)) = \int_{-\infty}^{\infty} dt\, f(t + i\beta)\omega(\tau_t(B)A)$$

is valid for all $A, B \in \mathfrak{A}$ and all f with $\hat{f} \in \mathscr{D}$.

Proof. (1) $\Rightarrow$ (2): If $B \in \mathfrak{A}_\tau$, then $z \mapsto \omega(A\tau_z(B))$ is entire analytic and

$$\omega(A\tau_t(B)) = \omega(\tau_{t-i\beta}(B)A)$$

for all $t \in \mathbb{R}$. The function

$$z \mapsto f(z)\omega(\tau_z(B)A)$$

is entire analytic and decreases faster than $|\mathrm{Re}\ z|^{-2}$ as $\mathrm{Re}\ z \to \infty$, provided $|\mathrm{Im}\ z| \leq \beta$, by Proposition 5.3.11. Hence, by Cauchy's theorem

$$\begin{aligned}\int_{-\infty}^{\infty} dt\, f(t)\omega(A\tau_t(B)) &= \int_{-\infty}^{\infty} dt\, f(t)\omega(\tau_{t-i\beta}(B)A) \\ &= \int_{-\infty}^{\infty} dt\, f(t + i\beta)\omega(\tau_t(B)A)\ .\end{aligned}$$

The condition for general $B \in \mathfrak{A}$ follows by continuity and the decay properties of f.

(2) $\Rightarrow$ (1): If (2) holds and $B \in \mathfrak{A}_\tau$ then inversion of the foregoing argument establishes that

$$\int_{-\infty}^{\infty} dt\, f(t)\omega(A\tau_t(B)) = \int_{-\infty}^{\infty} dt\, f(t)\omega(\tau_{t-i\beta}(B)A)\ .$$

Choose $\hat{f}_n \in \mathfrak{D}$ such that $0 \leq \hat{f}_n \leq 1, \hat{f}_n(x) = 1$ if $|x| \leq n$ and $\hat{f}_n(x) = 0$ if $|x| \geq n + 1$. Thus, for any bounded, continuous function g,

$$\lim_{n\to\infty}\int_{-\infty}^{\infty} dx\, f_n(x)g(x) = g(0)$$

and hence

$$\omega(AB) = \omega(\tau_{-i\beta}(B)A)\ .$$

Replacement of B by $\tau_{i\beta}(B)$ then gives the τ-KMS condition.

The utility of Proposition 5.3.12 can be illustrated by consideration of a sequence τ^n of strongly continuous one-parameter groups of *-automorphisms of $\mathfrak{A}$ converging strongly to a group τ, i.e., $\|\tau_t^n(A) - \tau_t(A)\| \to 0$ as $n \to \infty$ for all $A \in \mathfrak{A}$ and $t \in \mathbb{R}$. Assume that ω_n is a sequence of (τ^n, β)-KMS states which converges in the weak*-topology to a state ω. It then follows that $\omega_n(A\tau_t^n(B)) \to \omega(A\tau_t(B))$ and hence if $\hat{f} \in \mathscr{D}$ the Lebesgue-dominated convergence theorem and Proposition 5.3.12 imply that

$$\begin{aligned}\int_{-\infty}^{\infty} dt\, f(t)\omega(A\tau_t(B)) &= \lim_{n\to\infty}\int_{-\infty}^{\infty} dt\, f(t)\omega_n(A\tau_t^n(B))\\ &= \lim_{n\to\infty}\int_{-\infty}^{\infty} dt\, f(t+i\beta)\omega_n(\tau_t^n(B)A)\\ &= \int_{-\infty}^{\infty} dt\, f(t+i\beta)\omega(\tau_t(B)A)\ ,\end{aligned}$$

i.e., ω is a (τ, β)-KMS state. This same type of reasoning can be applied under weaker assumptions to the convergence of Green functions.

EXAMPLE 5.3.13. Let τ^n be a sequence of strongly continuous one-parameter groups of *-automorphisms of a C^*-algebra $\mathfrak{A}$ and ω_n a sequence of τ^n-invariant states. Assume that the limits

$$G(A, B; t) = \lim_{n\to\infty} \omega_n(A\tau_t^n(B))$$

exist, for all $A, B \in \mathfrak{A}$ and $t \in \mathbb{R}$, and in particular the weak*-limit ω of ω_n exists. It follows automatically that the functions $G; t \mapsto G(A, B; t)$ are measurable but they are not necessarily continuous. If one assumes, however, that the G are continuous and the ω_n are (τ^n, β)-KMS states for some $\beta \in \mathbb{R}$, then Proposition 5.3.12 implies that Ω_ω is separating for $\pi_\omega(\mathfrak{A})''$. For this one first applies the Lebesgue-dominated convergence theorem to conclude that

$$\int_{-\infty}^{\infty} dt\, f(t)G(A, B; t) = \int_{-\infty}^{\infty} dt\, f(t+i\beta)G(B, A; -t)$$

for all f with $\hat{f} \in \mathscr{D}$. Second, one estimates that

$$|G(A, B; t)|^2 \le \lim_{n\to\infty} \omega_n(AA^*)\omega_n(B^*B) = \|\pi_\omega(A^*)\Omega_\omega\|^2\|\pi_\omega(B)\Omega_\omega\|^2$$

and hence

$$G(A, B; t) = (\pi_\omega(A^*)\Omega_\omega, X_t\pi_\omega(B)\Omega_\omega)\ ,$$

where $t \mapsto X_t$ is a weakly continuous one-parameter family of bounded operators with $\|X_t\| \le 1$. Next, for $A \in \pi_\omega(\mathfrak{A})''$ one chooses $A_n \in \mathfrak{A}$ such that $\pi_\omega(A_n)\Omega_\omega \to A\mathfrak{A}_\omega$ and $\pi_\omega(A_n^*)\Omega_\omega \to A^*\Omega_\omega$. Finally one has

$$\begin{aligned}\int_{-\infty}^{\infty} dt\, f(t)(A^*\Omega_\omega, X_t A^*\Omega_\omega) &= \lim_{n\to\infty} \int_{-\infty}^{\infty} dt\, f(t) G(A_n, A_n^*; t) \\ &= \lim_{n\to\infty} \int_{-\infty}^{\infty} dt\, f(t+i\beta) G(A_n^*, A_n; -t) \\ &= \int_{-\infty}^{\infty} dt\, f(t+i\beta)(A\Omega_\omega, X_{-t} A\Omega_\omega) \ .\end{aligned}$$

Thus if $A\Omega_\omega = 0$, then

$$\int_{-\infty}^{\infty} dt\, f(t)(A^*\Omega_\omega, X_t A^*\Omega_\omega) = 0$$

and as $t \mapsto X_t$ is continuous one must have $A^*\Omega_\omega = 0$. But then Ω_ω is separating for $\pi_\omega(\mathfrak{A})''$ by Lemma 5.3.8.

The next reformulation of the KMS condition emphasizes the measure-theoretic structure which is an inherent consequence of the τ-invariance of KMS states.

If $(\mathfrak{A}, \tau)$ is a C^*-dynamical system, and ω is a τ-invariant state on $\mathfrak{A}$, consider the functionals μ_A and ν_A defined on $\mathscr{D}$ by

$$\mu_A(\hat{f}) = \int_{-\infty}^{\infty} dt\, f(t)\omega(A^*\tau_t(A)) \ ,$$

$$\nu_A(\hat{f}) = \int_{-\infty}^{\infty} dt\, f(t)\omega(\tau_t(A)A^*) \ .$$

If

$$U_\omega(t) = \int_{-\infty}^{\infty} e^{-ipt}\, dE(p)$$

is the spectral decomposition of the canonical unitary group implementing τ in the representation $(\mathfrak{H}_\omega, \pi_\omega, \Omega_\omega)$, one has

$$\begin{aligned}\mu_A(\hat{f}) &= \int_{-\infty}^{\infty} dt \int_{-\infty}^{\infty} dp \int_{-\infty}^{\infty} (\pi_\omega(A)\Omega_\omega, dE(q)\pi_\omega(A)\Omega_\omega) \frac{1}{2\pi} e^{ipt} \hat{f}(p) e^{-iqt} \\ &= \int_{-\infty}^{\infty} (\pi_\omega(A)\Omega_\omega, dE(q)\pi_\omega(A)\Omega_\omega) \hat{f}(q) \ .\end{aligned}$$

Hence μ_A is actually a positive Radon measure on $\mathbb{R}$, i.e., μ_A extends by continuity to a positive functional on $C_0(\mathbb{R})$, which is given by

$$d\mu_A(p) = (\pi_\omega(A)\Omega_\omega, dE(p)\pi_\omega(A)\Omega_\omega) \ .$$

Analogously, ν_A is the measure given by

$$d\nu_A(p) = (\pi_\omega(A^*)\Omega_\omega, dE(-p)\pi_\omega(A^*)\Omega_\omega) \ .$$

We now characterize the KMS condition by means of these measures.

Proposition 5.3.14. *Let $(\mathfrak{A}, \tau)$ be a C^*-dynamical system, ω a τ-invariant state over $\mathfrak{A}$, and μ_A and ν_A the positive Baire measures on $\mathbb{R}$ associated with ω.*

The following conditions are equivalent:

(1) *ω is a τ-KMS state at value β.*

(2) *The measures μ_A and ν_A are equivalent, with Radon-Nikodym derivative*

$$\frac{d\mu_A}{d\nu_A}(p) = e^{-\beta p}$$

for all $A \in \mathfrak{A}$.

PROOF. (1) $\Rightarrow$ (2): Using Proposition 5.3.12 (2) we deduce that

$$\begin{aligned}\mu_A(\hat{f}) &= \int_{-\infty}^{\infty} dt\, f(t)\omega(A^*\tau_t(A)) \\ &= \int_{-\infty}^{\infty} dt\, f(t+i\beta)\omega(\tau_t(A)A^*) = \nu_A(k\hat{f}) \ ;\end{aligned}$$

where $k(p) = e^{-\beta p}$. The proof of (2) $\Rightarrow$ (1) follows by inversion of the argument.

Note that condition (2) of the last proposition can be stated as a set of inequalities

$$d\mu_A(p) \geq e^{-\beta p}\, d\mu_{A^*}(-p) \tag{2'}$$

because iteration of this latter condition gives

$$d\mu_A(p) \geq e^{-\beta p}\, d\mu_{A^*}(-p) \geq d\mu_A(p)$$

and then the identity $d\nu_A(p) = d\mu_{A^*}(-p)$ implies that (2) and (2′) are equivalent. The following characterizations of the KMS condition are all expressed in terms of inequalities which stem from a stability property of the KMS states. It is remarkable that these inequalities can be expressed in terms of the infinitesimal generator δ of the group τ and do not directly involve the global behavior of the group.

The stability properties which are inherent in the following characterizations of the KMS condition can be partially explained through the principle of maximum entropy for the Gibbs equilibrium states. For simplicity let $\mathfrak{A} = M_n$, the C^*-algebra of all $n \times n$-matrices, acting on the n-dimensional Hilbert space $\mathfrak{H}_n$ and hence each state over $\mathfrak{A}$ is of the form ω_ρ where

$$\omega_\rho(A) = \mathrm{Tr}_{\mathfrak{H}_n}(\rho A)$$

and ρ is a density matrix. In particular, if $H = H^* \in \mathfrak{A}$ and $\beta \in \mathbb{R}$, the Gibbs state $\omega_{\rho\beta H}$ is defined by setting

$$\rho_{\beta H} = \frac{e^{-\beta H}}{\mathrm{Tr}_{\mathfrak{H}_n}(e^{-\beta H})} \ .$$

Now one can define an entropy function $S; \omega \in E_{\mathfrak{A}} \mapsto S(\omega) \in [0, \log n]$ by

$$S(\omega_\rho) = -\mathrm{Tr}_{\mathfrak{H}_n}(\rho \log \rho) \ .$$

(The function $-x \log x$ is defined by continuity to be zero at $x = 0$). It then follows that the Gibbs state is the unique state which maximizes the function

$$F(\omega_\rho) = \beta^{-1} S(\omega_\rho) - \omega_\rho(H) \ .$$

This follows basically from the convexity inequality

$$-\mathrm{Tr}(A \log A - A \log B) \ \leq \ \mathrm{Tr}(A - B)$$

for Hermitian matrices A and B and the identification

$$F(\omega_\rho) = -\beta^{-1} \mathrm{Tr}_{\mathfrak{H}_n}(\rho \log \rho - \rho \log \rho_{\beta H}) + \beta^{-1} \log \mathrm{Tr}_{\mathfrak{H}_n}(e^{-\beta H})$$

(see Chapter 6, Section 2.3). Thus the Gibbs state is characterized by the principle of maximum entropy at fixed energy.

The maximum entropy principle leads to various stability criteria. For example, if φ is any map from $E_{\mathfrak{A}}$ to $E_{\mathfrak{A}}$, then

$$F(\omega_{\rho_{\beta H}}) \ \geq \ F(\varphi(\omega_{\rho_{\beta H}})) \ .$$

The simplest illustration of this rule occurs if $(\varphi(\omega))(A) = \omega(U^* A U)$ for some unitary $U \in \mathfrak{A}$. For this transformation one has $S(\varphi(\omega)) = S(\omega)$, and hence the inequality for F gives

$$-\mathrm{Tr}_{\mathfrak{H}_n}(\rho_{\beta H} H) \ \geq \ -\mathrm{Tr}_{\mathfrak{H}_n}(\rho_{\beta H} U^* H U)$$

which can be rephrased as

$$\omega_{\rho_{\beta H}}(U^*[H, U]) \ \geq \ 0 \ .$$

But the dynamical group τ corresponding to H is given by

$$\tau_t(A) = e^{itH} A e^{-itH}$$

and the infinitesimal generator δ of τ by

$$\delta(A) = [iH, A] \ .$$

Thus one concludes that the Gibbs state satisfies the stability requirements

$$i^{-1} \omega(U^* \delta(U)) \ \geq \ 0$$

for each unitary $U \in \mathfrak{A}$. In Section 5.4.4 we will demonstrate that this criterion expresses the fact that systems in equilibrium are unable to perform mechanical work in cyclic processes. For this last reason states which satisfy the criterion are said to be passive. In Theorem 5.3.22 we also demonstrate that passivity of a state is to a large extent equivalent to the KMS condition. The two conditions cannot be completely equivalent because the passivity criterion carries no reference to the temperature, i.e., the value of β^{-1}, and convex combinations of passive states are passive.

A second type of stability criterion follows from consideration of continuous semigroups $t \geq 0 \mapsto T_t$ such that $T_t E_{\mathfrak{A}} \subseteq E_{\mathfrak{A}}$. If γ denotes the infinitesimal generator of T, then the maximum entropy principle gives

$$t^{-1}(F(\omega_{\rho_{\beta H}}) - F(T_t\,\omega_{\rho_{\beta H}})) \geq 0$$

and hence

$$-F(\gamma\omega_{\rho_{\beta H}}) \geq 0\,.$$

For an example of this latter principle consider the operator $\gamma_B; \mathfrak{A} \mapsto \mathfrak{A}$ defined by

$$\gamma_B(A) = B^*AB - \{B^*B,\, A\}/2$$

for some fixed $B \in \mathfrak{A}$. Clearly, γ_B is bounded and $\gamma_B(\mathbb{1}) = 0$. But one readily calculates that

$$\gamma_B(A^*A) - \gamma_B(A^*)A - A^*\gamma_B(A) = [A,\, B]^*[A,\, B] \geq 0$$

and hence γ_B is dissipative, by Proposition 3.2.22, and

$$\|A - \alpha\gamma_B(A)\| \geq \|A\|, \quad \alpha \geq 0,\, A \in \mathfrak{A}\,,$$

by Lemma 3.1.15. Therefore,

$$t \geq 0 \mapsto T_t = \exp\{t\gamma_B\} = \lim_{n\to\infty}\left(\imath - \frac{t}{n}\gamma_B\right)^{-n}$$

is a uniformly continuous semigroup of contractions. Moreover, $T_t\mathbb{1} = \mathbb{1}$. It then follows from Corollary 3.2.6 that the T_t are positive, i.e., $T_t\mathfrak{A}_+ \subseteq \mathfrak{A}_+$ and $T_t^*E_{\mathfrak{A}} \subseteq E_{\mathfrak{A}}$ for all $t \geq 0$. Application of this type of semigroup and convexity arguments leads to a set of inequalities for the Gibbs states which are sometimes referred to as *auto-correlation lower bounds*. These inequalities have been proved to be equivalent to the KMS condition.

Theorem 5.3.15 (Roepstorff-Araki-Sewell). *Let $(\mathfrak{A}, \tau)$ be a C^*-dynamical system, δ the infinitesimal generator of τ, and ω a state over $\mathfrak{A}$.*

The following conditions are equivalent:

(1) *ω is a (τ, β)-KMS state*

(2) $-i\beta\omega(A^*\delta(A)) \geq \omega(A^*A)\log(\omega(A^*A)/\omega(AA^*))$

for all $A \in D(\delta)$, where

$$u\log(u/v) = \begin{cases} u\log(u/v), & u > 0, v > 0\,, \\ 0, & u = 0, v \geq 0\,, \\ +\infty, & u > 0, v = 0\,. \end{cases}$$

Proof. (1) $\Rightarrow$ (2): A routine calculation shows that the function

$$u, v \in \mathbb{R}_+ \times \mathbb{R}_+ \mapsto S(u, v) = u\log(u/v)$$

is lower semicontinuous, jointly convex in (u, v) and homogeneous of degree 1 in (u, v), i.e.,

$$S(\lambda u,\, \lambda v) = \lambda S(u, v)$$

for $u, v, \lambda \in \mathbb{R}_+$. Hence it follows that

$$S\left(\sum_i \lambda_i u_i, \sum_i \lambda_i v_i\right) \leq \sum_i \lambda_i S(u_i, v_i)$$

for all finite sequences $\{\lambda_i\}$, $\{u_i\}$, and $\{v_i\}$ in $\mathbb{R}_+$. If f_1 and f_2 are continuous bounded non-negative functions on $\mathbb{R}$, and μ is a positive finite Baire measure on $\mathbb{R}$, it follows from Proposition 4.1.1 that μ can be approximated by measures of finite support, and the lower semicontinuity of S implies.

$$S(\mu(f_1), \mu(f_2)) \leq \mu(S(f_1, f_2)) .$$

If ω is a (τ, β)-KMS state, we may form the measures

$$\begin{aligned} d\mu_A(p) &= (\pi_\omega(A)\Omega_\omega, dE(p)\pi_\omega(A)\Omega_\omega) \ , \\ d\nu_A(p) &= (\pi_\omega(A^*)\Omega_\omega, dE(-p)\pi_\omega(A^*)\Omega_\omega) \end{aligned}$$

as in the introduction to Proposition 5.3.14, unless $\beta = 0$, in which case ω is a trace-state, and both sides of the inequality in (2) are zero. Define $k(p) = e^{-\beta p}$. Proposition 5.3.14 and the above inequality then imply

$$\begin{aligned} S(\omega(A^*A), \omega(AA^*)) &= S(\mu_A(1), \nu_A(1)) \\ &= S(\mu_A(1), \mu_A(k^{-1})) \\ &\leq \mu_A(S(1, k^{-1})) \\ &= \mu_A(\log k) \\ &= -i\beta(\pi_\omega(A)\Omega_\omega, iH_\omega\pi_\omega(A)\Omega_\omega) = -i\beta\omega(A^*\delta(A)) \ , \end{aligned}$$

where we have used the notation $U_\omega(t) = e^{itH_\omega}$.

To prove (2) $\Rightarrow$ (1) we need the following lemma.

Lemma 5.3.16. *Let $(\mathfrak{A}, \tau)$ be a C^*-dynamical system, let δ be the infinitesimal generator of τ, and assume that $\omega(A\delta(A)) \in i\mathbb{R}$ for all $A = A^* \in D(\delta)$.*

It follows that ω is τ-invariant, i.e.,

$$\omega(\tau_t(A)) = \omega(A)$$

for all $A \in \mathfrak{A}$ and $t \in \mathbb{R}$.

Proof. As $\delta(A)^* = \delta(A)$ for $A = A^* \in D(\delta)$ it follows that

$$\omega(\delta(A)A) = \overline{\omega(A\delta(A))} = -\omega(A\delta(A)) \ ,$$

where the last equality is a consequence of the hypothesis of the lemma. Hence

$$\omega(\delta(A^2)) = \omega(\delta(A)A) + \omega(A\delta(A)) = 0 \ ,$$

and it follows that

$$\omega(\tau_t(A^2)) - \omega(A^2) = \int_0^t ds\, \omega(\delta(\tau_s(A)^2)) = 0 \ .$$

The τ-invariance then follows by continuity from Proposition 2.2.10 and Theorem 2.2.11, i.e., each element of $\mathfrak{A}$ is a linear combination of four positive elements.

End of proof of Theorem 5.3.15. (2) $\Rightarrow$ (1). If $\beta \neq 0$ the auto-correlation lower bounds and Lemma 5.3.16 imply that ω is τ-invariant and we may form the measures

μ_A and ν_A for all $A \in \mathfrak{A}$. If $\hat{f} \in \mathscr{D}$ it follows essentially from Propositions 5.3.11 and 2.5.22 that

$$\tau_f(A) = \int dt\, f(t)\tau_t(A)$$

is entire analytic for δ and, in particular, $\tau_f(A) \in D(\delta)$. Now we compute

$$\begin{aligned} U_\omega(f) &= \int dt\, f(t) U_\omega(t) \\ &= \int dt\, f(t) \int dE(p) e^{-ipt} \\ &= \int \hat{f}(p) dE(p) = \hat{f}(-H_\omega)\,. \end{aligned}$$

Defining $h(p) = |\hat{f}(p)|^2$ and $k(p) = e^{-\beta p}$ we deduce further that

$$\begin{aligned} &-i\beta\omega(\tau_f(A)^*\delta(\tau_f(A))) \\ &\quad = -i\beta(U_\omega(f)\pi_\omega(A)\Omega_\omega,\, iH_\omega\, U_\omega(f)\pi_\omega(A)\Omega_\omega) \\ &\quad = (\pi_\omega(A)\Omega_\omega, \hat{f}(-H_\omega)\beta H_\omega \hat{f}(-H_\omega)\pi_\omega(A)\Omega_\omega) = \mu_A(\log(k)h)\,. \end{aligned}$$

By similar computations, one finds

$$\begin{aligned} \omega(\tau_f(A)^*\tau_f(A)) &= \mu_A(h)\,, \\ \omega(\tau_f(A)\tau_f(A)^*) &= \nu_A(h)\,, \\ -i\beta\omega(\tau_f(A)\delta(\tau_f(A)^*)) &= -\nu_A(\log(k)h)\,. \end{aligned}$$

Thus the auto-correlation lower bounds, applied to $\tau_f(A)$ and $\tau_f(A)^*$, respectively, give

$$\begin{aligned} \mu_A(\log(k)h) &\geq S(\mu_A(h),\, \nu_A(h))\,, \\ -\nu_A(\log(k)h) &\geq S(\nu_A(h),\, \mu_A(h))\,. \end{aligned}$$

Now, define $\bar{p}(h) = \sup(\operatorname{supp} h)$ and $\underline{p}(h) = \inf(\operatorname{supp} h)$. Assuming for the moment that $\beta > 0$, we deduce from $\log k(p) = -\beta p$ that

$$-\beta\bar{p}(h)h \leq h \log k \leq -\beta\underline{p}(h)h\,.$$

The auto-correlation lower bound then implies that

$$\begin{aligned} -\beta\underline{p}(h)\mu_A(h) &\geq \mu_A(h)\log(\mu_A(h)/\nu_A(h))\,, \\ \beta\bar{p}(h)\nu_A(h) &\geq \nu_A(h)\log(\nu_A(h)/\mu_A(h))\,, \end{aligned}$$

or, equivalently

$$e^{-\beta\underline{p}(h)}\nu_A(h) \geq \mu_A(h) \geq e^{-\beta\bar{p}(h)}\nu_A(h)\,.$$

Also, since

$$e^{-\beta\underline{p}(h)}h \geq hk \geq e^{-\beta\bar{p}(h)}h\,,$$

we have

$$e^{-\beta\underline{p}(h)}\nu_A(h) \geq \nu_A(hk) \geq e^{-\beta\bar{p}(h)}\nu_A(h)\,.$$

Let $\varepsilon > 0$ and let $\{h_n\}_{n\geq 1}$ be a sequence of positive elements in $\mathscr{D}$ such that $\sum_n h_n = 1$ pointwise, and

$$|e^{-\beta\underline{p}(h_n)} - e^{-\beta\bar{p}(h_n)}| < \varepsilon\,.$$

Then the above inequalities imply that

$$|\mu_A(hh_n) - \nu_A(hh_nk)| \leq \varepsilon\nu_A(hh_n)$$

and so, by Lebesgue's theorem,

$$|\mu_A(h) - \nu_A(hk)| \leq \varepsilon\nu_A(h) .$$

Hence

$$\mu_A(h) = \nu_A(hk)$$

for all $h \in \mathscr{D}$. But this is just the measure-theoretic form of the KMS condition, Theorem 5.3.14. When $\beta < 0$ the reasoning is the same.

Finally if $\beta = 0$ the auto-correlation lower bound implies that $\omega(A^*A) \leq \omega(AA^*)$ for all $A \in \mathfrak{A}$; thus by interchanging A and A^*, $\omega(A^*A) = \omega(AA^*)$, and ω is a trace-state.

We next derive a characterization of the KMS condition by "auto-correlation upper bounds." This is formulated in terms of a quantity which occurs in a perturbation expansion of the free energy, and is known alternatively as the Duhamel two-point function, Bogoliubov scalar product, Kubo-Mari scalar product, or the canonical correlation. If $(\mathfrak{A}, \tau)$ is a C^*-dynamical system and ω a τ-invariant state on $\mathfrak{A}$, this quantity is *a priori* defined as a sesquilinear form on the entire analytic elements $\mathfrak{A}_\tau$ by

$$(A, B)_\sim = \frac{1}{\beta}\int_0^\beta d\lambda\, \omega(A^*\tau_{i\lambda}(B)) = (\pi_\omega(A)\Omega_\omega, (\beta H_\omega)^{-1}(\mathbb{1} - e^{-\beta H_\omega})\pi_\omega(B)\Omega_\omega)$$

for $A, B \in \mathfrak{A}_\tau$. Here and later we define $p \mapsto p^{-1}(1 - e^{-p})$ by continuity to be equal to one when $p = 0$.

Formally, this quantity appears in the second-order term of a perturbation expansion of the partition function. Let us reconsider the example $\mathfrak{A} = M_n$ and the Gibbs state

$$\omega_{\beta H}(A) = \frac{\mathrm{Tr}_{\mathfrak{H}_n}(e^{-\beta H}A)}{\mathrm{Tr}_{\mathfrak{H}_n}(e^{-\beta H})} .$$

The quantity

$$Z(\beta H) = \mathrm{Tr}_{\mathfrak{H}_n}(e^{-\beta H})$$

is usually referred to as the partition function and one computes that

$$\begin{aligned}
\beta^2(A, B)_\sim &= \beta^2 \int_0^1 dt\ \omega_{\beta H}(A^*\tau_{it\beta}(B)) \\
&= \mathrm{Tr}_{\mathfrak{H}_n}(\beta A^* \int_0^1 dt\, e^{-\beta tH}\beta B e^{-\beta(1-t)H}) \Big/ Z(\beta H) \\
&= \frac{d}{dy}\mathrm{Tr}_{\mathfrak{H}_n}(\int_0^1 dt\ e^{-\beta t(H-yB)}\beta A^* e^{-\beta(1-t)(H-yB)})_{y=0} \Big/ Z(\beta H) \\
&= \frac{\partial^2}{\partial x \partial y}\mathrm{Tr}_{\mathfrak{H}_n}(e^{-\beta(H-xA^*-yB)})_{x=y=0} \Big/ Z(\beta H) \\
&= \frac{\partial^2}{\partial x \partial y} Z(\beta(H - xA^* - yB))_{x=y=0} \Big/ Z(\beta H) .
\end{aligned}$$

The name canonical correlation comes from the following formula which is derived in a similar manner

$$\frac{d}{dx}\,\omega_{\beta(H-xB)}(A)\big|_{x=0} = \beta\{(A^*, B)_\sim - \omega_{\beta H}(A)\omega_{\beta H}(B)\}\ .$$

Subsequently, in Theorem 5.4.12, we show that if ω is a (τ,β)-KMS state which is strongly clustering, i.e.,

$$\lim_{t\to\infty}\ \omega(A\tau_t(B)) = \omega(A)\omega(B)$$

for all $A, B \in \mathfrak{A}$, then

$$i\beta(A,B)_\sim = i\beta\omega(A)\omega(B) + \lim_{T\to\infty}\int_0^T dt\,\omega([A,\tau_t(B)]).$$

The last term represents the first-order change of $\omega(A)$ when ω is allowed to envolve under a perturbed dynamics, with perturbation B. Thus it is often called the *linear response*. This is fully discussed in Section 5.4.

The inequalities occurring in the following theorem will be referred to as the *auto-correlation upper bounds*.

Theorem 5.3.17 (Roepstorff-Fannes-Verbeure). *Let $(\mathfrak{A},\tau)$ be a C^*-dynamical system, and ω a τ-invariant state over $\mathfrak{A}$.*

The following conditions are equivalent:

(1) *ω is a (τ,β) - KMS state*

(2) $\beta^{-1}\displaystyle\int_0^\beta d\lambda\,\omega(A^*\tau_{i\lambda}(A)) \le (\omega(A^*A) - \omega(AA^*))/\log(\omega(A^*A)/\omega(AA^*))$

for all $A \in \mathfrak{A}_\tau$, where we define

$$(u-v)/\log(u/v) = \begin{cases} (u-v)/\log(u/v), & u>0,\ v>0, u\neq v,\\ u, & u=v>0,\\ 0, & uv=0\ . \end{cases}$$

Proof. We consider only the case $\beta \neq 0$ and leave the marginal case $\beta = 0$ as an exercise.

(1) $\Rightarrow$ (2): If $A \in \mathfrak{A}_\tau$ define the measures μ_A and ν_A as in the introduction to Proposition 5.3.14, and again define $k(p) = e^{-\beta p}$. By Proposition 5.3.14 the KMS condition implies

$$\mu_A(k^{-1}) = \nu_A(1)\,,$$

while the auto-correlation upper bound states that

$$\mu_A\big((1-k^{-1})/\log k\big) \le (\nu_A(1) - \mu_A(1))/\log(\nu_A(1)/\mu_A(1))\ .$$

Hence we must prove

$$\mu_A\big((1-k^{-1})/\log k\big) \le (\mu_A(k^{-1}) - \mu_A(1))/\log(\mu_A(k^{-1})/\mu_A(1))\ .$$

By a change of scale, it is enough to prove that

$$\int d\mu(p)p^{-1}(e^p-1) \le \left(\int d\mu(p)e^p - \int d\mu(p)\right)\Big/\log\left(\int d\mu(p)e^p \Big/ \int d\mu(p)\right)$$

for any positive finite Baire measure μ on $\mathbb{R}$ such that $\int d\mu(p)e^{tp} < \infty$ for all $t \in \mathbb{R}$. Define a function f by

$$f(t) = \log\left(\int d\mu(p)e^{tp}\right) .$$

This function is convex in t because

$$f'(t) = \int d\mu(p)pe^{tp} \Big/ \int d\mu(p)e^{tp} ,$$

$$f''(t) = \left(\int d\mu(p)e^{tp} \int d\mu(p)p^2e^{tp} - \left(\int d\mu(p)pe^{tp}\right)^2\right)\Big/\left(\int d\mu(p)e^{tp}\right)^2 \ge 0 ,$$

where the last inequality is a consequence of the Cauchy-Schwarz inequality, In particular,

$$f(t) \le (1-t)f(0) + tf(1)$$

and hence

$$\begin{aligned}\int_0^1 dt\, \exp\{f(t)\} &\le \int_0^1 dt\, \exp\{f(0)\}\exp\{t(f(1)-f(0))\} \\ &= (\exp\{f(1)\} - \exp\{f(0)\})/(f(1)-f(0)) .\end{aligned}$$

But

$$\int_0^1 dt\, \exp\{f(t)\} = \int d\mu(p)p^{-1}(e^p-1)$$

and so we obtain the desired inequality

$$\int d\mu(p)p^{-1}(e^p-1) \le \left(\int d\mu(p) - \int d\mu(p)e^p\right)\Big/\log\left(\int d\mu(p)\Big/\int d\mu(p)e^p\right) .$$

(2) $\Rightarrow$ (1). We will prove that the auto-correlation upper bound implies the auto-correlation lower bound and then appeal to Theorem 5.3.15. Again we may assume $\beta = 1$ by changing scale. Consider the function

$$f(p) = p^{-1}(e^p-1) = \int_0^1 dt\, e^{pt} .$$

It follows from the integral representation that f is strictly increasing and convex, and hence the inverse function g,

$$g(p^{-1}(e^p-1)) = p ,$$

exists on $\mathbb{R}^+$ and is strictly increasing and concave.

Defining $x = \omega(AA^*)/\omega(A^*A)$, the auto-correlation upper bound for $\beta = 1$ takes the form

$$\int d\mu_A(p)p^{-1}(e^p-1)/\omega(A^*A) \le (x-1)/\log x$$

and hence

$$g\left(\int d\mu_A(p)p^{-1}(e^p-1)/\omega(A^*A)\right) \leq \log\ x\ .$$

But as g is concave and continuous, and $d\mu_A(p)/\omega(A^*A)$ is a probability measure, it follows that

$$\begin{aligned} g\left(\int d\mu_A(p)p^{-1}(e^p-1)/\omega(A^*A)\right) &\geq \int d\mu_A(p)g(p^{-1}(e^p-1))/\omega(A^*A) \\ &= \int d\mu_A(p)\,p/\omega(A^*A) \\ &= (\pi_\omega(A)\Omega_\omega, -H_\omega\pi_\omega(A)\Omega_\omega)/\omega(A^*A) \\ &= i\omega(A^*\delta(A))/\omega(A^*A) \end{aligned}$$

and hence

$$i\omega(A^*\delta(A)) \leq \omega(A^*A)\log(\omega(AA^*)/\omega(A^*A))\ .$$

Multiplying both sides by -1 one obtains the auto-correlation lower bound at $\beta = 1$. As $\mathfrak{A}_\tau$ is a core for the infinitesimal generator δ of τ, by Corollary 3.1.7, the inequalities of Theorem 5.3.15 follow for general $A \in D(\delta)$ by continuity.

In order to proceed further in the analysis of KMS states, and in particular to examine the condition of passivity as a criterion for the KMS property, we must broaden slightly the latter notion. In statistical mechanics the parameter β which occurs in the definition of a (τ, β)-KMS state is proportional to the inverse temperature. Thus $\beta = 0$ corresponds to infinite temperature and the associated KMS states, the τ-invariant traces, are therefore called chaotic states. At the other extreme one has the zero-temperature case $\beta = +\infty$ and the definition of a KMS state extends in a natural fashion to these states. They are states of minimal energy in the corresponding representation, or ground states. One can also formally consider negative temperatures and the extreme case $\beta = -\infty$ and for contrast the corresponding states are called ceiling states.

Definition 5.3.18. Let $(\mathfrak{A}, \tau)$ be a C^*-dynamical system, δ the generator of τ, and ω a state over $\mathfrak{A}$.

Then ω is called a τ *ground state* if

$$-i\omega(A^*\delta(A)) \geq 0$$

for all $A \in D(\delta)$. In this case ω is also called a τ-KMS state at value $+\infty$, or a $(\tau, +\infty)$-KMS state. Similarly ω is called a τ *ceiling state* if

$$i\omega(A^*\delta(A)) \geq 0$$

for all $A \in D(\delta)$, and in this case ω is also called a τ-KMS state at value $-\infty$, or a $(\tau, -\infty)$-KMS state.

There are many other ways of characterizing ground states. We collect some of them in the next proposition. A corresponding proposition exists, of course, for ceiling states.

Proposition 5.3.19. *Let $(\mathfrak{A}, \tau)$ be a C^*-dynamical system, and let ω be a state on $\mathfrak{A}$.*

The following conditions are equivalent:

(1) *ω is a τ ground state.*

(2) *If $A, B \in \mathfrak{A}_\tau$, then the entire analytic function*

$$z \mapsto \omega(A\tau_z(B))$$

is uniformly bounded in the region $\{z;\, z \in \mathbb{C},\ \operatorname{Im} z \geq 0\}$.

(3) *For any $A, B \in \mathfrak{A}$, there exists a function $F_{A,B}$ which is continuous in $\operatorname{Im} z \geq 0$, analytic and bounded in $\operatorname{Im} z > 0$ such that*

$$F_{A,B}(t) = \omega(A\tau_t(B))$$

for all $t \in \mathbb{R}$.

(4) *If f is a function with Fourier transform $\hat{f} \in \mathscr{D}$, and $\operatorname{supp} \hat{f} \subseteq (-\infty, 0)$, then*

$$\omega(\tau_f(A)^* \tau_f(A)) = 0$$

for all $A \in \mathfrak{A}$.

(5) *ω is τ-invariant, and if*

$$e^{itH_\omega} \pi_\omega(A)\Omega_\omega = \pi_\omega(\tau_t(A))\Omega_\omega$$

is the corresponding unitary representation of $\mathbb{R}$ on $\mathfrak{H}_\omega$, then

$$H_\omega \geq 0 \ .$$

If these conditions are satisfied, then $e^{itH_\omega} \in \pi_\omega(\mathfrak{A})''$ for all $t \in \mathbb{R}$.

Proof. We will prove (1) $\Leftrightarrow$ (5), (4) $\Leftrightarrow$ (5), and subsequently (5) $\Rightarrow$ (3) $\Rightarrow$ (2) $\Rightarrow$ (5).

(1) $\Rightarrow$ (5). If ω is a ground state then ω is τ-invariant by Lemma 5.3.16, and we may form e^{itH_ω}. But $\pi_\omega(D(\delta))\Omega_\omega \subseteq D(H_\omega)$ and

$$\begin{aligned}(\pi_\omega(A)\Omega_\omega,\, H_\omega\pi_\omega(A)\Omega_\omega) &= -i(\pi_\omega(A)\Omega_\omega,\, \pi_\omega(\delta(A))\Omega_\omega)\\ &= -i\omega(A^*\delta(A)) \ \geq\ 0\end{aligned}$$

for all $A \in D(\delta)$. But

$$e^{itH_\omega}\pi_\omega(D(\delta))\Omega_\omega = \pi_\omega(\tau_t(D(\delta)))\Omega_\omega = \pi_\omega(D(\delta))\Omega_\omega$$

and hence $\pi_\omega(D(\delta))\Omega_\omega$ is a core for H_ω by Corollary 3.1.7. It follows that

$$(\psi,\, H_\omega\psi) \geq 0$$

for all $\psi \in D(H_\omega)$.

(5) $\Rightarrow$ (1). This is immediate from the relation

$$-i\omega(A^*\delta(A)) = (\pi_\omega(A)\Omega_\omega\,,\, H_\omega\pi_\omega(A)\Omega_\omega)$$

for $A \in D(\delta)$.

(5) $\Rightarrow$ (4). If ω is τ-invariant we have

$$\pi_\omega(\tau_f(A))\Omega_\omega = U_\omega(f)\pi_\omega(A)\Omega_\omega = \hat{f}(-H_\omega)\pi_\omega(A)\Omega_\omega$$

by the calculation used in the proof of (2) $\Rightarrow$ (1) in Theorem 5.3.15. Hence if $H_\omega \geq 0$ and supp $\hat{f} \subseteq (-\infty, 0)$ then $\hat{f}(-H_\omega) = 0$ and thus

$$\omega(\tau_f(A)^*\tau_f(A)) = \|\pi_\omega(\tau_f(A))\Omega_\omega\|^2 = 0$$

for all $A \in \mathfrak{A}$.

(4) $\Rightarrow$ (5). If (4) is true it follows from the Cauchy-Schwarz inequality that

$$\omega(A\tau_f(B)) = 0$$

for all $A, B \in \mathfrak{A}$, and all $\hat{f} \in \mathscr{D}$ with supp $\hat{f} \subseteq (-\infty, 0)$. Replacing A by the elements of an approximate identity for $\mathfrak{A}$, Proposition 2.2.17, we obtain

$$\omega(\tau_f(B)) = 0$$

for all $B \in \mathfrak{A}$ and all $\hat{f} \in \mathscr{D}$ with supp $\hat{f} \subseteq (-\infty, 0)$. If $B = B^*$ it follows by taking the complex conjugate of the last relation, that the relation still holds for all $\hat{f} \in \mathscr{D}$ such that $0 \notin$ supp $\hat{f}$. But then Lemma 3.2.45 implies that

$$\omega(\tau_t(B)) = \omega(B)$$

for all $t \in \mathbb{R}$, i.e., ω is τ-invariant. It follows therefore that

$$(\pi_\omega(A)\Omega_\omega, \hat{f}(-H_\omega)\pi_\omega(B)\Omega_\omega) = \omega(A^*\tau_f(B)) = 0$$

whenever supp $\hat{f} \subseteq (-\infty, 0)$. Hence $H_\omega \geq 0$.

(5) $\Rightarrow$ (3). By spectral theory, we may define

$$\begin{aligned} F_{A,B}(z) &= (\pi_\omega(A^*)\Omega_\omega,\, e^{izH_\omega}\pi_\omega(B)\Omega_\omega) \\ &= \int_{-\infty}^{0} e^{-izp}(\pi_\omega(A^*)\Omega_\omega,\, dE(p)\pi_\omega(B)\Omega_\omega) \end{aligned}$$

for Im $z \geq 0$, where

$$e^{itH_\omega} = \int_{-\infty}^{0} e^{-itp} dE(p)$$

is the spectral decomposition of e^{itH_ω}. Lebesgue's theorem now implies that $F_{A,B}$ has the desired properties.

(3) $\Rightarrow$ (2). This is proved by using the edge of the wedge theorem, Proposition 5.3.6, as in the proof of (3) $\Rightarrow$ (1) in Proposition 5.3.7.

(2) $\Rightarrow$ (5). By an extension of the Phragmen–Lindelöf theorem, Proposition 5.3.5, we have that

$$|\omega(A\tau_z(B))| \leq \|A\|\,\|B\|$$

when Im $z \geq 0$. Hence, replacing A by the elements of an approximate identity,

$$|\omega(\tau_z(B))| \leq \|B\|$$

when Im $z \geq 0$. But if $B = B^*$ it follows from the Schwarz reflection principle that $\omega(\tau_{\bar{z}}(B)) = \overline{\omega(\tau_z(B))}$, and hence $|\omega(\tau_z(B))| \leq \|B\|$ for all $z \in \mathbb{C}$. By Liouville's theorem, ω is τ-invariant, and we can form H_ω.

If $B \in \mathfrak{A}_\tau$ then $\psi = \pi_\omega(B)\Omega_\omega$ is analytic for H_ω and

$$|(\psi, e^{izH_\omega}\psi)| = |\omega(B^*\tau_z(B))| \leq \omega(B^*B) = (\psi, \psi)$$

for $\operatorname{Im} z \geq 0$. Therefore, taking the derivative at 0 in the direction $\operatorname{Im} z > 0$, $\operatorname{Re} z = 0$, we obtain

$$(\psi, -H_\omega\psi) \leq 0 \ .$$

But $\pi_\omega(\mathfrak{A}_\tau)\Omega_\omega$ is e^{itH_ω}-invariant and thus a core for H_ω by Corollary 3.1.7. It follows that

$$H_\omega \geq 0 \ .$$

The last statement in the proposition is a consequence of Corollary 3.2.60.

EXAMPLE 5.3.20. Let $\mathfrak{A}(\mathfrak{h})$ be the CAR algebra over a Hilbert space $\mathfrak{h}$ and τ a one-parameter group of Bogoliubov transformations such that $\tau_t(a(f)) = a(e^{itH}f)$, etc. In Example 5.3.2 we have shown that there is a unique (τ, β)-KMS state for all $\beta \in \mathbb{R}$ and we next argue that there is a unique τ ground state (τ ceiling state) if, and only if, there are no nonzero $f \in \mathfrak{h}$ invariant under the unitary group $U_t = e^{itH}$. First, assume there are no invariant f and let ω be a ground state. It follows from Lemma 5.3.16 that ω is τ-invariant and then it follows as in Example 5.2.21 that ω is even. Now by linearity, anti-linearity, and positivity

$$\omega(a^*(f)a(g)) = (g, Tf) \ ,$$

where $0 \leq T \leq \mathbb{1}$. The τ-invariance implies that T commutes with U_t and hence T commutes strongly with H. But the ground-state condition $-i\omega(A^*\delta(A)) \geq 0$ with the successive choices $A = a(f)$ and $A = a^*(f)$, $f \in D(H)$, yield the conditions

$$TH = HT \leq 0 \ , \quad TH = HT \leq H \ .$$

These conditions uniquely determine T by $T = E_H(-\infty, 0)$ where E_H denotes the spectral family of H. In particular

$$\pi_\omega(a((\mathbb{1} - T)f))\Omega_\omega = 0, \quad \pi_\omega(a^*(Tf))\Omega_\omega = 0 \ .$$

Therefore,

$$\begin{aligned}\omega(a(g_1)a(g_2)) &= \omega(a((\mathbb{1} - T)g_1)a(Tg_2)) \\ &= -\omega(a(Tg_2)a((\mathbb{1} - T)g_1)) = 0 \ .\end{aligned}$$

Moreover,

$$\begin{aligned}&\omega(a^*(f_1)a^*(f_2)a(g_1)a(g_2)) \\ &\quad = \omega(a^*(Tf_1)a^*(Tf_2)a(Tg_1)a(Tg_2)) \\ &\quad = -\omega(a^*(Tf_1)a(Tg_1)a^*(Tf_2)a(Tg_2)) + (g_1, Tf_2)(g_2\, Tf_1) \\ &\quad = -(g_2, Tf_2)(g_1, Tf_1) + (g_1, Tf_2)(g_2, Tf_1)\end{aligned}$$

by use of the CARs. A similar calculation for higher-order monomials proves that ω is the unique gauge-invariant quasi-free state with the above two-point function.

Conversely, assume that $U_t f = f$ with $f \neq 0$. Let $f^\perp$ denote the orthogonal complement of f in $\mathfrak{h}$. It follows from the construction in the proof of Theorem 5.2.5 that $\mathfrak{A}(\mathfrak{h}) \cong \mathfrak{A}(\mathbb{C}f) \otimes \mathfrak{A}(f^\perp)$. Thus, if ω_f is any state over $\mathfrak{A}(\mathbb{C}f)$ and ω_0 is a ground state for τ restricted to $\mathfrak{A}(f^\perp)$, then $\omega_f \otimes \omega_0$ is a ground state for τ. Thus the ground state is not unique.

After this diversion on ground states and ceiling states, which correspond intuitively to τ-KMS states at values $+\infty$, and $-\infty$, we return to the discussion of stability properties and the KMS condition. So far we have derived various characterizations of the (τ, β)-KMS condition for some fixed $\beta \in \mathbb{R} \cup \{\pm\infty\}$. We next consider a condition which implies the KMS property for some $\beta \in [0, \infty]$ but does not determine the precise value of β. This condition is the passivity condition introduced in the discussion of stability and the maximum entropy principle which preceded Theorem 5.3.15. We first give a precise definition of passivity for a general C^*-system together with a refinement of this notion, complete passivity.

Definition 5.3.21. Let $(\mathfrak{A}, \tau)$ be a C^*-dynamical system, where $\mathfrak{A}$ has an identity, let δ be the infinitesimal generator of τ, and let ω be a state on $\mathfrak{A}$.

Then ω is said to be a *passive state* if

$$-i\omega(U^*\delta(U)) \geq 0$$

for any $U \in \mathscr{U}_0(\mathfrak{A}) \cap D(\delta)$, where $\mathscr{U}_0(\mathfrak{A})$ denotes the connected component of the identity of the group $\mathscr{U}(\mathfrak{A})$ of all unitary elements of $\mathfrak{A}$ with the uniform topology.

Moreover, ω is said to be a *completely passive state* if $\bigotimes_{i=1}^n \omega$ is a passive state of the C^*-dynamical system $(\bigotimes_{i=1}^n \mathfrak{A}, \bigotimes_{j=1}^n \tau)$ for each $n \in \mathbb{N}$.

The principal characterizations of passivity are contained in the following.

Theorem 5.3.22 (Pusz-Woronowicz). *Let $(\mathfrak{A}, \tau)$ be a C^*-dynamical system, where $\mathfrak{A}$ has an identity, δ the infinitesimal generator of τ and ω a state on $\mathfrak{A}$. Let $\delta^{(n)}$ be the generator of $\bigoplus_{j=1}^n \tau$ on $\bigoplus_{j=1}^n \mathfrak{A}$. Consider the following conditions:*

(1) *ω is a (τ, β)-KMS state for a $\beta \in [0, +\infty]$, and ω is τ-invariant.*
(2) *ω is completely passive.*
(3) *ω is passive.*
(4) *$-i(\bigoplus_{j=1}^n \omega)(B\delta^{(n)}(B)) \geq 0$ for all $B = B^* \in D(\delta^{(n)})$ and all $n \in \mathbb{N}$.*
(5) *$-i\omega(A\delta(A)) \geq 0$ for all $A = A^* \in D(\delta)$.*

The following implications are valid: (1) $\Leftrightarrow$ (2) $\Leftrightarrow$ (4) $\Rightarrow$ (3) $\Rightarrow$ (5).

Furthermore, if there exists a group G and an action α of G as *-automorphisms of $\mathfrak{A}$ such that ω is α-invariant, α commutes with τ, and ω is weakly α-clustering, i.e.,

$$\omega \circ \alpha_g = \omega\,, \quad g \in G\,,$$

$$\alpha_g \tau_t = \tau_t \alpha_g\,, \quad g \in G, t \in \mathbb{R}\,,$$

and

$$\inf_{B' \in C_0(\alpha_G(B))} |\omega(AB') - \omega(A)\omega(B)| = 0\,, \quad A, B \in \mathfrak{A}\,,$$

then it follows that (5) $\Rightarrow$ (1) *and all the conditions are equivalent.*

Remarks

(1) Since conditions (3) and (5) are preserved under convex combinations of states, and convex combinations of (τ, β)-KMS states for different β are not KMS states, it is clear that a condition of purity of ω is needed for the implications (3) $\Rightarrow$ (1) and (5) $\Rightarrow$ 1.

(2) If ω is a (τ, β)-KMS state for a $\beta \in (0, \infty]$, then ω is automatically τ-invariant by Propositions 5.3.3 and 5.3.19, but this is no longer the case for $\beta = 0$. Condition (5) implies invariance, however, and thus the condition of τ-invariance cannot be dropped from (1) (see Lemma 5.3.16).

PROOF

(1) $\Rightarrow$ (2). If ω is an invariant KMS state at value β for $(\mathfrak{A}, \tau)$ then it follows that $\bigotimes_{j=1}^{n} \omega$ is a β-KMS state for $(\bigotimes_{j=1}^{n} \mathfrak{A}, \bigotimes_{j=1}^{n} \tau)$ and hence (1) $\Rightarrow$ (2) will follow from (1) $\Rightarrow$ (3).

(2) $\Rightarrow$ (3). Trivial.

(1) $\Rightarrow$ (3). When $\beta \in (0, +\infty)$ this is an immediate consequence of the autocorrelation lower bounds, Theorem 5.3.15, and when $\beta = +\infty$ it follows from the definition of a ground state, Definition 5.3.18. The remaining case is $\beta = 0$, i.e., ω is a τ-invariant trace-state. Assume first that $U \in D(\delta)$ is a unitary such that $\|U - \mathbb{1}\| < 2$. Then it follows from spectral theory and an extension of Theorem 3.2.32 that there exists an $A = A^* \in D(\delta)$ with $\|A\| < \pi$ such that $U = e^{iA}$. But Lemma 3.2.31 implies that

$$\delta(U) = i \int_0^1 dr\, e^{irA} \delta(A) e^{i(1-r)A}$$

and hence

$$\omega(U^* \delta(U)) = i \int_0^1 dr\, \omega(e^{i(r-1)A} \delta(A) e^{-i(r-1)A}) = i\omega(\delta(A)) = 0 \ ,$$

where the second step relies upon the trace property of ω and the third step follows from the τ-invariance.

Next, if $-i\omega(U^* \delta(U)) \geq 0$ for some $U \in \mathscr{U}(\mathfrak{A}) \cap D(\delta)$ and $V \in \mathscr{U}(\mathfrak{A}) \cap D(\delta)$ is an element such that $\|V - U\| < 2$, then

$$V = U_1 U \ ,$$

where $U_1 = VU^{-1} \in \mathscr{U}(\mathfrak{A}) \cap D(\delta)$ and $\|U_1 - \mathbb{1}\| = \|V - U\| < 2$. Thus

$$\omega(U_1^* \delta(U_1)) = 0$$

and

$$\begin{aligned} -i\omega(V^* \delta(V)) &= -i\omega(U^* U_1^* \delta(U_1 U)) \\ &= -i\omega(U^* U_1^* \delta(U_1) U) - i\omega(U^* U_1^* U_1 \delta(U)) \\ &= -i\omega(U_1^* \delta(U_1)) - i\omega(U^* \delta(U)) \geq 0 \ . \end{aligned}$$

Hence, the set of $U \in \mathscr{U}(\mathfrak{A}) \cap D(\delta)$ such that $-i\omega(U^* \delta(U)) \geq 0$ is open and closed, and thus $\mathscr{U}_0(\mathfrak{A}) \cap D(\delta)$ is contained in this set. (Note that $\mathscr{U}_0(\mathfrak{A}) \cap D(\delta) = (\mathscr{U}(\mathfrak{A}) \cap D(\delta))_0$ by the first part of the proof.)

(3) $\Rightarrow$ (5). If $A = A^* \in D(\delta)$, then

$$e^{i\varepsilon A} \in \mathscr{U}_0(\mathfrak{A}) \cap D(\delta)$$

for all $\varepsilon \in \mathbb{R}$ by Lemma 3.2.31, and

$$\delta(e^{i\varepsilon A}) = i\varepsilon \int_0^1 dr\, e^{i\varepsilon r A} \delta(A) e^{i\varepsilon(1-r)A} \ .$$

It follows that

$$\begin{aligned}
-i\omega(e^{-i\varepsilon A}\delta(e^{i\varepsilon A})) &= \varepsilon \int_0^1 dr\, \omega(e^{i\varepsilon(r-1)A}\delta(A)e^{-i\varepsilon(r-1)}A) \\
&= \varepsilon \int_0^1 dr \sum_{n=0}^{\infty} \frac{i^n \varepsilon^n (r-1)^n}{n!} \omega\Big(\underset{1}{[A,} \underset{2}{[A,} \dots \underset{n}{[A, \delta(A)]} \dots]\Big) \\
&= \sum_{n=0}^{\infty} \frac{(-i)^n \varepsilon^{n+1}}{(n+1)!} \omega\Big(\underset{1}{[A,} \underset{2}{[A,} \dots \underset{n}{[A, \delta(A)]} \dots]\Big) \\
&= \varepsilon\omega(\delta(A)) + \frac{\varepsilon^2}{2} i\omega([\delta(A), A]) + O(\varepsilon^3) \ .
\end{aligned}$$

But the passivity of ω implies that this expression is nonnegative for all $\varepsilon \in \mathbb{R}$. Therefore, one must have $\omega(\delta(A)) = 0$ and $i(\omega[\delta(A), A]) \geq 0$ for all $A = A^* \in D(\delta)$. But then the relation

$$[\delta(A), A] = \delta(A)A - A\delta(A) = \delta(A^2) - 2A\delta(A)$$

implies that

$$-i\omega(A\delta(A)) \geq 0$$

for all $A = A^* \in D(\delta)$.

(2) $\Rightarrow$ (4). This is a special case of (3) $\Rightarrow$ (5).

We now turn to the remaining proofs, namely, (4) $\Rightarrow$ (1) and (5) $\Rightarrow$ (1) under the weak-clustering assumption on ω. We first explore some consequences of (5).

If $B \in D(\delta)$, then $(B + B^*)/2$ and $(B - B^*)/2i$ are selfadjoint elements in $D(\delta)$, and condition (5) implies

$$-i\omega\big(2^{-1}(B+B^*)\delta(2^{-1}(B+B^*))\big) - i\omega\big((2i)^{-1}(B-B^*)\delta((2i)^{-1}(B-B^*))\big) \geq 0$$

and hence

$$-i\omega(B^*\delta(B)) - i\omega(B\delta(B^*)) \geq 0 \ .$$

Lemma 5.3.16 implies that ω is τ-invariant. Let $t \mapsto U_\omega(t) = \exp\{itH_\omega\}$ be the canonical unitary group implementing τ on $\mathfrak{H}_\omega$ The last condition then reads

$$(\pi_\omega(B)\Omega_\omega, H_\omega \pi_\omega(B)\Omega_\omega) + (\pi_\omega(B^*)\Omega_\omega, H_\omega \pi_\omega(B^*)\Omega_\omega) \geq 0$$

for all $B \in D(\delta)$. Next we use the relation

$$\pi_\omega(\tau_f(B))\Omega_\omega = U_\omega(f)\pi_\omega(B)\Omega_\omega \ = \ \hat{f}(-H_\omega)\pi_\omega(B)\Omega_\omega$$

which is valid for $f \in \mathscr{S}(\mathbb{R})$. Moreover, $\tau_f(B) \in D(\delta)$ for all $f \in \mathscr{S}$ and hence

$$(\pi_\omega(B)\Omega_\omega,\, H_\omega\chi(H_\omega)\pi_\omega(B)\Omega_\omega) + (\pi_\omega(B)^*\Omega_\omega,\, H_\omega\chi(-H_\omega)\pi_\omega(B)^*\Omega_\omega) \geq 0$$

for all $B \in \mathfrak{A}$ and all positive $\chi \in \mathscr{S}(\mathbb{R})$. By Corollary 2.4.15, $\pi_\omega(\mathfrak{A})$ is strong*-dense in $\pi_\omega(\mathfrak{A})'' = \mathfrak{M}_\omega$, and thus we have established

OBSERVATION 1

$$(A\Omega_\omega, H_\omega\chi(H_\omega)A\Omega_\omega) + (A^*\Omega_\omega, H_\omega\chi(-H_\omega)A^*\Omega_\omega) \geq 0$$

for all $A \in \mathfrak{M}_\omega$ and all positive $\chi \in \mathscr{S}(\mathbb{R})$.

Next, define $E = [\pi_\omega(\mathfrak{A})'\Omega_\omega]$. Then Ω_ω is cyclic and separating for $E\mathfrak{M}_\omega E$. Let Δ_E, J_E be the associated modular operator and antiunitary involution on $E\mathfrak{H}_\omega$. Extend Δ_E to $\mathfrak{H}_\omega$ by defining

$$\Delta = \Delta_E E \quad .$$

Then Δ is a nonnegative selfadjoint operator on $\mathfrak{H}_\omega$, and $\mathfrak{M}_\omega\Omega_\omega$ is a core for $\Delta^{1/2}$, since $E\mathfrak{M}_\omega\Omega_\omega = E\mathfrak{M}_\omega E\Omega_\omega$ is a core for $\Delta_E^{1/2}$. By standard results of the Tomita-Takesaki theory we obtain

$$\begin{aligned}(\Delta^{1/2}A\Omega_\omega, \Delta^{1/2}B\Omega_\omega) &= (\Delta_E^{1/2}EAE\Omega_\omega, \Delta_E^{1/2}EBE\Omega_\omega)\\ &= (EB^*E\,\Omega_\omega, EA^*E\Omega_\omega) \;=\; (EB^*\Omega_\omega, A^*\Omega_\omega)\end{aligned}$$

Since $U_\omega(t)\Omega_\omega = \Omega_\omega$ and $U_\omega(t)\pi_\omega(\mathfrak{A})'U_\omega(t)^* = \pi_\omega(\mathfrak{A})'$ for all t, we then find $U_\omega(t)E = EU_\omega(t)$ for all t, and hence

$$U_\omega(t)E\mathfrak{M}_\omega EU_\omega(t)^* = E\mathfrak{M}_\omega E \quad .$$

Since Δ_E is canonically related to $(E\mathfrak{M}_\omega E, \Omega_\omega)$, it follows that $U_\omega(t)E\Delta_E = \Delta_E U_\omega(t)E$, and hence Δ and H_ω commute strongly. Thus one has a joint spectral representation,

$$H_\omega = \int_\Lambda \varepsilon\, dE(\varepsilon, \lambda) \;, \qquad \Delta = \int_\Lambda e^\lambda dE(\varepsilon, \lambda) \;,$$

where $\Lambda = \mathbb{R} \times \tilde{\mathbb{R}}$ and $\tilde{\mathbb{R}} = \mathbb{R} \cup \{-\infty\}$. Let $\tilde{\sigma}(H_\omega, \log\Delta) \subseteq \Lambda$ be the support of $E(\cdot,\cdot)$, i.e., the joint spectrum of H_ω and $\log\Delta$.

OBSERVATION 2

$$\tilde{\sigma}(H_\omega, \log\Delta) \subseteq \{(\varepsilon, \lambda) \in \Lambda; \varepsilon\lambda \leq 0\} \quad .$$

To prove this, we apply Observation 1 with $\chi(t) = e^{-t^2}$ on $A = BE$ where $B \in \mathfrak{M}_\omega$. Therefore,

$$(B\Omega_\omega, H_\omega e^{-H_\omega^2}B\Omega_\omega) + (EB^*\Omega_\omega, H_\omega e^{-H_\omega^2}B^*\Omega_\omega) \geq 0 \;,$$

where we have used the fact that H_ω and E commute strongly. The function $\varepsilon \mapsto f(\varepsilon) = \varepsilon e^{-\varepsilon^2}$ is real and anti-symmetric and hence has purely imaginary Fourier transform $\hat{f}$. Let $C \in \mathfrak{M}_\omega$ be the element defined by

$$C^* \;=\; \int dt\; U_\omega(t)B^*U_\omega(t)^*\hat{f}(t) \quad .$$

Then

$$C \;=\; -\int dt\; U_\omega(t)BU_\omega(t)^*\hat{f}(t) \;,$$

and hence

$$C^*\Omega_\omega = H_\omega e^{-H_\omega^2} B^*\Omega_\omega \ , \qquad C\Omega_\omega = -H_\omega e^{-H_\omega^2} B\Omega_\omega \ .$$

Using the modular relation for Δ we obtain

$$\begin{aligned}(EB^*\Omega_\omega,\, H_\omega e^{-H_\omega^2} B^*\Omega_\omega) &= (EB^*\Omega_\omega,\, C^*\Omega_\omega)\\ &= (\Delta^{1/2} C\Omega_\omega,\, \Delta^{1/2} B\Omega_\omega)\\ &= -(\Delta^{1/2} H_\omega e^{-H_\omega^2} B\Omega_\omega,\, \Delta^{1/2} B\Omega_\omega)\ ,\end{aligned}$$

and hence

$$(B\Omega_\omega,\, H_\omega e^{-H_\omega^2} B\Omega_\omega) - (\Delta^{1/2} H_\omega e^{-H_\omega^2} B\Omega_\omega,\, \Delta^{1/2} B\Omega_\omega) \geq 0 \ .$$

As $\mathfrak{M}_\omega\Omega_\omega$ is a core for $\Delta^{1/2}$, and H_ω commutes strongly with $\Delta^{1/2}$, it follows by closure that

$$H_\omega\, e^{-H_\omega^2}(\mathbb{1} - \Delta) \geq 0 \ .$$

Observation 2 follows immediately from this inequality.

Define $\sigma(H_\omega, \log\Delta) = \tilde{\sigma}(H_\omega, \log\Delta) \cap \mathbb{R} \times \mathbb{R}$.

OBSERVATION 3

$$\sigma(H_\omega, \log\Delta) = -\sigma(H_\omega, \log\Delta) \ .$$

Note that $\sigma(H_\omega, \log\Delta) = \sigma(H_\omega E, \log\Delta_E)$. Hence Observation 3 follows from the identities.

$$J_E\, \Delta_E\, J_E = \Delta_E^{-1}, \qquad J_E\, H_\omega\, E J_E = -H_\omega\, E \ .$$

The first of these follows from Proposition 2.5.11, the second from the commutation of $e^{itH_\omega E}$ with $S_E = J_E \Delta_E^{1/2}$ which is established as in the proof of (3) $\Rightarrow$ (2) of Theorem 3.2.61.

OBSERVATION 4. Assume that there exists a set $\tilde{\Sigma} \subseteq \mathbb{R} \times \tilde{\mathbb{R}}$, such that

(1) $\tilde{\Sigma} + \Sigma \subseteq \tilde{\Sigma}$, where $\Sigma = \tilde{\Sigma} \cap (\mathbb{R} \times \mathbb{R})$,
(2) $\tilde{\Sigma} \subseteq \{(\varepsilon, \lambda) \in \mathbb{R} \times \tilde{\mathbb{R}};\ \varepsilon\lambda \leq 0\}$
(3) $\tilde{\sigma}(H_\omega, \log\Delta) \subseteq \tilde{\Sigma}$.

Then ω is a (τ, β)-KMS state for some $\beta \in [0, \infty]$.

In the proof of Observation 4 we consider two cases separately.

Case I. $\tilde{\sigma}(H_\omega, \log\Delta) = \sigma(H_\omega, \log\Delta)$. Thus, if $p, q \in \tilde{\sigma}$, then $-p, -q, \in \tilde{\sigma}$ by Observation 3, and hence $np + mq \in \tilde{\Sigma}$ for all integers n, m by assumption (1). But then assumption (2) implies that p and q must belong to the same straight line passing through (0,0) (otherwise $\{np + mq; n, m \in \mathbb{Z}\}$ would form a lattice in $\mathbb{R}^2$ which could not be contained in $\{(\varepsilon, \lambda) \in \mathbb{R}^2; \varepsilon\lambda \leq 0\}$). It follows that $\sigma(H_\omega, \log\Delta)$ itself is contained in a straight line passing through (0, 0). If this line is vertical, then $H_\omega = 0$ and ω is trivially a ground state. If the line is not vertical, there exists $\beta \geq 0$ such that $\lambda = -\beta\varepsilon$ for all $(\varepsilon, \lambda) \in \sigma(H_\omega, \log\Delta)$. But then

$$\Delta = e^{-\beta H_\omega} \ ,$$

and hence ω is a τ-KMS state at value β by Theorem 5.3.10.

Case II. $\tilde{\sigma}(H_\omega, \log\Delta) \neq \sigma(H_\omega, \log\Delta)$. Then there exists $\varepsilon_0 \in \mathbb{R}$ such that $(\varepsilon_0, -\infty) \in \tilde{\sigma}(H_\omega, \log\Delta)$. Assume that $(\varepsilon, \lambda) \in \tilde{\sigma}(H_\omega, \log\Delta)$ for some $\varepsilon < 0$. Then (3)

and (2) imply that $\lambda \geq 0$, and $(\varepsilon, \lambda) \in \sigma(H_\omega, \log\Delta)$. But (1) then implies that $n(\varepsilon, \lambda) + (\varepsilon_0, -\infty) = (n\varepsilon + \varepsilon_0, -\infty) \in \tilde{\Sigma}$ for all $n \in \mathbb{N}$, and when n is so large that $n\varepsilon + \varepsilon_0 < 0$ this contradicts (2). Therefore, $\varepsilon \geq 0$ for any $(\varepsilon, \lambda) \in \tilde{\sigma}(H_\omega, \log\Delta)$. This means that $H_\omega \geq 0$ and ω is a ground state.

We are now able to prove (4) $\Rightarrow$ (1) of Theorem 5.3.22. The proof is based on the following formula:

$$\tilde{\sigma}\left(H_{\bigotimes_{j=1}^{n}\omega}, \log\left(\Delta_{\bigotimes_{j=1}^{n}\omega}\right)\right) = \sum_{j=1}^{n} \tilde{\sigma}(H_\omega, \log\Delta)$$

which follows from the obvious facts that

$$H_{\bigotimes_{j=1}^{n}\omega} = \sum_{j=1}^{n} \mathbb{1} \otimes \ldots \otimes \mathbb{1} \otimes \underset{j}{H_\omega} \otimes \mathbb{1} \otimes \ldots \otimes \mathbb{1} \ , \qquad \Delta^{it}_{\bigotimes_{j=1}^{n}\omega} = \bigotimes_{j=1}^{n} \Delta^{it} \ .$$

Hence, if ω satisfies condition (4), i.e., $\otimes_{j=1}^{n}\omega$ satisfies condition (5) for all n, it follows from Observation 2 that the set

$$\tilde{\Sigma} = \bigcup_{n \geq 1} \left(\sum_{j=1}^{n} \tilde{\sigma}(H_\omega, \log\Delta) \right)$$

satisfies condition (2) of Observation 4. Conditions (1) and (3) of this observation are clearly satisfied, and hence Observation 4 implies that ω is a τ-KMS state at value $\beta \in [0, \infty]$. In particular, ω is τ-invariant by Proposition 5.3.3 or Lemma 5.3.16.

Finally, we prove that (5) $\Rightarrow$ (1) if ω is weakly G-clustering for an action α of a group G on $\mathfrak{A}$ such that $\alpha_g \tau_t = \tau_t \alpha_g$, for all $g \in G$ and $t \in \mathbb{R}$, and if ω is α- invariant. We show in this case that the requirements of Observation 4 are fulfilled with

$$\tilde{\Sigma} = \tilde{\sigma}(H_\omega, \log\Delta) \ .$$

Condition (3) is then trivial, while condition (2) follows from Observation 2. It remains to show condition (1). Let $\hat{\omega}$, $\hat{\tau}$, and $\hat{\alpha}$ be the normal extensions of ω, τ, and α to $\mathfrak{M}_\omega = \pi_\omega(\mathfrak{A})''$. Theorems 4.3.22 and 4.3.23 then imply that $\hat{\alpha}$, restricted to $E\mathfrak{M}_\omega E$, has the three point cluster property:

$$\inf_{B' \in Co(\alpha_G(B))} | \hat{\omega}(AB'C) - \hat{\omega}(AC)\hat{\omega}(B) | = 0$$

for all $A, B, C \in E\mathfrak{M}_\omega E$. Hence it follows from Theorem 4.3.33 and the subsequent remark that

$$\Sigma = \sigma(H_\omega, \log\Delta) = \sigma(H_\omega E, \log\Delta_E)$$

has the semigroup property

$$\Sigma + \Sigma \subseteq \Sigma \ .$$

(Observation 3 even implies that Σ is a group.) Thus to show condition (1) in Observation 4, it is enough to show that $(\varepsilon, -\infty) \in \tilde{\Sigma}$ and $(\varepsilon', \lambda) \in \Sigma$ implies $(\varepsilon + \varepsilon', -\infty) \in \tilde{\Sigma}$. But these conditions mean that

$$\varepsilon \in \sigma(H_\omega(\mathbb{1} - E)) \ , \quad \varepsilon' \in \sigma(H_\omega E) \ .$$

Now as E is τ-invariant, it follows from Proposition 3.2.40 that for any $\delta > 0$ there exists $A, B \in \mathfrak{M}_\omega$ such that

$$A = (\mathbb{1} - E)AE \ , \quad A\Omega_\omega \neq 0 \ , \quad B = EBE \ , \quad B\Omega_\omega \neq 0 \ ,$$
$$\sigma_\tau(A) \subseteq (\varepsilon - \delta, \varepsilon + \delta) \ , \quad \sigma_\tau(B) \subseteq (\varepsilon' - \delta, \varepsilon' + \delta) \ .$$

But as α commutes with τ the last condition implies that

$$\sigma_\tau(U_\omega(g)BU_\omega(g)^*) \subseteq (\varepsilon' - \delta, \varepsilon' + \delta)$$

for all $g \in G$. Hence it follows from Lemma 3.2.42 that

$$\sigma_{U_\omega}(AU_\omega(g)BU_\omega(g)^*\Omega_\omega) \subseteq (\varepsilon + \varepsilon' - 2\delta, \varepsilon + \varepsilon' + 2\delta)$$

for all $g \in G$. As $(\mathbb{1} - E)A = A$, the latter vector lies in $(\mathbb{1} - E)\mathfrak{H}_\omega$ for all $g \in G$. Hence if we can show that the vector is nonzero for some $g \in G$, it follows that

$$\sigma(H_\omega(\mathbb{1} - E)) \cap (\varepsilon + \varepsilon' - 2\delta, \varepsilon + \varepsilon' + 2\delta) \neq \varnothing \ .$$

As δ was arbitrary, this implies

$$(\varepsilon + \varepsilon', -\infty) \in \tilde{\Sigma} \ .$$

Assume, *ad absurdum*, that

$$AU_\omega(g)BU_\omega(g)^*\Omega_\omega = 0$$

for all $g \in G$. Then $AU_\omega(g)BU_\omega(g)^*E = 0$ by the definition of E. As

$$U_\omega(g)BU_\omega(g)^*(\mathbb{1} - E) = U_\omega(g)B(\mathbb{1} - E)U_\omega(g)^* = 0$$

by the assumption $BE = B$, it follows that

$$AU_\omega(g)BU_\omega(g)^* = 0$$

for all g, or $AU_\omega(g)B = 0$. Thus

$$(A\Omega_\omega, AU_\omega(g)BB^*\Omega_\omega) = 0 \ .$$

But the weak G-clustering of ω with respect to α and Theorem 4.3.22 next imply that

$$\|A\Omega_\omega\|^2\|B^*\Omega_\omega\|^2 = 0 \ .$$

But as $A\Omega_\omega \neq 0$ this implies $B^*\Omega_\omega = 0$. But Ω_ω is separating for $E\mathfrak{M}_\omega E \ni B^*$ and hence $B^* = 0$. This contradicts the assumption $B\Omega_\omega \neq 0$. Thus

$$\tilde{\Sigma} + \Sigma \subseteq \tilde{\Sigma}$$

and the proof of Theorem 5.3.22 is complete.

We conclude this subsection with a discussion of various convergence properties and several comments and examples concerning the existence of KMS states. First we derive a justification for a terminology "KMS state at $\pm\infty$" used in the definition of ground states and ceiling states.

Proposition 5.3.23. *Let $(\mathfrak{A}, \tau)$ be a C^*-dynamical system, and $\{\omega_\alpha\}$ a net of states on $\mathfrak{A}$ such that ω_α converges to a state ω in the weak*-topology, i.e.,*

$$\lim_\alpha \omega_\alpha(A) = \omega(A)$$

for all $A \in \mathfrak{A}$. Assume that ω_α is a (τ, β_α)-KMS state, where $\beta_\alpha \in \mathbb{R} \cup \{\pm\infty\}$, and that

$$\lim_\alpha \beta_\alpha = \beta$$

exists in $\mathbb{R}\cup\{\pm\infty\}$.

It follows that ω *is a* (τ,β)*-KMS state.*

PROOF. If $|\beta|<\infty$, we may assume that $|\beta_\alpha|<\infty$ for all α by passing to a subnet. Hence the corollary is an immediate consequence of the auto-correlation lower bounds in Theorem 5.3.15, since $u,v\mapsto u\log(u/v)$ is lower semi-continuous.

If $\beta=+\infty$, we may either assume that $\beta_\alpha=+\infty$ for all α, or $0<\beta_\alpha<+\infty$ for all α. In the first case

$$-i\omega(A^*\delta(A))=\lim_\alpha -i\omega_\alpha(A^*\delta(A))\geq 0$$

for all $A\in D(\delta)$. In the second case note that by the auto-correlation lower bound

$$\begin{aligned}-i\omega(A^*\delta(A)) &= \lim_\alpha -i\omega_\alpha(A^*\delta(A))\\ &\geq \overline{\lim_\alpha}\,\frac{1}{\beta_\alpha}\,\omega_\alpha(A^*A)\log(\omega_\alpha(A^*A)/\omega_\alpha(AA^*))\\ &\geq \overline{\lim_\alpha}\,\frac{1}{\beta_\alpha}(\omega_\alpha(A^*A)-\omega_\alpha(AA^*))=0\end{aligned}$$

for all $A\in D(\delta)$. The last inequality follows because

$$u\log(u/v) = v((u/v)\log(u/v)) \geq v(u/v-1) = u-v$$

by convexity of $x\mapsto x\log x$.

The case $\beta=-\infty$ is similar.

EXAMPLE 5.3.24. Adopt the assumptions of Examples 5.3.2 and 5.3.20. The unique (τ,β)-KMS state over the CAR algebra $\mathfrak{A}(\mathfrak{h})$, for $\beta\in\mathbb{R}$, is the gauge-invariant quasi free-state ω_β with two-point function

$$\omega_\beta(a^*(f)a(g))=(g,\,e^{-\beta H}(\mathbb{1}+e^{-\beta H})^{-1}f)\ .$$

If there are no nonzero $f\in\mathfrak{h}$ invariant under $U_t=e^{itH}$, then

$$\lim_{\beta\to\infty}\omega_\beta(a^*(f)a(g))=(g,\,E_H(-\infty,0)f)\ ,$$

where E_H is the spectral family of H. Thus the KMS states converge in the weak*-topology to the unique ground state constructed in Example 5.3.20. Note that if $f,g\in\mathfrak{h}$ are invariant under U_t then

$$\omega_\beta(a^*(f)a(g))=(g,f)/2\ .$$

Thus the ω_β are trace-states on the CAR subalgebra over the subspace of U-invariant vectors.

The next proposition, which is similar to the previous one, is sometimes useful for proving existence of ground states and KMS states in C^*-dynamical systems which are thermodynamic limits. It also implies that if $\mathfrak{A}$ has an identity, the set of β such that (τ,β)-KMS states exist, for a given group τ, is a closed subset of $\mathbb{R}\cup\{\pm\infty\}$.

Proposition 5.3.25. *Let* $\mathfrak{A}$ *be a* C^**-algebra with identity* $\mathbb{1}$*, and* $\{\tau^n\}_{n\geq 1}$ *a sequence of strongly continuous one-parameter groups of* $*$*-automorphisms of* $\mathfrak{A}$ *converging strongly to a one-parameter group* τ*, i.e.,*

$$\lim_{n\to\infty} \|\tau_t^n(A) - \tau_t(A)\| = 0$$

for each $t \in \mathbb{R}$ and $A \in \mathfrak{A}$. Assume that there exists a (τ_t^n, β_n)-KMS state ω_n on $\mathfrak{A}$ for each n, where $\{\beta_n\}_{n\geq 1} \subseteq \mathbb{R} \cup \pm\infty$ converges to a $\beta \in \mathbb{R} \cup \{\pm\infty\}$, i.e.,

$$\lim_{n\to\infty} \beta_n = \beta .$$

It follows that each weak-limit point ω of the sequence $\{\omega_n\}$ is a (τ, β)-KMS state on $\mathfrak{A}$. In particular there exists a (τ, β)-KMS state on $\mathfrak{A}$.*

PROOF. Let δ_n be the generator of τ^n and δ the generator of τ. By Theorems 3.1.26 and 3.1.28 there exists for each $A \in D(\delta)$ a sequence $\{A_n\}_{n\geq 1}$ in $\mathfrak{A}$ such that

$$\lim_{n\to\infty} A_n = A , \qquad \lim_{n\to\infty} \delta_n(A_n) = \delta(A) .$$

Let ω_n be a (τ^n, β_n)-KMS state of $\mathfrak{A}$. Since $\mathfrak{A}$ has an identity, $E_{\mathfrak{A}}$ is compact in the weak*-topology, Theorem, 2.3.15. Thus there exists a subset $\{\omega_{n_\alpha}\}_\alpha$ of $\{\omega_n\}_n$ such that $n_\alpha \to \infty$ and ω_{n_α} converges to some state ω in the weak*-topology. We will show that ω is a (τ, β)-KMS state.

If $|\beta| < \infty$, we may assume that $|\beta_n| < \infty$ for all n, and by the auto-correlation lower bounds, Theorem 5.3.15,

$$-i\beta_{n_\alpha}\omega_{n_\alpha}(A_{n_\alpha}^*\delta_{n_\alpha}(A_{n_\alpha})) \geq \omega_{n_\alpha}(A_{n_\alpha}^* A_{n_\alpha}) \log\left(\frac{\omega_{n_\alpha}(A_{n_\alpha}^* A_{n_\alpha})}{\omega_{n_\alpha}(A_{n_\alpha} A_{n_\alpha}^*)}\right) .$$

Hence, by limiting

$$\begin{aligned} -i\beta\omega(A\delta(A)) &\geq \overline{\lim_\alpha}\left\{\omega_{n_\alpha}(A_{n_\alpha}^* A_{n_\alpha}) \log\left(\omega_{n_\alpha}(A_{n_\alpha}^* A_{n_\alpha})/\omega_{n_\alpha}(A_{n_\alpha} A_{n_\alpha}^*)\right)\right\} \\ &\geq \omega(A^*A)\log(\omega(A^*A)/\omega(AA^*)) \end{aligned}$$

where the last step uses the lower semi-continuity of $u, v \mapsto u\log(u/v)$.

If $\beta = +\infty$, we may either assume $\beta_{n_\alpha} = +\infty$ for all α, or $0 < \beta_{n_\alpha} < +\infty$ for all α. In the first case

$$-i\omega_{n_\alpha}(A_{n_\alpha}^*\delta(A_{n_\alpha})) \geq 0$$

for all α, and ω is a ground state by limiting. In the second case ω is a ground state essentially by the reasoning used in the proof of Proposition 5.3.23.

EXAMPLE 5.3.26. Let $\mathfrak{A}$ be a C^*-algebra with identity, ω a trace-state over $\mathfrak{A}$ such that $(\mathfrak{H}_\omega, \pi_\omega)$ is a faithful representation, and consider a sequence $H_n = H_n^* \in \mathfrak{A}$ such that

$$\delta(A) = \lim_{n\to\infty} i[H_n, A]$$

exists for all A in a dense *-subalgebra $D(\delta)_0$ of $\mathfrak{A}$. Now $\omega \circ \delta = 0$ and δ is closable by Proposition 3.2.26 and if the subspaces $(\imath \pm \delta)(D(\delta)_0)$ are dense in $\mathfrak{A}$, the closure $\overline{\delta}$ of δ is the generator of a group τ of *-automorphisms of $\mathfrak{A}$ by Corollary 3.2.57. If $\tau_t^n(A) = e^{itH_n}Ae^{-itH_n}$, then $\tau_t^n(A) \to \tau_t(A)$ uniformly for t in compacts, Theorem 3.1.28. Now

$$\omega_{\beta,n}(A) = \omega(e^{-\beta H_n}A)/\omega(e^{-\beta H_n})$$

is a (τ^n, β)-KMS state on $\mathfrak{A}$, since

$$\begin{aligned}\omega_{\beta,n}(AB) &= \omega(e^{-\beta H_n}AB)/\omega(e^{-\beta H_n})\\ &= \omega(e^{-\beta H_n}e^{\beta H_n}Be^{-\beta H_n}A)/\omega(e^{-\beta H_n}) = \omega_n(\tau^n_{-i\beta}(B)A)\end{aligned}$$

for all $A, B \in \mathfrak{A}$, and it is in fact not hard to see that this establishes a one-to-one correspondence between (τ^n, β)-KMS states and trace-states on $\mathfrak{A}$. By Proposition 5.3.25, $\mathfrak{A}$ has (τ, β)-KMS states for all $\beta \in \mathbb{R} \cup \{\pm\infty\}$.

Our fascination with KMS states throughout this section might mislead one into thinking that such states always exist. We conclude with an example which shows that this is not necessarily the case.

EXAMPLE 5.3.27. Our aim is to exhibit some C^*-dynamical systems $(\mathfrak{A}, \tau)$, where the $\mathfrak{A}$ are simple C^*-algebras with identity, and there exists a τ-KMS state at one and only one value $\beta \in \mathbb{R} \cup \{\pm\infty\}$. This state will be unique. Furthermore, this is possible both for finite and infinite β, and hence by rescaling of τ for any $\beta \in \mathbb{R} \cup \{\pm\infty\}$.

For $n = 2, 3, \ldots, +\infty$, let $\mathcal{O}_n$ be the C^*-algebra generated by a sequence $\{S_i\}_{i=1}^n$ of isometries

$$S_i^* S_i = \mathbb{1}; \quad i = 1, 2, \ldots \tag{1}$$

and if $n < +\infty$, assume that

$$\sum_{i=1}^{n} S_i^* S_i = \mathbb{1}\ . \tag{2.n}$$

If $n = +\infty$, assume that

$$\sum_{i=1}^{n} S_i S_i^* \leq \mathbb{1}; \quad k = 1, 2, \ldots. \tag{2.∞}$$

It can be proved (see Notes and Remarks) that if $\mathcal{O}_n'$ is another C^*-algebra generated by elements $S_i', i = 1 \ldots, n$ satisfying (1) and (2.n), then there exists a *-isomorphism $\alpha; \mathcal{O}_n \mapsto \mathcal{O}_n'$ such that $\alpha(S_i) = S_i'$. Hence $\mathcal{O}_n$ is uniquely determined up to *-isomorphism by relations (1) and (2.n), and by the arguments used in the uniqueness proofs of CARs and CCRs, Theorems 5.2.5 and 5.2.8, it follows that each $\mathcal{O}_n$ is a simple C^*-algebra. Now for each t

$$S_i' = \tau_t(S_i) = e^{it} S_i$$

satisfies (1) and (2.n), and hence τ_t extends uniquely to a *-automorphism of $\mathcal{O}_n$. (This is the only point in the argument at which we use the uniqueness of the $\mathcal{O}_n$. Alternatively one could regard each τ_t as a representation of relations (1) and (2.n), and then form the direct sum representation $\bigoplus_{s \in \mathbb{R}} \tau_s$. Trivially $(\bigoplus_{s \in \mathbb{R}} \tau_s)(S_i) \mapsto e^{it} \times (\bigoplus_{s \in \mathbb{R}} \tau_s)(S_i)$ defines a*-automorphism of the C^*-algebra $\mathcal{O}_n$ generated by this representation, and the remaining arguments do not change. Of course, the simplicity of $\mathcal{O}_n$ would need another proof.) Clearly $t \mapsto \tau_t$ is a strongly continuous one-parameter group, which is periodic with period 2π. Hence

$$\Phi(A) = \frac{1}{2\pi} \int_0^{2\pi} dt\ \tau_t(A)$$

defines a projection of norm one from $\mathcal{O}_n$ onto the fixed-point algebra $\mathcal{O}_n^\tau$ for τ.

We next analyze this fixed-point algebra. It follows immediately from (1) and (2.n) that

$$S_j^* S_i = \delta_{ij} \mathbb{1}; \quad i, j = 1, 2 \ldots, n \tag{3}$$

and hence each element in the *-algebra generated by $\{S_i\}_{i=1}^n$ is a linear combination of elements of the form

$$S_\mu S_\nu^* \ ,$$

where μ, ν are multiindices, e.g., $\mu = (j_1, \ldots, j_k), j_i \in \{1, 2, \ldots, n\}$, and

$$S_\mu = S_{j_1} S_{j_2} \ldots S_{j_k} \ .$$

Define the length of $\mu = (j_1, \ldots, j_k)$ as $L(\mu) = k$. Then

$$\tau_t(S_\mu S_\nu^*) = e^{it(L(\mu) - L(\nu))} S_\mu S_\nu^*$$

and hence

$$\Phi(S_\mu S_\nu^*) = \delta_{L(\mu), L(\nu)} S_\mu S_\nu^* \ .$$

It follows that $\mathcal{O}_n^\tau$ is just the closure of the linear combinations of elements of the form $S_\mu S_\nu^*$, where $L(\mu) = L(\nu)$. But if $L(\mu) = L(\nu) = L(\mu') = L(\nu')$ it follows from (3) that

$$S_\mu S_\nu^* S_{\mu'} S_{\nu'}^* = \delta_{\nu, \mu'} \, S_\mu S_{\nu'}^* \ ,$$

i.e., the set of $S_\mu S_\nu^*$ with $L(\mu) = L(\nu) = k$ form a set of $n^k \times n^k$ matrix units. It follows from (2.n) when $n < +\infty$ that these matrix units are linear combinations of n of the corresponding matrix units for $L(\mu) = L(\nu) = k + 1$, and hence $\mathcal{O}_n^\tau$ is a UHF-algebra, i.e., $\mathcal{O}_n^\tau$ is generated by an increasing sequence $\{\mathfrak{B}_k\}_{k \geq 1}$ of full $n^k \times n^k$ matrix algebras, all with the same unit. If $n = +\infty$, a variation of the argument above shows that $\mathcal{O}_\infty^\tau$ can be represented as follows: If $\mathfrak{H}$ is an infinite-dimensional separable Hilbert space, then $\mathcal{O}_\infty^\tau$ is the C^*-algebra on $\mathfrak{H} \otimes \mathfrak{H} \otimes \cdots$ generated by $\mathbb{1}$, $\mathscr{L}\mathscr{C}(\mathfrak{H}) \otimes \mathbb{1} \otimes \mathbb{1} \otimes \cdots, \mathscr{L}\mathscr{C}(\mathfrak{H} \otimes \mathfrak{H}) \otimes \mathbb{1} \otimes \cdots$, etc. It follows that $\mathcal{O}_n^\tau$ admits a unique tracial state which is faithful if $n < \infty$ and is a character if $n = +\infty$.

Now, let ω be a state on $\mathcal{O}_n$ which is a τ-KMS state at a finite value $\beta \in \mathbb{R}$. As

$$\omega(\tau_t(S_\mu S_\nu^*)) = e^{it(L(\mu) - L(\nu))} \omega(S_\mu S_\nu^*) \ ,$$

it follows from the τ-invariance of ω, Proposition 5.3.3, that $\omega(S_\mu S_\nu^*) = 0$ unless $L(\mu) = L(\nu)$. (Note that $\mathcal{O}_n$ does not admit any tracial state because of relations (1) and (2.n) and hence the case $\beta = 0$ is immediately excluded.) Now, Proposition 5.3.28 implies that the restriction of ω to $\mathcal{O}_n^\tau$ is a trace, which is faithful, since $\mathcal{O}_n$ is simple. This shows that $(\mathcal{O}_\infty, \tau)$ does not have any KMS states for finite values of β, and if $n < +\infty$ we have shown that

$$\omega(S_\mu S_\nu^*) = \delta_{\mu, \nu} \, n^{-L(\mu)} \tag{4}$$

(where $\delta_{\mu,\nu} = 0$ if $L(\mu) \neq L(\nu)$). Hence ω is unique, if it exists. But ω is a KMS state at value β if, and only if,

$$\omega(S_{\mu'} S_{\nu'}^* \tau_{i\beta}(S_\mu S_\nu^*)) = \omega(S_\mu S_\nu^* S_{\mu'} S_{\nu'}^*) \ ,$$

i.e.,

$$e^{-\beta(L(\mu) - L(\nu))} \omega(S_{\mu'} S_{\nu'}^* S_\mu S_\nu^*) = \omega(S_\mu S_\nu^* S_{\mu'} S_{\nu'}^*) \ .$$

It follows from (3) and (4) by tedious arguments that the left-hand side (LHS) of this equation is nonzero if, and only if, the right-hand side (RHS) is nonzero, and in this case

$$L(\mu') + L(\mu) = L(\nu') + L(\nu) \ .$$

Furthermore, when this condition is fulfilled, one has

$$\text{LHS} = e^{-\beta(L(\mu)-L(\nu))} \begin{cases} n^{-L(\nu)}, & \text{if } L(\mu) \geq L(\nu') \\ n^{-L(\mu')}, & \text{if } L(\mu) \leq L(\nu') \ , \end{cases}$$

$$\text{RHS} = \begin{cases} n^{-L(\nu')}, & \text{if } L(\mu') \geq L(\nu) \\ n^{-L(\mu)}, & \text{if } L(\mu') \leq L(\nu) \ . \end{cases}$$

But $L(\mu) + L(\mu') = L(\nu) + L(\nu')$ and hence $L(\mu) \geq L(\nu')$ if, and only if, $L(\mu') \leq L(\nu)$, etc. Hence it follows that the equation is satisfied if and only if

$$e^{-\beta(L(\mu)-L(\nu))} = n^{-(L(\mu)-L(\nu))}$$

for all μ, ν, i.e., if and only if,

$$\beta = \log n \ .$$

Now, assume $n < +\infty$ and let ω be a ground on $\mathcal{O}_n$. Then

$$t \mapsto \omega(S_i \tau_t(S_i^*)) = e^{-it}\omega(S_i S_i^*)$$

has a bounded analytic extension to the upper half-plane, and hence $\omega(S_i S_i^*) = 0$. But then

$$\omega(\mathbb{1}) = \sum_{i=1}^{n} \omega(S_i S_i^*) = 0$$

which is a contradiction. To show nonexistence of ceiling states for all n, one notes that

$$\tau \mapsto \omega(S_i^* \tau_t(S_i)) = e^{-it}\omega(\mathbb{1}) = e^{it}$$

does not have a bounded analytic extension to the lower half-plane. If $n = +\infty$, choose a representation for $\{S_i\}_{i=1}^{\infty}$ such that there exists a unit vector $\Omega \in R(S_i)^{\perp}$ for all i. If ω is the corresponding state, then

$$\omega(S_\mu S_\nu^*) = \begin{cases} 1, & \text{for } \mu = \nu = \varnothing, \quad (S_\mu S_\nu^* = \mathbb{1}) \\ 0, & \text{otherwise.} \end{cases}$$

It follows immediately that ω is a ground state. Conversely, it follows from the reasoning showing nonexistence of ground states for finite n that this is the only ground state.

Conclusion. The C^*-dynamical system $(\mathcal{O}_n, \tau)$, $n = 2, 3, ..., +\infty$ admits a (τ, β)-KMS state if, and only if, $\beta = \log n$, ($\beta = +\infty$ if $n = +\infty$). The corresponding KMS state is unique.

5.3.2. The Set of KMS States

The KMS condition originated as a characteristic of Gibbs equilibrium states in quantum statistical mechanics and for finite systems the condition com-

pletely characterizes the Gibbs states (see Example 5.3.31). This coincidence between KMS and Gibbs states appears to persist in many models after the thermodynamic limit. The ideal Fermi gas provides a specific example. Thus if a thermodynamic system is described by a C^*-dynamical system $(\mathfrak{A}, \tau)$ and one accepts the Gibbs formalism it is natural to interpret the set K_β of (τ, β)-KMS states as the set of equilibrium states at inverse temperature β. We will give more fundamental reasons for this interpretation later in this chapter and in the next chapter. If the model reflects the basic elements of physical reality one expects for high temperatures that K_β contains a unique element but at lower temperatures, i.e., larger β, it should contain many elements corresponding to the various thermodynamic phases and their possible mixtures. Our next intention is to analyze the set K_β with this interpretation in mind. In particular it is of interest to characterize the elements of K_β corresponding to pure phases and to examine the decomposition of a general $\omega \in K_\beta$ in terms of these special elements.

It is evident that the set K_β is a convex subset of the state space $E_{\mathfrak{A}}$ but it follows immediately from the auto-correlation lower bounds in Theorem 5.3.15 that this set is closed in the weak*-topology. Thus if $\mathfrak{A}$ has an identity, K_β is a convex subset of $E_{\mathfrak{A}}$ and consequently it is the convex closure of its extreme points. These extremal (τ, β)-KMS states appear as natural candidates for the description of pure thermodynamic phases and then the separation of phases coincides with the barycentric decomposition of KMS states.

In order to analyze K_β it is necessary to study the set of KMS states over an associated W^*-dynamical system $(\mathfrak{M}, \tau)$. We begin our analysis with a proposition which implies, among other things, that a nontrivial one-parameter group on an abelian algebra does not admit faithful KMS states. This indicates that the KMS condition is not an appropriate characterization of equilibrium for classical systems (see Notes and Remarks).

Proposition 5.3.28. *Let $\mathfrak{M}$ be a von Neumann algebra with a cyclic unit vector Ω, ω the corresponding state, and τ a σ-weakly continuous one-parameter group of *-automorphisms of $\mathfrak{M}$. Let*

$$\mathfrak{M}^\tau = \{A \in \mathfrak{M};\ \tau_t(A) = A \text{ for all } t \in \mathbb{R}\}$$

be the fixed-point algebra of τ and let

$$\mathfrak{C}_\omega = \{A \in \mathfrak{M};\ \omega(AB) = \omega(BA) \text{ for all } B \in \mathfrak{M}\}$$

be the centralizer of ω.

If ω is a τ-KMS state then it follows that

$$\mathfrak{C}_\omega = \mathfrak{M}^\tau.$$

In particular

$$\mathfrak{M} \cap \mathfrak{M}' \subseteq \mathfrak{M}^\tau$$

and if $\mathfrak{M}$ is abelian, one has $\tau_t = \iota$, for all $t \in \mathbb{R}$.

PROOF. If $A \in \mathfrak{M}^\tau$, then $A \in \mathfrak{M}_\tau$ and $\tau_i(A) = A$. Hence by the τ-KMS condition

$$\omega(BA) = \omega(AB)$$

for all $B \in \mathfrak{M}_\tau$, and by the density of $\mathfrak{M}_\tau$ in $\mathfrak{M}$ one concludes that $A \in \mathfrak{C}_\omega$.

Conversely, if $\omega(AB) = \omega(BA)$ for all $B \in \mathfrak{M}$, then

$$\omega(B\tau_t(A)) - \omega(\tau_t(A)B) = \omega(\tau_{-t}(B)A) - \omega(A\tau_{-t}(B)) = 0$$

because ω is τ-invariant, Proposition 5.3.3. Hence, if $F_{B,A}$ is the KMS function associated with the couple B, A, we have

$$F_{B,A}(t-i) = F_{B,A}(t),\ t \in \mathbb{R}\ .$$

Now, if $B \in \mathfrak{M}_\tau$, we have that

$$F_{B,A}(z) = \omega(\tau_{-z}(B)A)$$

by the edge of the wedge argument used in the proof of (3) $\Rightarrow$ (1) of Proposition 5.3.7. Hence $F_{B,A}$ has an entire analytic extension in this case. But as an entire analytic function it is determined by its restriction to $\mathbb{R}$. It follows that

$$F_{B,A}(z-i) = F_{B,A}(z)$$

for all $z \in \mathbb{C}$, i.e., $F_{B,A}$ is periodic with period i. As $F_{B,A}$ is bounded in the strip $-1 \leq \operatorname{Im} z \leq 0$, it follows that $F_{B,A}$ is bounded, and hence $F_{B,A}$ is constant by Liouville's theorem, i.e.,

$$(B^*\Omega, \tau_t(A)\Omega) = F_{B,A}(t) = F_{B,A}(0) = (B^*\Omega, A\,\Omega)\ .$$

Therefore as $\mathfrak{M}_\tau\Omega$ is dense in $\mathfrak{H}$,

$$\tau_t(A)\Omega = A\Omega$$

for all $t \in \mathbb{R}$. But Ω is separating for $\mathfrak{M}$ by Corollary 5.3.9, and therefore $\tau_t(A) = A$, i.e., $A \in \mathfrak{M}^\tau$, and $\mathfrak{C}_\omega = \mathfrak{M}^\tau$. The last statement of the proposition follows from the fact that

$$\mathfrak{M} \cap \mathfrak{M}' \subseteq \mathfrak{C}_\omega\ .$$

The next result is a key lemma in the analysis of K_β.

Proposition 5.3.29. *Let $\mathfrak{M}$ be a von Neumann algebra with a faithful normal state ω, σ_t the corresponding modular group, and φ any other normal state on $\mathfrak{M}$.*

The following statements are equivalent.

(1) *φ is a σ-KMS state.*

(2) *There exists a positive operator T affiliated with $\mathfrak{M} \cap \mathfrak{M}'$ such that*

$$\varphi(A) = \omega(T^{1/2}AT^{1/2})$$

for all $A \in \mathfrak{M}$.

If these statements are true, then T is unique.

In particular ω is the unique σ-KMS state on $\mathfrak{M}$ if, and only if, $\mathfrak{M}$ is a factor.

PROOF. We may assume the existence of a separating and cyclic vector Ω such that

$$\omega(A) = (\Omega, A\Omega)$$

for all $A \in \mathfrak{M}$. Let J and Δ be the modular conjugation and modular operator associated with $(\mathfrak{M}, \Omega)$, Definition 2.5.10.

(1) $\Rightarrow$ (2). Assume first that there exists a $\lambda > 0$ such that

$$\varphi \leq \lambda\omega \ .$$

By Theorem 2.3.19, there then exists a positive $T' \in \mathfrak{M}'$ such that

$$\varphi(A) = (\Omega, AT'\Omega) \ .$$

As φ is σ-KMS it is σ-invariant by Proposition 5.3.3. It follows that

$$\begin{aligned}(A\Omega, \Delta^{it}T'\Delta^{-it}B\Omega) &= (\Omega, \sigma_{-t}(A^*B)T'\Omega)\\ &= \varphi(\sigma_{-t}(A^*B))\\ &= \varphi(A^*B) = (A\Omega, T'B\Omega) \ ,\end{aligned}$$

for all $A, B \in \mathfrak{M}$ and hence

$$\Delta^{it}T'\Delta^{-it} = T'$$

for all $t \in \mathbb{R}$. Now, define

$$T = JT'J \ .$$

Then

$$\begin{aligned}T\Omega &= JT'\Omega\\ &= JT'\Delta^{-1/2}\Omega\\ &= J\Delta^{-1/2}T'\Omega = T'\Omega \ ,\end{aligned}$$

where the third equality follows from the strong commutation of T' and Δ that we have proved previously. The fourth stems from the fact that $J\Delta^{-1/2}A'\Omega = A'^*\Omega$ for $A' \in \mathfrak{M}'$, Proposition 2.5.11. It follows that

$$\varphi(A) = (\Omega, AT\Omega) = \omega(AT) \ ,$$

and it remains to prove that $T \in \mathfrak{M}'$. To this end, assume $A, B, C \in \mathfrak{M}_\sigma$ and use the KMS condition to compute

$$\begin{aligned}\omega(ATBC) &= \omega(\sigma_i(BC)AT)\\ &= \varphi(\sigma_i(BC)A)\\ &= \varphi(\sigma_i(B)\sigma_i(C)A)\\ &= \varphi(\sigma_i(C)AB)\\ &= \omega(\sigma_i(C)ABT) = \omega(ABTC) \ .\end{aligned}$$

It follows that B and T commute and hence $T \in \mathfrak{M}'$.

It φ is not bounded by a positive multiple of ω, we form the new state $\rho = (\omega + \varphi)/2$. As ρ is a σ-KMS state and faithful on $\mathfrak{M}$, it follows from the first part of the proof that there exist positive operators $T_1, T_2 \in \mathfrak{M} \cap \mathfrak{M}'$ such that

$$\omega(A) = \rho(AT_1) = \rho(T_1^{1/2}AT_1^{1/2}) \ ,$$
$$\varphi(A) = \rho(AT_2) = \rho(T_2^{1/2}AT_2^{1/2}) \ .$$

Since ω is faithful, the kernel of T_1 must be zero, and hence T_1^{-1} exists as a positive, possibly unbounded, operator affiliated with $\mathfrak{M}\cap\mathfrak{M}'$. Thus $T = T_2T_1^{-1}$ is a positive operator affiliated with $\mathfrak{M}\cap\mathfrak{M}'$. But then

$$\begin{aligned}\omega(T^{1/2}AT^{1/2}) &= \omega(T_1^{1/2}\,T_2^{1/2}\,AT_2^{1/2}\,T_1^{-1/2})\\ &= \rho(T_2^{1/2}AT_2^{1/2}) \ = \ \varphi(A)\end{aligned}$$

for all $A \in \mathfrak{M}$.

(2) $\Rightarrow$ (1). Approximating T strongly by an increasing sequence of positive, bounded elements in $\mathfrak{M}\cap\mathfrak{M}'$ we may assume that T is bounded. But then, if $A, B \in \mathfrak{M}_\tau$

$$\begin{aligned}\varphi(AB) &= \omega(ABT)\\ &= \omega(ATB)\\ &= \omega(\sigma_i(B)AT) = \varphi(\sigma_i(B)A) \ .\end{aligned}$$

The uniqueness of T follows because T and Δ commute strongly by Proposition 5.3.28, and hence

$$T^{1/2}\Omega \ = \ \Delta^{1/4}\,T^{1/2}\,\Omega \in \mathscr{P} \ ,$$

where $\mathscr{P}$ is the natural cone associated with the pair $\{\mathfrak{M}, \Omega\}$ by Proposition 2.5.26. But the representative vector for φ in this cone is unique, by Theorem 2.5.31, and hence $T \in (\mathfrak{M}\cap\mathfrak{M}')_+$ is unique.

The last statement of the proposition is now trivial.

We are now in a position to establish the principal affine properties of the set of KMS states of a C^*-dynamical system $(\mathfrak{A}, \tau)$. We will assume that $\mathfrak{A}$ possesses an identity but this does not lead to any essential loss of generality. If $\mathfrak{A}$ does not have an identity, one can introduce $\tilde{\mathfrak{A}} = \mathbb{C}\mathbb{1} + \mathfrak{A}$ and extend τ to $\tilde{\mathfrak{A}}$ by the definition

$$\tilde{\tau};\ (\alpha, A) \ \in \ \tilde{\mathfrak{A}} \mapsto \tilde{\tau}_t((\alpha, A)) \ = \ (\alpha, \tau_t(A)) \in \tilde{\mathfrak{A}} \ .$$

There is a one-to-one correspondence between states ω over $\mathfrak{A}$ and states $\tilde{\omega}$ over $\tilde{\mathfrak{A}}$ for which $\|\tilde{\omega}|_{\mathfrak{A}}\| = 1$. This correspondence is given by extension and restriction, i.e.,

$$\tilde{\omega}((\alpha, A)) \ = \ \alpha + \omega(A) \ .$$

Moreover, as $\tilde{\mathfrak{A}}_{\tilde{\tau}} = \mathbb{C}\mathbb{1} + \mathfrak{A}_\tau$ if follows by using an approximate identity as in the proof of Proposition 5.3.3 that this gives a one-to-one correspondence between the (τ, β)-KMS states of $(\mathfrak{A}, \tau)$ and the $(\tilde{\tau}, \beta)$-KMS states of the C^*-dynamical system $(\tilde{\mathfrak{A}}, \tilde{\tau})$ with $\|\tilde{\omega}|_{\mathfrak{A}}\| \ = \ 1$. The principal advantage in assuming the existence of an identity is that $E_{\mathfrak{A}}$ is compact in the weak*-topology.

Theorem 5.3.30. *Let $(\mathfrak{A}, \tau)$ be a C^*-dynamical system and assume that $\mathfrak{A}$ has an identity. For $\beta \in \mathbb{R}$ let K_β be the set of τ-KMS states at value β.*

It follows that:

(1) *K_β is convex and weak*-compact.*
(2) *K_β is a simplex*
(3) *$\omega \in K_\beta$ is an extremal point of K_β if, and only if, ω is a factor state.*
(4) *Let ω_1 and ω_2 be extremal points of K_β, then ω_1 and ω_2 are either equal or disjoint.*
(5) *If $\omega \in K_\beta$, the unique maximal measure on K_β corresponding to ω is identical to the central measure corresponding to ω.*

PROOF. If $\beta \neq 0$, we may assume $\beta = -1$ by rescaling τ. Moreover, we already proved (1) in the introductory remarks of this subsection.

(2) $R_+ K_{-1}$ is just the set of positive functionals on $\mathfrak{A}$ which satisfy the τ-KMS condition. If $\omega, \varphi \in \mathbb{R}_+ K_{-1}$, define $\rho = \omega + \varphi$. Since $\omega \leq \rho, \varphi \leq \rho$, it follows from Theorem 2.3.19 that ω and φ and π_ρ-normal, and Corollary 5.3.4 and Proposition 5.3.29 imply that there exist positive operators $T_1, T_2 \in \pi_\rho(\mathfrak{A})'' \cap \pi_\rho(\mathfrak{A})'$ such that

$$\omega(A) = \hat{\rho}(A(T_1)\ , \quad \varphi(A) = \hat{\rho}(AT_2)$$

for $A \in \mathfrak{A}$, where $\hat{\rho}$ is the normal extension of ρ to $\pi_\rho(\mathfrak{A})''$. As $\mathfrak{Z}_\rho = \pi_\rho(\mathfrak{A})'' \cap \pi_\rho(\mathfrak{A})'$ is abelian, the greatest lowest bound $T_1 \wedge T_2$ of T_1 and T_2 exists in $\mathfrak{Z}_\rho$. Define

$$(\omega \wedge \varphi)(A) = \hat{\rho}(A(T_1 \wedge T_2))$$

for $A \in \mathfrak{A}$. Then $\omega \wedge \varphi$ is a KMS positive functional by Proposition 5.3.29. If τ is a KMS positive functional such that $\tau \leq \omega$, $\tau \leq \varphi$, then $\tau \leq \rho$ and there exists a $T \in (\mathfrak{Z}_\rho)_+$ such that

$$\tau(A) = \hat{\rho}(AT)\ .$$

But as T, T_1, $T_2 \in \mathfrak{Z}_\rho$ it follows that

$$T \leq T_1\ , \qquad T \leq T_2\ ,$$

and hence

$$T \leq T_1 \wedge T_2\ .$$

Thus $\tau \leq \omega \wedge \varphi$, and so $\omega \wedge \varphi$ is a unique greatest lower bound of ω and φ in $\mathbb{R}_+ K_{-1}$. It follows that $\mathbb{R}_+ K_{-1}$ is a lattice, and K_{-1} is a simplex

(3) From Proposition 5.3.29 it follows that if $\omega \in K_{-1}$ is given, then the $\varphi \in \mathbb{R}_+ K_{-1}$ which are dominated by ω are of the form

$$\varphi(A) = \hat{\omega}(AT)\ ,$$

where $T \in \pi_\omega(\mathfrak{A})' \cap \pi_\omega(\mathfrak{A})''$ and $0 \leq T \leq \mathbb{1}$, and the correspondence between φ and T is one to one. Hence ω is extremal in K_{-1} if, and only if,

$$\pi_\omega(\mathfrak{A})'' \cap \pi_\omega(\mathfrak{A})' = \mathbb{C}\mathbb{1}\ .$$

(4) As ω_1 and ω_2 are factor states they are either quasi-equivalent or disjoint by the proof of Proposition 2.4.27. (Compare also Lemma 4.2.8). But if they are quasi-equivalent they are equal by Proposition 5.3.29.

(5) Let μ_K be the unique maximal measure on K_{-1} with barycenter ω, which exists by Theorem 4.1.15. Let μ_C be the central measure of ω, i.e., μ_C is the orthogonal measure in $M_\omega(E_{\mathfrak{A}})$ corresponding to $\pi_\omega(\mathfrak{A})'' \cap \pi_\omega(\mathfrak{A})'$. If $\mu \in M_\omega(K_{-1})$ is a measure of finite support, then $\mu = \sum_i \lambda_i \delta_{\omega_i}$ where $\lambda_i > 0$ and $\sum_i \lambda_i = 1$, and since

$b(\mu) = b(\mu_K) = \omega$ it follows that $\omega_i \leq \omega/\lambda_i$. By Proposition 5.3.29, there exist positive operators $T_i \in \pi_\omega(\mathfrak{A}'')\cap\pi_\omega(\mathfrak{A})'$ such that

$$\omega_i(A) = \hat{\omega}(AT_i) \;=\; (\Omega_\omega, \pi_\omega(A)T_i\Omega_\omega)\ .$$

Applying Lemma 4.1.26 and approximating T_i by a linear combination of spectral projections it is now simple to show that $\mu \prec \mu_C$ in the ordering of measures in $M_\omega(E\mathfrak{A})$. As μ_k can be approximated by finite support measures in $M_\omega(K_{-1})$, it follows that

$$\mu_K \prec \mu_C\ .$$

On the other hand, Lemma 4.1.26 implies that μ_C is a limit of finite support measures in $M_\omega(E_{\mathfrak{A}})$ of the form

$$\mu = \sum_i \lambda_i \delta_{\omega_i}\ ,$$

where

$$\omega_i(A) = \hat{\omega}(AP_i)$$

and P_i are projections in $\pi_\omega(\mathfrak{A})'' \cap \pi_\omega(\mathfrak{A})'$. But Proposition 5.3.29 then implies that $\omega_i \in K_{-1}$, and thus $\mu \prec \mu_K$, since μ_K is maximal in $M_\omega(K_{-1})$. Hence

$$\mu_C \prec \mu_K$$

and we conclude from Lemma 4.1.4 that

$$\mu_C = \mu_K\ .$$

The remaining case, $\beta = 0$, can be deduced from the above by remarking that K_0 is just the set of trace-states on $\mathfrak{A}$ and these are just the KMS states on $\mathfrak{A}$ for the trivial dynamics $\tau_t = \iota$.

Theorem 5.3.30 does not have an obvious analogue for W*-dynamical systems $(\mathfrak{M}, \tau)$ since τ is then strongly continuous if, and only if, it is norm-continuous (see Example 3.2.36). If one defines K_β as the set of normal states of $\mathfrak{M}$ which satisfy the τ-KMS condition at value β then K_β is a weakly closed convex subset of the normal states but it is not necessarily compact nor does it always have extremal points. For example, if the centre of $\mathfrak{M}$ has no minimal projections then K_β has no extremal points. The simplex property (2) is replaced by the property that if $\omega \in K_\beta$ and ρ is a state such that $\rho \leq \lambda\omega$ for some $\lambda > 0$ then $\rho \in K_\beta$ if and only if there is positive operator $T \in \mathfrak{M}\cap\mathfrak{M}'$ such that $\rho(A) = \omega(AT)$ for all $A \in \mathfrak{M}$. Properties (3) and (4) remain true whilst (5) no longer makes sense.

Theorem 5.3.30 has many interesting implications especially for the tentative physical interpretation of K_β as the set of equilibrium states, of the system $(\mathfrak{A}, \tau)$, at inverse temperature β. If K_β consists of one, and only one, state ω, this state is automatically a factor state. Thus if there is a unique equilibrium state, it is a factor state. This is of particular interest because we have already established that factor states can often be characterized by cluster properties which reflect the absence of long-range correlations, or the absence of large fluctuations for the values of space-averaged observables. In Section 2.6 we elaborated these characterizations for quasi-local algebras and in Section 4.3

for invariant states (see in particular, Example 4.3.24 and the discussion in the Notes and Remarks to Section 4.3). But the absence of correlations or large fluctuations is typical of pure thermodynamic phases and these various points all indicate that pure phases should correspond to factor states and more precisely to extremal KMS states. But if one adopts this interpretation, the simplex property of K_β has a clear significance.

Under suitable separability conditions, e.g., $\mathfrak{H}_\omega$ separable, the unique maximal measure μ_ω on K_β with barycenter $\omega \in K_\beta$ is concentrated on the extreme points $\mathscr{E}(K_\beta)$ of K_β. Thus ω is represented in a unique manner as a convex superposition of extremal KMS states. This decomposition then corresponds to the physical separation of an equilibrium state into pure thermodynamic phases. The symmetry, or lack of symmetry, of these phases is then automatically determined and phenomena of broken symmetry, as discussed in Section 4.3.4, occur if $\mathfrak{Z}_\omega$ is not pointwise invariant under the corresponding symmetry group.

Theorem 5.2.30 also has interest in the analysis of concrete models. In such applications one essentially reverses the foregoing reasoning. For example, if one can show that a particular model predicts a unique (τ, β)- KMS state, then this state is a factor state and has good cluster properties. In particular this demonstrates that the equilibrium states of the ideal Fermi gas described in Theorem 5.2.24 are factor states. This could also be deduced by direct construction of the corresponding representations as in Example 5.2.20 but in more complex models, such as the quantum spin systems discussed in Chapter 6, the direct construction is not possible and the abstract proof of factoriality and cluster properties is particularly convenient. On the other hand, for finite systems, one can again reverse the line of reasoning and deduce uniqueness from factoriality.

EXAMPLE 5.3.31. Let $\mathfrak{A} = M_n$ be the algebra of $n \times n$ matrices acting on the n-dimensional space $\mathfrak{H}_n$. For $H = H^* \in M_n$ define τ by

$$\tau_t(A) = e^{itH} A e^{-itH} ,$$

then the Gibbs state

$$\omega_\beta(A) = \frac{\mathrm{Tr}_{\mathfrak{H}_n}(e^{-\beta H} A)}{\mathrm{Tr}_{\mathfrak{H}_n}(e^{-\beta H})}$$

is a (τ, β)-KMS state but it is also the unique such state for the following reason. If ω is a second (τ, β)-KMS state and $\omega \neq \omega_\beta$, then $(\omega + \omega_\beta)/2 \in K_\beta$ but $(\omega + \omega_\beta)/2 \notin \mathscr{E}(K_\beta)$. Thus the mixed state $(\omega + \omega_\beta)/2$ is not a factor state. But all states over M_n are type-I factor states and this gives a contradiction. If $\mathfrak{A} = \mathscr{L}\mathscr{C}(\mathfrak{H})$ and $\mathfrak{H}$ is infinite dimensional, a similar argument yields uniqueness. It is, however, necessary to argue with the aid of the extension $\tilde{\mathfrak{A}} = \mathbb{C}\mathbb{1} + \mathfrak{A}$ of $\mathfrak{A}$ obtained by adjoining an identity.

Theorem 5.3.30 establishes that the unique decomposition of a KMS state ω into extremal KMS states coincides with the central decomposition and we have argued that this should be interpreted as the separation of ω into pure

thermodynamic phases. But there are other possible natural definitions of a pure phase and one might well suspect that purity corresponds to ergodicity among the τ-invariant states. Therefore, we next study conditions under which the KMS decomposition coincides with the ergodic decomposition of ω relative to τ. Once again a condition of asymptotic abelianness is of crucial importance.

Theorem 5.3.32 *Let $(\mathfrak{A}, \tau)$ be a C^*-dynamical system, assume that $\mathfrak{A}$ has an identity $\mathbb{1}$, and let K_β be the set of τ- KMS states at value β if $\beta \in \mathbb{R}\backslash\{0\}$, and K_0 the set of τ-invariant trace-states on $\mathfrak{A}$. Take $\omega \in K_\beta$, and let $\mu_K \in M_\omega(K_\beta)$ be the unique maximal measure with barycenter ω.*

The following conditions are equivalent:

(1) *There exists a unique maximal measure $\mu_E \in M_\omega(E_{\mathfrak{A}}^{\mathbb{R}})$, and*

$$\mu_E = \mu_K \ ,$$

where $E_{\mathfrak{A}}^{\mathbb{R}}$ denotes the τ-invariant states on $\mathfrak{A}$.

(2) *$\{\mathfrak{A}, \omega\}$ is weakly asymptotic abelian in mean in the sense that*

$$\lim_{T-S\to\infty} \frac{1}{T-S} \int_S^T dt\ \omega(A[\tau_t(B),\ C]D) = 0$$

for all A, B, C, $D \in \mathfrak{A}$.

(3) *$\{\mathfrak{A}, \omega\}$ is $\mathbb{R}$-central.*

In particular an extremal invariant $(\tau,\ \beta)$–KMS state ω is extremal invariant if, and only if

$$\lim_{T-S\to\infty} \frac{1}{T-S} \int_S^T dt\ \omega(A[\tau_t(B), C]D) = 0$$

for all A, B, C, $D \in \mathfrak{A}$, where $\beta \in \mathbb{R}$.

Proof. Let $\mathfrak{M} = \pi_\omega(\mathfrak{A})''$, and let $\hat{\omega}$ and $\hat{\tau}$ denote the normal extensions of ω and τ to $\mathfrak{M}$. If $\beta \neq 0$, then $\hat{\omega}$ satisfies the $\hat{\tau}$-KMS condition at β by Corollary 5.3.4 and hence Ω_ω is separating for $\mathfrak{M}$ by Corollary 5.3.9. If ω is a trace-state, $\hat{\omega}$ is a trace-state on $\mathfrak{M}$, and Ω_ω is again separating for $\mathfrak{M}$ by a simple application of Lemma 5.3.8. In any case $[\mathfrak{M}'\Omega_\omega] = \mathbb{1}$ by Proposition 2.5.3, and the Kovacs-Szücs theorem, Proposition 4.3.8, implies the existence of a unique normal G-invariant projection M from $\mathfrak{M}$ to $\mathfrak{M}^{\hat{\tau}}$ where $\mathfrak{M}^{\hat{\tau}} = \{A \in \mathfrak{M};\ \hat{\tau}_t(A) = A \text{ for all } t \in \mathbb{R}\}$.

Proposition 4.3.8 and Example 4.3.5 imply that

$$\begin{aligned} M(A)\Omega_\omega &= \lim_{T-S\to\infty} \frac{1}{T-S} \int_S^T dt\ U_\omega(t)A\Omega_\omega \\ &= \lim_{T-S\to\infty} \frac{1}{T-S} \int_S^T dt\ \hat{\tau}_t(A)\Omega_\omega \end{aligned}$$

for all $A \in \mathfrak{M}$ and in particular the limit exists.

But then

$$\begin{aligned} M(A)B'\Omega_\omega &= B'M(A)\Omega_\omega \\ &= \lim_{T-S\to\infty} B'\frac{1}{T-S}\int_S^T dt\ \hat{\tau}_t(A)\Omega_\omega \\ &= \lim_{T-S\to\infty} \frac{1}{T-S}\int_S^T dt\ \hat{\tau}_t(A)B'\Omega_\omega \end{aligned}$$

for all $B' \in \mathfrak{M}'$, and since the net $T-S \mapsto (T-S)^{-1}\int_S^T dt\ \hat{\tau}_t(A)$ is uniformly bounded, it follows that

$$M(A) = \lim_{S-T\to\infty} \frac{1}{T-S}\int_S^T dt\ \hat{\tau}_t(A)$$

exists in the strong operator topology. This ensures that the limit in condition (2) of the theorem always exists, and as $\mathfrak{M}'\Omega_\omega$ is dense in $\mathfrak{H}_\omega$ it follows from Definition 4.3.6 and Theorem 2.3.19 that conditions (2) and (3) are equivalent, and in fact both conditions are equivalent to

$$\mathfrak{M}^{\hat{\tau}} \subseteq \mathfrak{M} \cap \mathfrak{M}' . \tag{$*$}$$

If J and Δ are the modular conjugation and the modular operator associated with $\{\mathfrak{M}, \Omega\}$, one has

$$U_\omega(t)J\Delta^{1/2}A\Omega_\omega = U_\omega(t)A^*\Omega_\omega = \hat{\tau}_t(A)^*\Omega_\omega = J\Delta^{1/2}U_\omega(t)A\Omega_\omega$$

for $A \in \mathfrak{M}$, and from the uniqueness of the polar decomposition $S = J\Delta^{1/2}$ it follows that $U_\omega(t)J = JU_\omega(t)$ for all $t \in \mathbb{R}$. It follows that $(*)$ is equivalent to

$$\begin{aligned} \mathfrak{M}'^{\hat{\tau}} = \mathfrak{M}' \cap U_\omega(\mathbb{R})' &= J(\mathfrak{M} \cap U_\omega(\mathbb{R})')J \\ &\subseteq J(\mathfrak{M} \cap \mathfrak{M}')J \ = \ \mathfrak{M} \cap \mathfrak{M}' . \end{aligned} \tag{$**$}$$

By Proposition 4.3.3 this is, however, equivalent to $M_\omega(E_{\mathfrak{A}}^{\mathbb{R}})$ containing a unique maximal measure μ_E, which is subcentral, i.e.,

$$\mu_E \prec \mu_C ,$$

where μ_C is the central measure. Now, if $\beta \neq 0$, then $\mu_K = \mu_C$ by Theorem 5.3.30 and since trivially $\mu_K \prec \mu_E$, it follows that

$$\mu_K = \mu_E .$$

If $\beta = 0$, note that for any projection $E \in \mathfrak{M}'^{\hat{\tau}}$ we have that

$$A \in \mathfrak{A} \mapsto (\Omega_\omega, AE\Omega_\omega)$$

is a τ-invariant trace on $\mathfrak{A}$, and it follows as in the proof of Theorem 5.3.30 that the extremal decomposition coincides with the decomposition into invariant traces, i.e.,

$$\mu_K = \mu_E .$$

Conversely Theorem 5.3.30 implies that $\mu_K = \mu_C$ for $\beta \neq 0$, while $\mu_k \prec \mu_C$ for $\beta = 0$ since μ_K is dominated by the measure corresponding to the tracial decomposition, and the latter measure is equal to μ_C by Theorem 5.3.30 applied in the case $\tau = \imath$.

The last statement of the theorem follows from the fact that $\omega \in \mathscr{E}(K_\beta)$ is extremal invariant if, and only if,

$$\mu_E = \mu_K = \delta_\omega .$$

Remark 1. In the course of the above proof it was established that condition (2) and condition (3) are equivalent for any τ-invariant state ω such that Ω_ω is separating for $\pi_\omega(\mathfrak{A})''$. This gives a version of Theorem 4.3.14 in the case that Ω_ω is separating and $G = \mathbb{R}$.

Remark 2. An immediate consequence of Theorem 5.3.32 is the following global statement concerning the set K_β of KMS states at value $\beta \in \mathbb{R}$. (We adopt the convention that K_0 is the set of τ-invariant traces.)

The following conditions are equivalent for each fixed $\beta \in \mathbb{R}$.

(1) *K_β is a face in $E^{\mathbb{R}}_{\mathfrak{A}}$,*
(2) *$(\mathfrak{A}, \omega)$ is weakly asymptotically abelian in mean for all $\omega \in K_\beta$,*
(3) *$(\mathfrak{A}, \omega)$ is $\mathbb{R}$-central for all $\omega \in K_\beta$.*

We only have to show that (1) is equivalent to

(1′) *For each $\omega \in K_\beta$ there exists a unique maximal measure $\mu_E \in M_\omega(E^{\mathbb{R}}_{\mathfrak{A}})$, and*

$$\mu_E = \mu_K$$

where μ_K is the unique maximal measure in $M_\omega(K_\beta)$.

Since K_β is a simplex, this is again equivalent to

(1″) *For each $\omega \in K_\beta$ and each maximal measure $\mu \in M_\omega(E^{\mathbb{R}}_{\mathfrak{A}})$ one has*

$$\mu(K_\beta) = 1\,.$$

((1′) clearly implies (1″) but (1″) and the simplex property of K_β imply that each pair of maximal measures in $M_\omega(E^{\mathbb{R}}_{\mathfrak{A}})$ must coincide.) The equivalence between (1) and (1″) is a general characterization of closed faces in compact convex sets, and is proved as follows.

(1) $\Rightarrow$ (1″). If μ is any measure in $M_\omega(E^{\mathbb{R}}_{\mathfrak{A}})$, there exists a net $\mu_\alpha \in M_\omega(E^{\mathbb{R}}_{\mathfrak{A}})$ of measures with finite support converging in the weak*-topology to μ, by Proposition 4.1.1. But $\mu_\alpha(K_\beta) = 1$ by the facial property of K_β, and hence $\mu(K_\beta) = 1$.

(1″) $\Rightarrow$ (1). Assume that $\omega \in K_\beta$, and that

$$\omega = \sum_{i=1}^{n} \lambda_i \omega_i$$

is a convex decomposition of ω with $\omega_i \in E^{\mathbb{R}}_{\mathfrak{A}}$. We have to show that $\omega_i \in K_\beta$. Let $\mu \in M_\omega(E^{\mathbb{R}}_{\mathfrak{A}})$ be a maximal measure such that

$$\sum_{i=1}^{n} \lambda_i \delta_{\omega_i} \prec \mu\ .$$

By the Cartier – Fell – Meyer theorem, Proposition 4.2.1, there exist measures $\mu_i \in M_{\omega_i}(E^{\mathbb{R}}_{\mathfrak{A}})$ such that

$$\mu = \sum_{i=1}^{n} \lambda_i \mu_i \ .$$

But as $\mu(K_\beta) = 1$ by assumption (1″) it follows that $\mu_i(K_\beta) = 1$ for $i = 1, \ldots, n$ and hence

$$\omega_i = \int d\mu_i(\omega')\omega' \in K_\beta \ .$$

It follows that K_β is a face in $E_{\mathfrak{A}}^{\mathbb{R}}$.

Remark 3. In the preceding remark we saw that K_β is a face in $E_{\mathfrak{A}}^{\mathbb{R}}$ under quite general circumstances when $\beta \in \mathbb{R}$, but K_β is very seldom a face in $E_{\mathfrak{A}}$, i.e., *the following conditions are equivalent:*

(1) *K_β is a face in $E_{\mathfrak{A}}$.*
(2) *$\pi_\omega(\mathfrak{A})$ is abelian for all $\omega \in K_\beta$*

(Here we use the convention that K_0 is the set of all trace states.)

(1) $\Rightarrow$ (2). Let $\omega \in K_\beta$ and let T be a positive element in $\pi_\omega(\mathfrak{A})'$. The positive linear functional

$$\omega_T(A) = (T\Omega_\omega, \pi_\omega(A)\Omega_\omega)\,, \quad A \in \mathfrak{A}\,,$$

is dominated by a positive multiple of ω, by Theorem 2.3.19, and condition (1) implies that $\omega_T/\|\omega_T\|$ is in K_β. It follows from Proposition 5.3.29 that $T \in \pi_\omega(\mathfrak{A})' \cap \pi_\omega(\mathfrak{A})''$, and we have proved that

$$\pi_\omega(\mathfrak{A})' \subseteq \pi_\omega(\mathfrak{A})' \cap \pi_\omega(\mathfrak{A})'' \ .$$

Since $\pi_\omega(\mathfrak{A})''$ is anti-isomorphic to $\pi_\omega(\mathfrak{A})'$ by the Tomita-Takesaki theorem, it follows that $\pi_\omega(\mathfrak{A})$ is abelian.

(2) $\Rightarrow$ (1). If $\omega \in K_\beta$ is such that $\pi_\omega(\mathfrak{A})$ is abelian, one has that

$$\pi_\omega(\mathfrak{A})'' = \pi_\omega(\mathfrak{A})' = \pi_\omega(\mathfrak{A})'' \cap \pi_\omega(\mathfrak{A})'$$

and hence all states dominated by a multiple of ω are (τ, β)-KMS states by Theorem 2.3.19 and Proposition 5.3.29. It follows that K_β is a face in $E_{\mathfrak{A}}$.

We shall see later that K_∞ always is a face of $E_{\mathfrak{A}}$, Theorem 5.3.37.

Next we examine various relationships between automorphisms and KMS states. In physical applications the automorphisms correspond to symmetry transformations and thus the following result gives information concerning symmetry properties of equilibrium states.

In Proposition 5.3.29 we proved that if σ is a one-parameter group of *-automorphisms of a von Neumann algebra $\mathfrak{M}$, then the set of σ-KMS states is affinely isomorphic with the set of normal states on a hereditary subalgebra of the center of $\mathfrak{M}$. This implies various relations between automorphisms and KMS states.

Proposition 5.3.33. *Let $(\mathfrak{M}, \sigma)$ be a W^*-dynamical system, and ω a faithful normal state on $\mathfrak{M}$ satisfying the (σ, β) -KMS condition, for some $\beta \in \mathbb{R}$. Let α be a *-automorphism of $\mathfrak{M}$.*

It follows that:

(1) *$\omega \circ \alpha$ is a $(\alpha^{-1}\sigma\alpha, \beta)$-KMS state on $\mathfrak{M}$.*
(2) *If $\omega \circ \alpha = \omega$ and $\beta \neq 0$ then $\alpha\sigma_t = \sigma_t\alpha$ for all $t \in \mathbb{R}$.*
(3) *If $\alpha\sigma_t = \sigma_t\alpha$ for all $t \in \mathbb{R}$ then $\omega \circ \alpha$ is (α, β)-KMS.*
(4) *If $\alpha\sigma_t = \sigma_t\alpha$ for all $t \in \mathbb{R}$, $\alpha|_{\mathfrak{M} \cap \mathfrak{M}'}$ is the identity and $\beta \neq 0$, then $\omega \circ \alpha = \omega$.*

Proof. (1) If $A, B \in \mathfrak{M}$, then by applying Proposition 5.3.7 to the pair $\alpha(A), \alpha(B)$, we obtain a function F in $C_b(\overline{\mathfrak{D}}_\beta)$, analytic in $\mathfrak{D}_\beta$ such that

$$F(t) = \omega(\alpha(A)\sigma_t(\alpha(B))) = \omega \circ \alpha(A(\alpha^{-1}\sigma_t\alpha)(B)) \ ,$$
$$F(t + i\beta) = \omega(\sigma_t(\alpha(B))\alpha(A)) = \omega \circ \alpha((\alpha^{-1}\sigma_t\alpha)(B)A) \ .$$

Hence $\omega \circ \alpha$ is a $(\alpha^{-1}\sigma\alpha, \beta)$-KMS state by the same proposition.

(2) follows from the uniqueness of the β-KMS group associated with ω, Theorem 5.3.10, and (1).

(3) is an immediate consequence of (1).

(4) It follows from (3) and Proposition 5.3.29 that

$$(\omega \circ \alpha)(A) = \omega(T^{1/2}AT^{1/2})$$

for all $A \in \mathfrak{M}$, where T is a positive operator affiliated with $\mathfrak{Z} = \mathfrak{M} \cap \mathfrak{M}'$. In particular

$$\omega(A) = \omega(T^{1/2}AT^{1/2})$$

for $A \in \mathfrak{Z}$. But if $\mathfrak{Z} = C(K)$ is the Gelfand representation of $\mathfrak{Z}$, there exists by the Riesz representation theorem a unique probability Radon measure μ on the compact Hausdorff space K such that

$$\omega(A) = \int_K d\mu(x)\hat{A}(x) \ ,$$

where $A \mapsto \hat{A}$ is the Gelfand transform. But then

$$\int_K d\mu(x)\hat{A}(x) = \int_K d\mu(x)\hat{T}(x)\hat{A}(x)$$

for all $A \in \mathfrak{Z}$, and hence $\hat{T} = 1$ by the uniqueness of μ. Thus

$$\omega \circ \alpha = \omega \ .$$

The statements (1)–(3) of Proposition 5.3.33 are also true for C^*-dynamical systems $(\mathfrak{A}, \tau)$ by the same reasoning. If α is a symmetry of the system, i.e., a *-automorphism of $\mathfrak{A}$ which commutes with τ, and if ω is a (τ, β)-KMS state then $\omega \circ \alpha$ is also a (τ, β)-KMS state. If $\omega \circ \alpha \neq \omega$ the symmetry is said to be broken by ω. The following theorem states that under some apparently general circumstances symmetries are not broken.

Theorem 5.3.33A (Fannes–Vanheuverzwijn–Verbeure). *Let* $(\mathfrak{A}, \tau)$ *be a* C^**-dynamical system,* δ *the generator of* τ, ω *a* (τ, β)*-KMS state of* $\mathfrak{A}$ *with* $\beta \in \mathbb{R}$ *and* α *a* **-automorphism of* $\mathfrak{A}$ *such that* $\alpha\tau_t = \tau_t\alpha$ *for all* $t \in \mathbf{R}$. *Assume there exists a sequence of unitaries* $U_n \in D(\delta)$ *such that*

$$\alpha(A) = \lim_{n\to\infty} U_n A U_n^*$$

for all $A \in \mathfrak{A}$ *and*

$$\sup_n \|\delta(U_n)\| < \infty \ .$$

It follows that

$$\omega \circ \alpha = \omega \ ,$$

i.e., the symmetry α *is not broken by* ω.

PROOF. Replacing τ_t by τ_{-t} if necessary we may assume $\beta \geq 0$. But the case $\beta = 0$ is trivial so we may assume $\beta > 0$.

OBSERVATION 1. *Let* $I = [a, b]$ *be a finite interval in* $\hat{\mathbb{R}} = \mathbb{R}$ *and assume that the* τ*-spectrum* $\sigma_\tau(A) \subseteq I$. *It follows that*

$$0 \leq -i\beta\omega(A^*\delta(A)) - \omega(A^*A)\log(\omega(A^*A)/\omega(AA^*)) \leq \beta(b-a)\omega(A^*A) \ .$$

PROOF. The first inequality is the auto-correlation lower bound of Theorem 5.3.15. For the second inequality note that the spectral restriction on A implies that the measure

$$d\mu_A(\lambda) = (\pi_\omega(A)\Omega_\omega, dE(\lambda)\pi_\omega(A)\Omega_\omega)$$

introduced prior to Proposition 5.3.14 is supported on I. Therefore this proposition implies that

$$\begin{aligned}
&-i\beta\omega(A^*\delta(A)) - \omega(A^*A)\log(\omega(A^*A)/\omega(AA^*)) \\
&\qquad = \beta(\pi_\omega(A)\Omega_\omega, H_\omega\pi_\omega(A)\Omega_\omega) - \omega(A^*A)\log(\omega(A^*A)/\omega(AA^*)) \\
&\qquad = -\beta\int_a^b d\mu_A(\lambda)\lambda - \int_a^b d\mu_A(\lambda)\log\left(\int_a^b d\mu_A(\lambda)\Big/\int_a^b d\mu_A(\lambda)e^{\beta\lambda}\right) \\
&\qquad \leq -a\beta\int_a^b d\mu_A(\lambda) - \int_a^b d\mu_A(\lambda)\log\left(\int_a^b d\mu_A(\lambda)\Big/\int_a^b d\mu_A(\lambda)e^{\beta b}\right) \\
&\qquad = \beta(b-a)\int_a^b d\mu_A(\lambda) = \beta(b-a)\omega(A^*A) \ .
\end{aligned}$$

OBSERVATION 2. *There exists a* $C > 0$ *such that*

$$\omega(AA^*) \leq C\,\omega(\alpha(AA^*))$$

for all $A \in \mathfrak{A}$.

PROOF. Set $K = \sup_n \|\delta(U_n)\|$. If $A \in \mathfrak{A}$ has bounded τ-spectrum we can find a finite sequence h_n of positive C^∞-functions on $\hat{\mathbb{R}} = \mathbb{R}$, each with compact support in an interval of length at most one, such that $\sum_n h_n^2 = 1$ in a neighborhood of $\sigma_\tau(A)$. Define

$$A_n = \int dt\, \hat{h}_n(-t)\tau_t(A) \ .$$

Then

$$\omega(AA^*) = \int d\nu_A(-\lambda) = \sum_n \int d\nu_A(-\lambda) h_n(\lambda)^2 = \sum_n \omega(A_n A_n^*) \ .$$

For each n such that $A_n \neq 0$ we now apply the auto-correlation lower bound to $U_m A_n$ to obtain the first of the following inequalities:

$$\begin{aligned}
&\omega(A_n^* A_n) \log(\omega(A_n A_n^*)/\omega(U_m A_n A_n^* U_m^*)) + i\beta\, \omega(A_n^* U_m^* \delta(U_m) A_n) \\
&\qquad = \omega(A_n^* A_n) \log(\omega(A_n^* A_n)/\omega(U_m A_n A_n^* U_m^*)) + i\beta\omega(A_n^* U_m^* \delta(U_m A_n)) \\
&\qquad - i\beta\omega(A_n^* \delta(A_n)) - \omega(A_n^* A_n) \log(\omega(A_n^* A_n)/\omega(A_n A_n^*)) \\
&\qquad \leq -i\beta\omega(A_n^* \delta(A_n)) - \omega(A_n^* A_n) \log(\omega(A_n^* A_n)/\omega(A_n A_n^*)) \\
&\qquad \leq \beta\, \omega(A_n^* A_n) \ .
\end{aligned}$$

The second inequality follows from Observation 1. But

$$|i\beta\omega(A_n^* U_m^* \delta(U_m) A_n)| \leq \beta\, \|\delta(U_m)\| \omega(A_n^* A_n) \leq \beta\, K\omega(A_n^* A_n)$$

so from the previous inequality

$$\log(\omega(A_n^* A_n)/\omega(U_m A_n A_n^* U_m^*)) \leq \beta(K+1)$$

or

$$\omega(A_n^* A_n) \leq C\omega(U_m A_n A_n^* U_m^*)$$

where $C = \exp(\beta(K+1))$. Now taking the limit $m \to \infty$ one obtains

$$\omega(A_n^* A_n) \leq C\omega(\alpha(A_n A_n^*)) \ .$$

But as $[\alpha, \tau_t] = 0$, $\alpha(A_n) = (\alpha(A))_n$ so adding these inequalities over n one finds

$$\omega(A^* A) \leq C\omega(\alpha(AA^*)) \ .$$

Since the elements with bounded τ-spectrum are dense in $\mathfrak{A}$, by Lemma 3.2.39 (4), this inequality extends to all $A \in \mathfrak{A}$, and Observation 2 follows.

END OF PROOF OF THEOREM 5.3.33A: It is sufficient to prove $\omega \circ \alpha = \omega$ for extremal (τ, β)-KMS states ω. But then $\omega \circ \alpha$ is an extremal (τ, β)-KMS state. By Observation 2 and Theorem 2.3.19, ω is a normal state in the representation defined by $\omega \circ \alpha$. But as $\omega \circ \alpha$ is a factor state, by Theorem 5.3.30 (3), it follows from Proposition 5.3.29 (or the simplex property of K_β) that $\omega = \omega \circ \alpha$. This completes the proof of the theorem.

Any normal faithful state of a von Neumann algebra $\mathfrak{M}$ is a KMS state for a unique automorphism group of $\mathfrak{M}$, by Theorem 5.3.10. The converse is not true however; an automorphism group does not necessarily have KMS states. Proposition 5.3.28 implies, for example, that if τ is an automorphism group

which allows a faithful KMS state, then τ leaves the center of $\mathfrak{M}$ pointwise fixed. Even this condition on τ is not sufficient however, by the following theorem, which states that any two groups which allow faithful KMS states are related by an inner cocycle. This theorem is a partial restatement of Theorem 2.7.16.

Theorem 5.3.34 (Connes). *Let ω and φ be faithful normal states on a von Neumann algebra $\mathfrak{M}$, and let σ^ω and σ^φ be the corresponding modular groups. It follows that there exists a strongly continuous one-parameter family $t \mapsto \Gamma_t$ of unitaries in $\mathfrak{M}$ such that*

$$\sigma_t^\varphi(A) = \Gamma_t \sigma_t^\omega(A) \Gamma_t^* \ ,$$
$$\Gamma_{t+s} = \Gamma_t \sigma_t^\omega(\Gamma_s) \ ,$$

for all $A \in \mathfrak{M}$, and all $s, t \in \mathbb{R}$.

Proof. Define a faithful normal state ρ on $\mathfrak{M} \otimes M_2$ by

$$\rho\left(\begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix}\right) = \frac{1}{2}(\omega(A_{11}) + \varphi(A_{22})) \ .$$

Let σ^ρ be the modular group associated with ρ. As

$$\rho\left(\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}\begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix}\right) = \frac{1}{2}\omega(A_{11}) = \rho\left(\begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}\right)$$

it follows from Proposition 5.3.28 that

$$\sigma_t^\rho\left(\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}\right) = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

for all $t \in \mathbb{R}$. The same is true for $\left(\begin{smallmatrix} 0 & 0 \\ 0 & 1 \end{smallmatrix}\right)$ and hence σ^ρ leaves the subalgebra

$$\mathfrak{M} \oplus \mathfrak{M} = \left\{\begin{pmatrix} A_{11} & 0 \\ 0 & A_{22} \end{pmatrix} \ ; \quad A_{ii} \in \mathfrak{M}\right\}$$

invariant. But ρ satisfies the KMS condition with respect to the automorphism group defined by

$$\begin{pmatrix} A_{11} & 0 \\ 0 & A_{22} \end{pmatrix} \mapsto \begin{pmatrix} \sigma_t^\omega(A_{11}) & 0 \\ 0 & \sigma_t^\varphi(A_{22}) \end{pmatrix} \ .$$

Therefore, it follows from the uniqueness statement of Theorem 5.3.10 that

$$\sigma_t^\rho\left(\begin{pmatrix} A_{11} & 0 \\ 0 & A_{22} \end{pmatrix}\right) = \begin{pmatrix} \sigma_t^\omega(A_{11}) & 0 \\ 0 & \sigma_t^\varphi(A_{22}) \end{pmatrix}$$

Now, from the relations

$$\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} = 0 = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \ ,$$

it follows that

$$\sigma_t^\rho\left(\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}\right)\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} = 0 = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}\sigma_t^\rho\left(\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}\right)$$

and hence there exists a σ-weakly continuous one-parameter family $t \mapsto \Gamma_t \in \mathfrak{M}$ determined by

$$\begin{pmatrix} 0 & 0 \\ \Gamma_t & 0 \end{pmatrix} = \sigma_t^\rho\left(\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}\right) .$$

Applying σ_t^ρ to the relation

$$\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}^* + \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}^*\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} = \mathbb{1} ,$$

it follows that

$$\Gamma_t\Gamma_t^* = \mathbb{1} = \Gamma_t^*\Gamma_t ,$$

i.e., each Γ_t is unitary.

Similarly, from

$$\begin{pmatrix} 0 & 0 \\ 0 & A \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} A & 0 \\ 0 & 0 \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} ,$$

it follows that

$$\sigma_t^\varphi(A) = \Gamma_t\sigma_t^\omega(A)\Gamma_t^* .$$

Finally,

$$\begin{aligned}\begin{pmatrix} 0 & 0 \\ \Gamma_{t+s} & 0 \end{pmatrix} &= \sigma_{t+s}^\rho\left(\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}\right) = \sigma_t^\rho\left(\begin{pmatrix} 0 & 0 \\ \Gamma_s & 0 \end{pmatrix}\right) \\ &= \sigma_t^\rho\left(\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}\right)\sigma_t^\rho\left(\begin{pmatrix} \Gamma_s & 0 \\ 0 & 0 \end{pmatrix}\right) = \begin{pmatrix} 0 & 0 \\ \Gamma_t\sigma_t^\omega(\Gamma_s) & 0 \end{pmatrix} .\end{aligned}$$

We conclude the analysis of (τ, β)-KMS states for finite β with an examination of disjointness properties.

In Theorem 2.7.17 we stated, and sketched a proof, that a von Neumann algebra $\mathfrak{M}$ with a faithful normal state ω is purely infinite, or type-III, if, and only if, $\sigma^\omega|_{\mathfrak{M}E}$ is not an inner group of automorphisms of $\mathfrak{M}E$ for any nonzero projection E in the center $\mathfrak{M} \cap \mathfrak{M}'$. In fact it is this latter characterization of type-III von Neumann algebras which is most useful in proving that a given von Neumann algebra is type-III, and for our purposes it could be taken as a definition.

Theorem 5.3.34 shows that this definition is independent of the particular choice of faithful, normal state ω. The next theorem shows that the (τ, β)-KMS states are highly sensitive to variations of the temperature, i.e., variations of β.

Theorem 5.3.35. *Let $(\mathfrak{A}, \tau)$ be a C^*-dynamical system, and suppose that ω_1 and ω_2 are KMS-states corresponding to two different values $\beta_1, \beta_2 \in \mathbb{R}$. Assume that $\pi_{\omega_1}(\mathfrak{A})''$ is a type-III von Neumann algebra.*

It follows that the states ω_1 and ω_2 are disjoint.

Proof. Recall from the beginning of Section 4.2.2 that ω_1 and ω_2 are disjoint if, and only if, π_{ω_1} and π_{ω_2} have no quasi-equivalent subrepresentations. Suppose

ad absurdum that π_{ω_1} and π_{ω_2} have quasi-equivalent subrepresentations. Then it follows from Theorem 2.4.26 that there exist projections $E_i \in \mathfrak{Z}_{\omega_i} = \pi_{\omega_i}(\mathfrak{A})'' \cap \mathfrak{A}' \pi_{\omega_i}(\mathfrak{A})'$ and an isomorphism $\alpha; \pi_{\omega_1}(\mathfrak{A})'' E_1 \mapsto \pi_{\omega_2}(\mathfrak{A})'' E_2$ such that $\alpha(\pi_{\omega_1}(A)E_1) = \pi_{\omega_2}(A)E_2$.

Now $\beta_1 \neq 0$ because if $\beta_1 = 0$ then $\hat{\omega}_1$ would be a finite trace on $\pi_{\omega_1}(\mathfrak{A})''$, contradicting the type-III assumption. If $\beta_2 = 0$ then $\pi_{\omega_1}(\mathfrak{A})'' E_1$ would be properly infinite and $\pi_{\omega_2}(\mathfrak{A})'' E_2$ finite, a contradiction. Hence we may assume $\beta_2 \neq 0$. By Corollary 5.3.4 it follows that τ extends to groups $\hat{\tau}^i$ on $\pi_{\omega_i}(\mathfrak{A})''$ with respect to which the normal extensions $\hat{\omega}_i$ satisfy the $(\hat{\tau}^i, \beta_i)$-KMS conditions. By Proposition 5.3.28 it follows that $\hat{\tau}^1_t(E_1) = E_1$ for all t, and hence τ^1 defines an automorphism group σ on $\mathfrak{M} = \pi_{\omega_1}(\mathfrak{A})'' E_1$ such that

$$\sigma_t(\pi_{\omega_1}(A)E_1) = \pi_{\omega_1}(\tau_t(A))E_1$$

for $A \in \mathfrak{A}, t \in \mathbb{R}$.

Next, Proposition 5.3.33 implies that the faithful normal states φ_i defined on $\mathfrak{M}$ by

$$\varphi_1(A) = \frac{\hat{\omega}_1(A)}{\hat{\omega}_1(E_1)} \quad , \quad \varphi_2(A) = \frac{\hat{\omega}_2(\alpha(A))}{\hat{\omega}_2(E_2)} \quad ,$$

for $i = 1, 2$, satisfy the (σ, β_i)-KMS condition. This follows because

$$\sigma_t(A) = (\alpha^{-1}\, \hat{\tau}^2_t \alpha)(A)$$

for $A \in \mathfrak{M}$. Theorem 5.3.10 then implies

$$t \mapsto \sigma_{-\beta_i t} \equiv \sigma^i_t$$

is the modular group for $\omega_i, i = 1, 2$. Hence, by Theorem 5.3.34 there exists a unitary cocycle Γ in $\mathfrak{M}$ such that

$$\sigma^2_t(A) = \Gamma_t \sigma^1_t(A) \Gamma^*_t$$

for all $t \in \mathbb{R}$. As the state φ_1 is both σ^1- and σ^2-invariant, it follows that

$$\varphi_1(A\Gamma_t) = \varphi_1(\sigma^2_t \sigma^1_{-t}(A\Gamma_t)) = \varphi_1(\Gamma_t A \Gamma_t \Gamma^*_t) = \varphi_1(\Gamma_t A)$$

for all $A \in \mathfrak{M}$, i.e., Γ_t is contained in the centralizer for φ_1. Hence Proposition 5.3.28 implies that $\sigma^1_s(\Gamma_t) = \Gamma_t$ for all s. It follows that

$$\Gamma_{s+t} = \Gamma_s \sigma^1_s(\Gamma_t) = \Gamma_s \Gamma_t \quad ,$$

i.e., $t \mapsto \Gamma_t$ is a unitary representation of $\mathbb{R}$. But now

$$\sigma_{(\beta_1 - \beta_2)t} = \sigma^2_t \sigma^1_{-t}(A) = \Gamma_t\, A \Gamma^*_t$$

is an inner group of *-automorphisms of $\mathfrak{M}$. Hence, by rescaling, σ^1_t is an inner group of *-automorphisms. It follows that $\mathfrak{M}$ is a semi-finite von Neumann algebra, which is a contradiction.

Theorem 5.3.35 applies in particular to KMS states satisfying the weak asymptotic abelianess condition of Theorem 5.3.32. Recall from the proof of that theorem that if ω is a (τ, β)-KMS state where $\beta \neq 0$, then

$$\lim_{S-T \to \infty} \frac{1}{S-T} \int_S^T dt\, \omega(A\tau_t(B)C)$$

exists for all $A, B, C \in \mathfrak{A}$.

Corollary 5.3.36. *Let $(\mathfrak{A}, \tau)$ be a C^*-dynamical system, let $\beta \in \mathbb{R}\backslash\{0\}$, and let ω be a (τ, β)-KMS state on $\mathfrak{A}$ such that*

$$\lim_{S-T\to\infty} \frac{1}{S-T}\int_S^T dt\, \omega(A[\tau_t(B), C]D) = 0 \qquad (*)$$

for all $A, B, C, D \in \mathfrak{A}$. Let $(\mathfrak{H}_\omega, \pi_\omega, \Omega_\omega)$ be the cyclic representation associated with ω.

It follows that there exists a projection $E \in \pi_\omega(\mathfrak{A})'' \cap \pi_\omega(\mathfrak{A})'$ such that

(1) *$\pi_\omega(\mathfrak{A})''E$ is type-III.*
(2) *$\pi_\omega(\mathfrak{A})''(\mathbb{1} - E)$ is abelian.*

In particular, assume that $\mathfrak{A}$ does not have any characters and let ω_1 and ω_2 be states on $\mathfrak{A}$ satisfying the τ-KMS condition at values $\beta_1, \beta_2 \in \mathbb{R}$, where $\beta_1 \neq \beta_2$. Assume furthermore that ω_i satisfies condition $(*)$ if $\beta_i \neq 0$ for $i = 1, 2$.

It follows that ω_1 and ω_2 are disjoint.

Proof. Assume that ω satisfies the hypotheses of the corollary and let $\hat{\omega}$ and $\hat{\tau}$ be the normal extensions of ω and τ to $\mathfrak{M} = \pi_\omega(\mathfrak{A})''$, which exist by Corollary 5.3.4. The center of $\mathfrak{M}$ is contained in $\mathfrak{M}^{\hat{\tau}}$ by Proposition 5.3.28, and it follows from the proof of Theorem 5.3.32 that condition $(*)$ is equivalent to

$$\mathfrak{M}^{\hat{\tau}} = \mathfrak{M} \cap \mathfrak{M}'$$

where $\mathfrak{M}^{\hat{\tau}}$ is the fixed-point algebra of $\mathfrak{M}$ under the action $\hat{\tau}$. Now, let $\mathbb{1} - E$ be the largest projection in $\mathfrak{M} \cap \mathfrak{M}'$ such that $\hat{\tau}|_{\mathfrak{M}(\mathbb{1}-E)}$ is an inner group of automorphisms. Then $\pi_\omega(\mathfrak{A})''E$ is type-III by the remark before Theorem 5.3.35, since $\hat{\tau}$ is a multiple of the modular group. We may henceforth assume $E = 0$. Then there exists a unitary group $t \mapsto U_t$ in $\mathfrak{M}$ such that

$$\hat{\tau}_t(A) = U_t A U_t^* \ .$$

But then

$$\hat{\tau}_t(U_s) = U_t U_s U_{-t} = U_s$$

and so

$$U_s \in \mathfrak{M}^{\hat{\tau}} = \mathfrak{M} \cap \mathfrak{M}' \ .$$

Hence

$$\hat{\tau}_s(A) = U_s A U_s^* = A$$

for all $A \in \mathfrak{M}$. But then

$$\mathfrak{M} = \mathfrak{M}^{\hat{\tau}} = \mathfrak{M} \cap \mathfrak{M}' ,$$

i.e., $\mathfrak{M}$ is abelian.

In particular, if $\mathfrak{A}$ has no characters then we must have $E = \mathbb{1}$ in the above construction, and thus the last statement of the corollary follows from Theorem 5.3.35.

5.3.3. The Set of Ground States

In the previous subsection we analyzed various properties of the set K_β of (τ, β)-KMS states over a C^*-dynamical system $(\mathfrak{A}, \tau)$. This analysis was restricted to the case $\beta \in \mathbb{R}$ and our next aim is to make an analogous analysis for $\beta = \pm\infty$. Since both these latter cases are similar we examine only the set K_∞ of (τ, ∞)-KMS states, i.e., the set of ground states of $(\mathfrak{A}, \tau)$.

It follows directly from Definition 5.3.18 that K_∞ is a weak*-closed convex subset of the state space $E_\mathfrak{A}$. But K_∞ need not be a simplex in contrast to the case of K_β with β finite. An example is given by the choice $\tau_t = \iota$ for all t, and thus $K_\infty = E_\mathfrak{A}$. Recall that $E_\mathfrak{A}$ is a simplex if, and only if, $\mathfrak{A}$ is abelian, Example 4.2.6. However, K_∞ has one simple geometric property not generally shared by K_β, it is a face in $E_\mathfrak{A}$ (see Remarks 2 and 3 after Theorem 5.3.32).

Theorem 5.3.37. *Let $(\mathfrak{A}, \tau)$ be a C^*-dynamical system and assume that $\mathfrak{A}$ has an identity.*

It follows that the set K_∞ of τ ground states is convex and compact in the weak-topology and K_∞ is a face in $E_\mathfrak{A}$.*

Let $\omega \in K_\infty$, and consider the following conditions:

(1) *The pair $(\mathfrak{A}, \omega)$ is $\mathbb{R}$-abelian.*
(2) *$\pi_\omega(\mathfrak{A})'$ is abelian.*
(3) *There exists a unique maximal measure μ_K in $M_\omega(K_\infty)$.*
(4) *There exists a unique maximal measure μ_E in $M_\omega(E_\mathfrak{A}^\mathbb{R})$.*
(5) *There exists a unique maximal measure μ_X in $M_\omega(E_\mathfrak{A})$.*

It follows that (1) $\Rightarrow$ (2) $\Leftrightarrow$ (3) $\Leftrightarrow$ (4) $\Leftrightarrow$ (5).

If any of these conditions are fulfilled, then

$$\mu_K = \mu_E = \mu_X = \mu_C \ ,$$

where μ_C is the central measure in $M_\omega(E_\mathfrak{A})$, and these measures are pseudo-supported by the intersection of the ground states, the $\mathbb{R}$-ergodic states and the pure states.

In particular, if ω is an extremal ground state, then ω is pure and

$$\pi_\omega(\mathfrak{A})'' = \mathscr{L}(\mathfrak{H}_\omega) \ .$$

Proof. K_∞ is convex and compact by the remarks before the theorem and Theorem 2.3.15. If $\omega \in K_\infty$ and $\varphi \in E_\mathfrak{A}$ with $\varphi \leq \lambda\omega$ then, by condition (4) of Proposition 5.3.19,

$$0 \leq \varphi(\tau_f(A)^*\tau_f(A)) \leq \lambda\omega(\tau_f(A)^*\tau_f(A)) = 0$$

for all $\hat{f} \in \mathscr{D}$ with supp $\hat{f} \subseteq \langle -\infty, 0\rangle$, and all $A \in \mathfrak{A}$. Hence φ is a ground state by the same condition. It follows that K_∞ is a face in $E_\mathfrak{A}$.

Let $\omega \in K_\infty$ be a fixed state, and let $(\mathfrak{H}_\omega, \pi_\omega, \Omega_\omega, U_\omega)$ be the associated representation. Then

$$U_\omega(t) \in \pi_\omega(\mathfrak{A})''$$

for all $t \in \mathbb{R}$, by Proposition 5.3.19. It follows that

$$\pi_\omega(\mathfrak{A})' = \pi_\omega(\mathfrak{A})' \cap U_\omega(\mathbb{R})'$$

and hence (1) $\Rightarrow$ (2) by Proposition 4.3.7. Furthermore (2) $\Leftrightarrow$ (4) by the same Proposition, and (2) $\Leftrightarrow$ (5) by Theorem 4.2.4. Since K_∞ is a face in $E_{\mathfrak{A}}$, we have the identification

$$M_\omega(K_\infty) = M_\omega(E_{\mathfrak{A}})$$

and (3) $\Leftrightarrow$ (5) follows.

Now, if condition (2) is fulfilled, we have

$$\pi_\omega(\mathfrak{A})' \cap \pi_\omega(\mathfrak{A})'' = \pi_\omega(\mathfrak{A})' = \pi_\omega(\mathfrak{A})' \cap U_\omega(\mathbb{R})'$$

and hence

$$\mu_C = \mu_X = \mu_E \ .$$

But $\mu_X = \mu_K$ by the facial property of K_∞.

Since this measure is maximal in $M_\omega(E_{\mathfrak{A}})$, the pseudo-support property is a consequence of Theorem 4.1.11.

If $\omega \in \mathscr{E}(K_\infty)$ then $\mu_K = \delta_\omega$ is unique maximal in $M_\omega(K_\infty)$. Thus condition (3) is valid. This implies condition (5) and the identification $\mu_X = \delta_\omega$, i.e., $\omega \in \mathscr{E}(E_{\mathfrak{A}})$.

Note that the implication (2) $\Rightarrow$ (1) in Theorem 5.3.37 is not true in general. A simple counterexample is provided by taking τ to be the trivial action on a non-abelian C^*-algebra $\mathfrak{A}$. Then any pure state on $\mathfrak{A}$ is a ground state satisfying condition (2), but $(\mathfrak{A}, \omega)$ is not $\mathbb{R}$-abelian if $\dim(\mathfrak{H}_\omega) \geq 2$. However, the implication corresponding to (2) $\Rightarrow$ (1) is true in a global version of the theorem. This global version can be formulated for more general faces F in $E_{\mathfrak{A}}^{\mathbb{R}}$ than the face of ground states and also for more general groups G than $\mathbb{R}$. Note in particular that if $\omega \in E_{\mathfrak{A}}^G$ and F is the closure of the set N_ω^G of π_ω-normal τ-invariant states on $\mathfrak{A}$, then F satisfies the hypotheses of the following theorem, and therefore this theorem is a partial generalization of Theorem 4.3.9. We emphasize that F is only assumed to be a face in $E_{\mathfrak{A}}^G$, not necessarily in $E_{\mathfrak{A}}$.

Theorem 5.3.38. *Let $(\mathfrak{A}, G, \tau)$ be a C^*-dynamical system, where G is a locally compact, σ-compact, topological group and $\mathfrak{A}$ has an identity. Let F be a closed face of $E_{\mathfrak{A}}^G$ with the property that if $\omega \in F$ and ψ is a unit vector in the space $E_\omega \mathfrak{H}_\omega$ of U_ω-invariant vectors in $\mathfrak{H}_\omega$, then the vector state ω' defined by*

$$\omega'(A) = (\psi, \pi_\omega(A)\psi) \ , \qquad A \in \mathfrak{A} \ ,$$

is included in F.

The following statements are equivalent.

(1) *The pair $(\mathfrak{A}, \omega)$ is G-abelian for all $\omega \in F$.*

(2) *$\{\pi_\omega(\mathfrak{A}) \cup U_\omega(G)\}'$ is abelian for all $\omega \in F$.*

(3) *F is a simplex.*

(4) *Each extremal state ω in F is weakly clustering in the sense that*

$$\inf_{A' \in Co(\tau_G(A))} |\omega(A'B) - \omega(A)\omega(B)| = 0$$

for all $A, B \in \mathfrak{A}$.

(5) *Any state ω in F such that $\{\pi_\omega(\mathfrak{A}) \cup U_\omega(G)\}'$ is a factor is ergodic.*

(6) *If ω_1 and ω_2 are ergodic states in F and $\omega_1 \neq \omega_2$, then the covariant representations $(\mathfrak{H}_{\omega_1}, \pi_{\omega_1}, U_{\omega_1})$ and $(\mathfrak{H}_{\omega_2}, \pi_{\omega_2}, U_{\omega_2})$ are not unitarily equivalent (as covariant representations).*

(7) *If ω_1 and ω_2 are distinct ergodic states in F, then the face generated by ω_1 and ω_2 in $E^G_{\mathfrak{A}}$ is equal to the convex set $\{\lambda\omega_1 + (1-\lambda)\omega_2;$ $\lambda \in [0,1]\}$ generated by ω_1 and ω_2.*

Remark. The special assumption on the closed face F used in this theorem is necessary but the theorem is true without the assumption that G is σ-compact (see Notes and Remarks).

PROOF. We will prove the following implications

$$\begin{tikzcd}
 & 4 \arrow[r, Rightarrow] & 1 \arrow[d, Rightarrow] & \\
7 \arrow[r, Leftrightarrow] & 6 \arrow[ur, Rightarrow] \arrow[dr, Rightarrow] & & 3 \arrow[ul, Rightarrow] \arrow[dl, Rightarrow] \\
 & 5 & 2 \arrow[l, Rightarrow] &
\end{tikzcd}$$

We have $1 \Rightarrow 2 \Leftrightarrow 3$ by Proposition 4.3.7 and Theorem 4.1.15. To prove $3 \Rightarrow 1$ we exploit a technique closely related to the one used in the proof of Theorem 4.3.9. By the latter it suffices to show that

$$N^G_\omega = \{\omega'; \omega' \in N^G_\omega, \omega'(F_\omega) = 1\}$$

is a simplex, where N^G_ω denotes the τ-invariant π_ω-normal states over $\mathfrak{A}$,

$$F_\omega = [\pi_\omega(\mathfrak{A})' E_\omega] \in \pi_\omega(\mathfrak{A})'' \cap U_\omega(G)' \ ,$$

E_ω is the projection onto the U_ω-invariant vectors in $\mathfrak{H}_\omega$, and we identify π_ω-normal states with their σ-weakly continuous extensions to $\pi_\omega(\mathfrak{A})''$. It follows from Theorem 2.4.21 that all $\omega' \in N^G_\omega$ have the form

$$\omega'(A) = \sum_{k \geq 1} (\xi_k, \pi_\omega(A)\xi_k) \ ,$$

where $\xi_k \in \mathfrak{H}_\omega$ and $\sum_{k \geq 1} \|\xi_k\|^2 = 1$. But $\omega'(F_\omega) = 1$ implies $\omega_{\xi_k}(F_\omega) = 1$ for all k and hence $F_\omega \xi_k = \xi_k$ for all k. But this means that ω' can be approximated in norm by states ω'' of the form

$$\omega''(A) = \sum_{k=1}^{n} (T_k \eta_k, \pi_\omega(A) T_k \eta_k)$$

where $E_\omega \eta_k = \eta_k$ and $T_k \in \pi_\omega(\mathfrak{A})'$. But then $\omega_{\eta_k} \in F$ by the special assumption on F, and we have

$$\omega' \leq \sum_{k=1}^{n} \|T_k\|^2 \omega_{\eta_k}$$

by Theorem 2.3.19. Since F is a closed face, it follows that $\omega' \in F$. Hence

$$N^G_\omega \subseteq F \ .$$

But since N_ω^G is a face of the simplex F, it follows that N_ω^G is a simplex, and $(\mathfrak{A}, \omega)$ is G-abelian by the argument used in the proof of Theorem 4.3.9.

(2) $\Rightarrow$ (5): If $\{\pi_\omega(\mathfrak{A}) \cup U_\omega(G)\}'$ is an abelian factor, then $\{\pi_\omega(\mathfrak{A}) \cup U_\omega(G)\}' = \mathbb{C}\mathbb{1}$ and ω is ergodic by Theorem 4.3.17.

(5) $\Rightarrow$ (6): Suppose that (6) does not hold, i.e., suppose that F contains two distinct extremal covariantly equivalent states ω_1 and ω_2. Let $\omega = (\omega_1 + \omega_2)/2$. Further let T be the unique positive element in $\pi_\omega(\mathfrak{A})'$ such that

$$\omega_1(A)/2 = (\Omega_\omega, \pi_\omega(A) T \Omega_\omega)$$

for all $A \in \mathfrak{A}$ (Theorem 2.3.19). It follows from the G-invariance of ω_1 that $T \in U_\omega(G)'$ and hence

$$T \in \{\pi_\omega(\mathfrak{A}) \cup U_\omega(G)\}' \ .$$

Furthermore

$$\omega_2(A)/2 = (\Omega_\omega, \pi_\omega(A)(\mathbb{1} - T)\Omega_\omega)$$

and hence

$$A \mapsto (\Omega_\omega, \pi_\omega(A)(\mathbb{1} - T) T \Omega_\omega)$$

is a positive, G-invariant, linear functional dominated by both ω_1 and ω_2 and it is, therefore, a multiple of both ω_1 and ω_2 by extremality. Since $\omega_1 \neq \omega_2$ it follows that $(\mathbb{1} - T)T = 0$, i.e., T is a projection. Hence $(\mathfrak{H}_\omega, T_\omega, U_\omega, \Omega_\omega)$ is unitarily equivalent to $(\mathfrak{H}_{\omega_1} \oplus \mathfrak{H}_{\omega_2}, \pi_{\omega_1} \oplus \pi_{\omega_2}, U_{\omega_1} \oplus U_{\omega_2}, \Omega_{\omega_1} \oplus \Omega_{\omega_2}/\sqrt{2})$ and, therefore, to $(\mathfrak{H}_{\omega_1} \oplus \mathfrak{H}_{\omega_1}, \pi_{\omega_1} \oplus \pi_{\omega_1}, U_{\omega_1} \oplus U_{\omega_1}, \Omega_{\omega_1} \oplus \eta/\sqrt{2})$ where η is a unit vector (distinct from $\exp\{i\theta\}\Omega_{\omega_1}$ for all $\theta \in \mathbb{R}$) in $E_\omega \mathfrak{H}_\omega$. As $\{\pi_{\omega_1}(\mathfrak{A}) \cup U_{\omega_1}(G)\}' = \mathbb{C}\mathbb{1}$, it follows that $\{\pi_\omega(\mathfrak{A}) \cup U_\omega\ (G)\}' \simeq M_2$, where M_2 is the algebra of 2×2 matrices. But M_2 is a factor, and $\omega = (\omega_1 \times \omega_2)/2$ is not ergodic. Hence condition (5) is not fulfilled.

(7) $\Rightarrow$ (6): If (6) does not hold, it follows from the preceding argument that there exist distinct ergodic states ω_1 and ω_2 in F such that

$$\{\pi_\omega(\mathfrak{A}) \cup U_\omega(G)\}' \simeq M_2 \ ,$$

where $\omega = (\omega_1 + \omega_2)/2$. Hence the face generated by ω_1 and ω_2 is affinely isomorphic to the positive 2×2 matrices of trace one, and hence isomorphic to the three-dimensional unit ball by Example 4.2.7. Thus condition (6) is not fulfilled.

(6) $\Rightarrow$ (7): If ω_1 and ω_2 are distinct ergodic states in F and property (6) holds, then it follows from the argument used in proving (5) $\Rightarrow$ (6) that

$$[\{\pi_{\omega_1} \oplus \pi_{\omega_2}(A);\ A \in \mathfrak{A}\} \cup \{U_{\omega_1} \oplus U_{\omega_2}(g);\ g \in G\}]' = \{\alpha_1 T + \alpha_2(\mathbb{1} - T);\ \alpha_1, \alpha_2 \in \mathbb{C}\} \ ,$$

where T is the projection from $\mathfrak{H}_{\omega_1} \oplus \mathfrak{H}_{\omega_2}$ onto $\mathfrak{H}_{\omega_1}$. As the face generated by ω_1 and ω_2 in $E_{\mathfrak{A}}^G$ is affinely isomorphic to the subset of positive operators of trace one, assertion (7) holds.

(6) $\Rightarrow$ (4): Assume that the state ω of condition (4) is ergodic, but not weakly clustering, i.e., E_ω has dimension larger than one. If $\eta \in E_\omega \mathfrak{H}_\omega$ is a unit vector orthogonal to Ω_ω, then the state ω_1 corresponding to η is contained in F by the special assumption on F and $\omega_1 \neq \omega$. By ergodicity

$$\{\pi_\omega(\mathfrak{A}) \cup U_\omega(G)\}'' = \mathscr{L}(\mathfrak{H}_\omega)$$

and hence

$$E_\omega \pi_\omega(\mathfrak{A})'' E_\omega = \mathscr{L}(E_\omega \mathfrak{H}_\omega) \ .$$

But this implies that η is cyclic for $\pi_\omega(\mathfrak{A})$, and hence the representation $(\mathfrak{H}_{\omega_1}, \pi_{\omega_1}, U_{\omega_1}, \Omega_{\omega_1})$ is canonically unitarily equivalent with $(\mathfrak{H}_\omega, \pi_\omega, U_\omega, \Omega_\omega)$. Hence condition (6) is not fulfilled.

In order to show (4) $\Rightarrow$ (1) and finish the proof of the theorem we need an unpleasant measure-theoretic lemma. The point of this lemma is to circumvent difficulties which could arise from the possible nonseparability of $\mathfrak{A}$.

Lemma 5.3.39. *Let ω be a state over a C^*-algebra $\mathfrak{A}$ with identity, $\mu \in M_\omega(E_\mathfrak{A})$ a probability measure with barycenter ω, η a vector in $\mathfrak{H}_\omega$, and $\{A_n\}_{n\geq 1}$ a sequence in $\mathfrak{A}$ such that*

$$\sum_{n\geq 1} \|\pi_\omega(A_n)\Omega_\omega - \eta\| < +\infty \ .$$

(1) *It follows that $\pi_\varphi(A_n)\Omega_\varphi$ converges to some vector $\eta_\varphi \in \mathfrak{H}_\varphi$ for μ-almost all $\varphi \in E_\mathfrak{A}$.*

(2) *If $B \in \mathfrak{A}$ let*

$$\omega_\varphi^\eta(B) = (\eta_\varphi, \pi_\varphi(B)\eta_\varphi) \ .$$

Then $\varphi \mapsto \omega_\varphi^\eta(B)$ is μ-integrable and

$$\omega_\omega^\eta(B) = \int d\mu(\varphi)\omega_\varphi^\eta(B) \ .$$

(3) *If $\{A_n'\}_{n\geq 1}$ is another sequence in $\mathfrak{A}$ such that*

$$\sum_{n\geq 1} \|\pi_\omega(A_n')\Omega_\omega - \eta\| < +\infty \ ,$$

then $\pi_\varphi(A_n')\Omega_\varphi$ converges to η_φ for μ-almost all $\varphi \in E_\mathfrak{A}$.

Proof. (1) Let f_n be the non-negative continuous function on $E_\mathfrak{A}$ defined by

$$f_n(\varphi) = \|\pi_\varphi(A_n - A_{n+1})\Omega_\varphi\| = \varphi((A_n - A_{n+1})^*(A_n - A_{n+1}))^{1/2} \ .$$

Then

$$\begin{aligned}\int d\mu(\varphi) f_n(\varphi)^2 &= \int d\mu(\varphi)\varphi((A_n - A_{n+1})^*(A_n - A_{n+1})) \\ &= \omega((A_n - A_{n+1})^*(A_n - A_{n+1})) = \|\pi_\omega(A_n - A_{n+1})\Omega_\omega\|^2 \ .\end{aligned}$$

Hence $\sum f_n$ is a convergent series in $L^2(\mu)$ and therefore in $L^1(\mu)$, and consequently

$$\sum_{n\geq 1} f_n(\varphi) < +\infty$$

for μ-almost all $\varphi \in E_\mathfrak{A}$. For any such $\varphi, \pi_\varphi(A_n)\Omega_\varphi$ is a Cauchy sequence which converges to some limit η_φ.

(2) Let

$$g_n(\varphi) = \|\pi_\varphi(BA_n)\Omega_\varphi\| \ .$$

By the triangle inequality

$$|g_n(\varphi) - g_{n+1}(\varphi)| \leq \|B\| f_n(\varphi)$$

and so $\{g_n\}_{n \geq 1}$ is a Cauchy sequence in $L^2(\mu)$ converging pointwise to $\omega_\varphi^\eta(B^*B)^{1/2}$. Thus this function of φ is square integrable, and

$$\begin{aligned}\int d\mu(\varphi)\omega_\varphi^\eta(B^*B) &= \lim_{n\to\infty}\int d\mu(\varphi) g_n(\varphi)^2 \\ &= \lim_{n\to\infty} \omega(A_n^* B^* B A_n) = \omega_\omega^\eta(B^*B) \ .\end{aligned}$$

Since $\mathfrak{A}$ is spanned linearly by its positive part, it follows that

$$\omega_\omega^\eta(B) = \int d\mu(\varphi)\omega_\varphi^\eta(B)$$

for all $B \in \mathfrak{A}$.

(3) The same argument as in the proof of (1) shows that

$$\|\pi_\varphi(A_n - A_n')\Omega_\varphi)\| \to 0$$

for μ-almost all $\varphi \in E_{\mathfrak{A}}$, and hence

$$\|\pi_\varphi(A_n')\Omega_\varphi - \eta_\varphi\| \to 0$$

for μ-almost all $\varphi \in E_{\mathfrak{A}}$.

End of proof of Theorem 5.3.38 It remains to prove that (4) $\Rightarrow$ (1).

Let $\omega \in F$, let $A, A' \in \mathfrak{A}$ and let $\mu \in M_\omega(F)$ be a maximal measure representing ω. Since F is a face in $E_{\mathfrak{A}}^G$, μ is pseudo-supported by the ergodic states in F, Theorem 4.1.11.

Let η be a unit vector in $E_\omega \mathfrak{H}_\omega$ and $\{B_n\}$ a sequence in $\mathfrak{A}$ such that

$$\|\pi_\omega(B_n)\Omega_\omega - \eta\| < 2^{-n-1}.$$

By Proposition 4.3.4 there exist elements

$$S_{\lambda^n}(U_\omega) = \sum_{i=1}^{k_n} \lambda_i^n U_\omega(g_i^n)$$

in $Co(U_\omega(G))$ such that

$$\|S_{\lambda^n}(U_\omega)\pi_\omega(AB_n)\Omega_\omega - E_\omega \pi_\omega(A)\eta\| < 2^{-n}$$

and

$$\|S_{\lambda^n}(U_\omega)\pi_\omega(A'B_n)\Omega_\omega - E_\omega \pi_\omega(A')\eta\| < 2^{-n} \ .$$

Now, define

$$A_n = S_{\lambda^n}(\tau(AB_n)) \ , \quad A_n' = S_{\lambda^n}(\tau(A'B_n)) \ .$$

The relations above may be written as

$$\|\pi_\omega(S_{\lambda^n}(\tau(AB_n)))\Omega_\omega - E_\omega \pi_\omega(A)\eta\| < 2^{-n}$$

and

$$\|\pi_\omega(S_{\lambda^n}(\tau(A'B_n)))\Omega_\omega - E_\omega \pi_\omega(A')\eta\| < 2^{-n} \ .$$

By Lemma 5.3.39 (1) there is a Baire subset E of F with $\mu(E) = 1$ such that for $\varphi \in E, \pi_\varphi(B_n)\Omega_\varphi$, $\pi_\varphi(A_n)\Omega_\varphi$ and $\pi_\varphi(A'_n)\Omega_\varphi$ converge to some limits $\eta_\varphi, \xi_\varphi$, and ξ'_φ respectively, in $\mathfrak{H}_\varphi$.

For fixed $g \in G$ one has

$$\|\pi_\omega(\tau_g(B_n))\Omega_\omega - \eta\| = \|U_\omega(g)(\pi_\omega(B_n)\Omega_\omega - \eta)\| < 2^{-n-1}$$

and it follows from Lemma 5.3.39 (3) that $\pi_\varphi(\tau_g(B_n))\Omega_\varphi$ converges μ-almost everywhere to η_φ. Since

$$\pi_\varphi(\tau_g(B_n))\Omega_\varphi = U_\varphi(g)\pi_\varphi(B_n)\Omega_\varphi \to U_\varphi(g)\eta_\varphi$$

for $\varphi \in E$, it follows that

$$U_\varphi(g)\eta_\varphi = \eta_\varphi$$

for μ-almost all $\varphi \in F$.

Now, define

$$\begin{aligned} D &= \{(g, \varphi) \in G \times E;\ U_\varphi(g)\eta_\varphi = \eta_\varphi\} \\ &= \{(g, \varphi) \in G \times E;\ \varphi((\tau_g(B_n) - B_n)^*(\tau_g(B_n) - B_n)) \to 0\} \ . \end{aligned}$$

Then D is a Baire subset of $G \times F$, and we have proved that $\{\varphi \in F; (g, \varphi) \in D\}$ supports μ for each $g \in G$. The Haar measure μ_0 on G is σ-finite by assumption and it follows from Fubini's theorem that $\mu_0 \otimes \mu$ is supported by D. Hence for μ-almost all $\varphi \in F$ one has that

$$U_\varphi(g)\eta_\varphi = \eta_\varphi$$

for μ_0-almost all $g \in G$, and hence this relation holds for all $g \in G$ by the strong continuity of U_φ. We conclude that

$$\eta_\varphi \in E_\varphi \mathfrak{H}_\varphi$$

for μ-almost all $\varphi \in F$.

Applying similar arguments to ξ_φ and ξ'_φ we find a Baire subset $E_1 \subseteq F$ such that $E_1 \subseteq E, \mu$ is supported by E_1 and

$$\eta_\varphi, \xi_\varphi, \xi'_\varphi \in E_\varphi \mathfrak{H}_\varphi$$

for all $\varphi \in E_1$. In particular, if $\varphi \in E_1$ is such that E_φ is one-dimensional, one has

$$\begin{aligned} \eta_\varphi &= (\Omega_\varphi, \eta_\varphi)\,\Omega_\varphi \ , \\ \xi_\varphi &= (\Omega_\varphi, \xi_\varphi)\,\Omega_\varphi = \lim_{n\to\infty} \varphi(A_n)\,\Omega_\varphi \ , \end{aligned}$$

and

$$E_\varphi \pi_\varphi(A)\eta_\varphi = (\Omega_\varphi, \pi_\varphi(A)\eta_\varphi)\Omega_\varphi = \lim_{n\to\infty} \varphi(AB_n)\Omega_\varphi \ .$$

But $\varphi(A_n) = \varphi(AB_n)$ and thus

$$\xi_\varphi = E_\varphi \pi_\varphi(A)\eta_\varphi = \varphi(A)(\Omega_\varphi, \eta_\varphi)\Omega_\varphi \ .$$

Similarly

$$\xi'_\varphi = \varphi(A')(\Omega_\varphi, \eta_\varphi)\Omega_\varphi$$

and hence

$$(\eta_\varphi, \pi_\varphi(A')\xi_\varphi) = \varphi(A')\varphi(A)|(\Omega_\varphi, \eta_\varphi)|^2 = (\eta_\varphi, \pi_\varphi(A)\xi'_\varphi)$$

for all $\varphi \in E_1$ such that E_φ is one-dimensional.

Condition (4) is equivalent to the condition that E_φ is one-dimensional for each ergodic state in F, by Theorem 4.3.22. Therefore, if we assume (4), it follows that the set

$$\{\varphi \in E_1; (\eta_\varphi, \pi_\varphi(A')\xi_\varphi) \neq (\eta_\varphi, \pi_\varphi(A)\xi'_\varphi)\}$$

contains no ergodic states. But this is a Baire subset of F, and it follows from the maximality of μ that the set has measure zero (see Theorem 4.1.11). By Lemma 5.3.9 (2) and the polarization identity, it now follows that

$$\begin{aligned}(\eta, \pi_\omega(A')E_\omega\pi_\omega(A)\eta) &= \lim_{n\to\infty}(\pi_\omega(B_n)\Omega_\omega,\ \pi_\omega(A')\pi_\omega(A_n)\Omega_\omega)\\ &= \lim_{n\to\infty}\int_F d\mu(\varphi)(\pi_\varphi(B_n)\Omega_\varphi,\ \pi_\varphi(A')\pi_\varphi(A_n)\Omega_\varphi)\\ &= \int_F d\mu(\varphi)(\eta_\varphi, \pi_\varphi(A')\xi_\varphi)\\ &= \int_F d\mu(\varphi)(\eta_\varphi, \pi_\varphi(A)\xi'_\varphi) = (\eta, \pi_\omega(A)E_\omega\pi_\omega(A')\eta)\ .\end{aligned}$$

Since this is true for all $\eta \in E_\omega\mathfrak{H}_\omega$, it follows that

$$E_\omega\pi_\omega(A')E_\omega\pi_\omega(A)E_\omega = E_\omega\pi_\omega(A)E_\omega\pi_\omega(A')E_\omega$$

for all $A, A' \in \mathfrak{A}$. The pair $(\mathfrak{A}, \omega)$ is then G-abelian by Proposition 4.3.7.

Theorem 5.3.38 has several interesting corollaries. First we consider the set of ground states of a C^*-dynamical system.

Corollary 5.3.40. *Let $(\mathfrak{A}, \mathbb{R}, \tau)$ be a C^*-dynamical system where $\mathfrak{A}$ has an identity, and let K_∞ be the set of ground states for the system.*

The following 15 statements are equivalent:

(1) *The pair $(\mathfrak{A}, \omega)$ is $\mathbb{R}$-abelian for all $\omega \in K_\infty$.*

(2) *$\pi_\omega(\mathfrak{A})'$ is abelian for all $\omega \in K_\infty$.*

(3) *K_∞ is a simplex.*

(4) *Each pure ground state is weakly clustering in the sense that*

$$\inf_{A' \in Co(\tau_{\mathbb{R}}(A))} |\omega(A'B) - \omega(A)\omega(B)| = 0$$

for all $A, B \in \mathfrak{A}$.

(5) *Any state ω in K_∞ such that $\pi_\omega(\mathfrak{A})'$ is a factor is pure.*

(6) *If ω_1 and ω_2 are pure states in K_∞ then ω_1 and ω_2 are either disjoint or equal, i.e.,*

$$\omega_1 \mathbin{\delta} \omega_2 \quad \text{or} \quad \omega_1 = \omega_2\ .$$

(7) *If ω_1 and ω_2 are distinct pure states in K_∞ then the face generated by ω_1 and ω_2 in $E_{\mathfrak{A}}^{\mathbb{R}}$ is equal to the convex set*

$$\{\lambda\omega_1 + (1-\lambda)\omega_2;\ \lambda \in [0,1]\}$$

generated by ω_1 and ω_2.

(4′), (5′), (6′), (7′): *The statements obtained by replacing "pure" by "ergodic" in* (4), (5), (6), (7), *respectively.*

(4″), (5″), (6″), (7″): *The statements obtained by replacing "pure" by "extremal in K_∞" in* (4), (5), (6), (7), *respectively.*

PROOF. The set K_∞ is a face in $E_{\mathfrak{A}}$ by Theorem 5.3.37, and hence K_∞ is a face in $E_{\mathfrak{A}}^{\mathbb{R}}$. It follows that if ω is a ground state, the statements "ω is pure," "ω is ergodic," and "ω is extremal in K_∞" are all equivalent, and hence the unprimed statements in the theorem are equivalent to the primed ones.

We next show that the face $F = K_\infty$ has the special property required in Theorem 5.3.38. If ω is a ground state and $\psi \in E_\omega \mathfrak{H}_\omega$ is a unit vector defining a state through

$$\omega'(A) = (\psi, \pi_\omega(A)\psi) \ ,$$

then the cyclic representation $(\mathfrak{H}_{\omega'}, \pi_{\omega'}, U_{\omega'}, \Omega_{\omega'})$ corresponding to ω' is unitary equivalent to the representation

$$(P\mathfrak{H}_\omega, P\pi_\omega P, PU_\omega P, \psi) \ ,$$

where $P \in \{\pi_\omega(\mathfrak{A}) \cup U_\omega(\mathbb{R})\}'$ is the projection defined by

$$P = [\pi_\omega(\mathfrak{A})\psi] \ .$$

It follows from Proposition 5.3.19 (5) that ω' is a ground state. Thus Theorem 5.3.38 applies to $F = K_\infty$, and it remains to show that the statements (1)–(7) of that theorem are equivalent to statements of (1)–(7) of this theorem in the special case of ground states. This is clear for statements (1), (3), (4), and (7), and since Proposition 5.3.19 implies that

$$U_\omega(\mathbb{R}) \subseteq \pi_\omega(\mathfrak{A})''$$

for all $\omega \in K_\infty$, the equivalence for statements (2) and (5) follows immediately. Statement (6) of Theorem 5.3.38 takes the form

(6‴). *If ω_1 and ω_2 are pure ground states and $\omega_1 \neq \omega_2$, then the representations $(\mathfrak{H}_{\omega_1}, \pi_{\omega_1})$ and $(\mathfrak{H}_{\omega_2}, \pi_{\omega_2})$ are not unitarily equivalent.*

But since two irreducible representations are either unitary equivalent or disjoint, this is equivalent to statement (6) of the corollary.

The implication (1) $\Rightarrow$ (6) in Corollary 5.3.40 is related to a result which was of fundamental importance in the development of quantum field theory, Haag's theorem. This theorem demonstrated that the examination of the ground states of a given dynamics necessitated the examination of a variety of unitary inequivalent representations. A more local version of this implication is as follows.

Corollary 5.3.41. *Let $(\mathfrak{A}, \mathbb{R}, \tau)$ be a C^*-dynamical system, and let ω_1 and ω_2 be extremal ground states on $\mathfrak{A}$ such that $(\mathfrak{A}, \omega_i)$ is $\mathbb{R}$-abelian for $i = 1, 2$.*

It follows that ω_1 and ω_2 are either disjoint or equal, i.e.,

$$\omega_1 \mathrel{\underline{\circ}} \omega_2 \quad \textit{or} \quad \omega_1 = \omega_2 \ .$$

PROOF. Assume that ω_1 and ω_2 are not disjoint. Then π_{ω_1} and π_{ω_2} have equivalent subrepresentations, and since $\pi_{\omega_i}(\mathfrak{A})'' = \mathscr{L}(\mathfrak{H}_{\omega_i})$ by Theorem 5.3.37, it follows that

ω_1 and ω_2 are quasi-equivalent (and even unitary equivalent). Hence $(\omega_1 + \omega_2)/2$ is a factor state by Proposition 2.4.27. Since the set of ground states is convex and the set of invariant states φ such that $(\mathfrak{A}, \varphi)$ is $\mathbb{R}$-abelian is convex as a consequence of Corollary 4.3.10, it follows that $(\omega_1 + \omega_2)/2$ is a ground state and $(\mathfrak{A}, (\omega_1 + \omega_2)/2)$ is G-abelian. Theorem 5.3.37 implies that $\pi_{(\omega_1+\omega_2)/2}(\mathfrak{A})'$ is abelian, but since this is a factor, one deduces that $(\omega_1 + \omega_2)/2$ is a pure state. Hence

$$\omega_1 = \omega_2 = (\omega_1 + \omega_2)/2 \ .$$

The last corollary concerns the set of all G-invariant states. It is a partial generalization of Corollary 4.3.11.

Corollary 5.3.42. *Let $(\mathfrak{A}, G, \tau)$ be a C^*-dynamical system, where G is a locally compact, σ-compact, topological group and $\mathfrak{A}$ has an identity, and define $F = E^G_{\mathfrak{A}}$ as the set of all G-invariant states on $\mathfrak{A}$.*

It follows that all the statements (1)–(7) *in Theorem* 5.3.38 *are equivalent for F.*

PROOF. $F = E^G_{\mathfrak{A}}$ clearly satisfies the requirements of Theorem 5.3.38.

We know that all extremal ground states are pure, by Theorem 5.3.37. It is remarkable that if ω is a general ergodic state on a C^*-dynamical system $(\mathfrak{A}, \mathbb{R}, \tau)$ with energy spectrum unequal to the whole real line, then ω is either pure or can be decomposed into pure states with lower symmetry in a manner analogous to that given in Theorem 4.3.37.

Theorem 5.3.43. *Let ω be an $\mathbb{R}$-ergodic state on a C^*-dynamical system $(\mathfrak{A}, \mathbb{R}, \tau)$, and assume that the spectrum of the associated unitary representation U_ω of $\mathbb{R}$ is not the whole real line.*

It follows that ω is either pure, or there exists a pure state $\tilde{\omega}$ and a positive real number T such that

(1) $$\omega(A) = \frac{1}{T}\int_0^T dt\, \tilde{\omega}(\tau_t(A))$$

for all $A \in \mathfrak{A}$,

(2) *$\tilde{\omega}$ is periodic with period T, i.e., $\tilde{\omega} \circ \tau_T = \tilde{\omega}$,*

(3) *$\tilde{\omega}$ and $\tilde{\omega} \circ \tau_t$ are disjoint, $\tilde{\omega} \overset{\downarrow}{\circ} \tilde{\omega} \circ \tau_t$, whenever $0 < t < T$.*

Furthermore, a pure state $\tilde{\omega}$ with the properties (1)–(3) *is unique up to transformations by τ_t.*

PROOF. Let $\mathfrak{M} = \pi_\omega(\mathfrak{A})''$. Since

$$U_\omega(t)\mathfrak{M}U_\omega(t)^* = \mathfrak{M}$$

for all $t \in \mathbb{R}$, one must have

$$U_\omega(t)\mathfrak{M}'U_\omega(t)^* = \mathfrak{M}'$$

for all $t \in \mathbb{R}$. Hence one can define τ on $\mathfrak{M}'$ by

$$\tau_t(A) = U_\omega(t) A U_\omega(t)^* \ , \qquad A \in \mathfrak{M}' \ .$$

But since Ω_ω is separating for $\mathfrak{M}'$, one has

$$\sigma_\tau(\mathfrak{M}') = \sigma(U_\omega|_{\mathfrak{M}'\Omega})$$

in the notation of Definition 3.2.37. Now it follows from the ergodicity of ω, and Theorem 4.3.17, that

$$\mathfrak{M}' \cap U_\omega(\mathbb{R})' = \mathbb{C}\mathbb{1}_\omega \ ,$$

i.e., τ is ergodic on $\mathfrak{M}'$ in the usual sense. Therefore, the argument used in the proof of Theorem 4.3.33 implies that $\sigma_\tau(\mathfrak{M}')$ is additive. But $\sigma_\tau(\mathfrak{M}')$ is symmetric by Lemma 3.2.42. Hence the spectrum $\sigma_\tau(\mathfrak{M}')$ is a group and since $\sigma(U_\omega)$ is not the whole real line there are only two possibilities.

Case 1. $\sigma_\tau(\mathfrak{M}') = 0$.

In this case the action τ on $\mathfrak{M}'$ is trivial, i.e.,

$$\mathfrak{M}' \subseteq U_\omega(\mathbb{R})'$$

and hence

$$\mathfrak{M}' = \mathfrak{M}' \cap U_\omega(\mathbb{R})' = \mathbb{C}\mathbb{1}_\omega \ .$$

It follows that π_ω is irreducible and ω is pure.

Case 2. $\sigma_\tau(\mathfrak{M}') = 2\pi\mathbb{Z}/T$ for some $T > 0$.

It follows from ergodicity, as in the proof of Theorem 4.3.31, that the spectral subspaces

$$(\mathfrak{M}')^\tau(\{2\pi n/T\})$$

are one-dimensional, and there exists a unitary operator

$$V \in (\mathfrak{M}')^\tau(\{-2\pi/T\})$$

such that the linear span of the powers V^n, $n \in \mathbb{Z}$, of V is dense in $\mathfrak{M}'$. In particular $\mathfrak{M}'$ is abelian.

Note that

$$\tau_t(V) = e^{i2\pi t/T} V$$

and hence the spectrum of V is equal to the unit circle,

$$\sigma(V) = \mathbb{T} \ .$$

The Gelfand transform, Theorem 2.1.11B, identifies the C^*-algebra $\mathfrak{C}$ generated by V with $C(\mathbb{T})$, and the restriction of τ_t to $\mathfrak{C}$ identifies with rotation through the angle $2\pi t/T$.

Define a probability measure μ on $\mathbb{T}$ by

$$\mu(\hat{C}) = (\Omega_\omega, C\Omega_\omega)$$

for $C \in \mathfrak{C}$, where $\hat{C}$ denotes the Gelfand transform of C. By τ-invariance, μ is the normalized Haar measure on $\mathbb{T}$. Put $F_\omega = [\mathfrak{M}'\Omega_\omega]$. If $A \in \mathfrak{A}$ is an element with bounded τ-spectrum, then

$$F_\omega \pi_\omega(A) F_\omega \in F_\omega \mathfrak{M} F_\omega = \mathfrak{M}' F_\omega$$

is an element in $\mathfrak{M}' F_\omega$ with bounded τ-spectrum and hence

$$F_\omega \pi_\omega(A) F_\omega \in \mathfrak{C} F_\omega \ .$$

It follows by norm continuity that

$$F_\omega \pi_\omega(\mathfrak{A}) F_\omega \subseteq \mathfrak{C} F_\omega \ .$$

Thus, if $A \in \mathfrak{A}$, there exists a unique $C \in \mathfrak{C}$ such that

$$F_\omega \pi_\omega(A) F_\omega = C F_\omega$$

and hence a unique function

$$\gamma \in \mathbb{T} \mapsto \tilde{\omega}_\gamma(A) = \hat{C}(\gamma)$$

in $C(\mathbb{T})$ corresponding to A. Since $\tilde{\omega}_\gamma(\mathbb{1}) = 1$ and $\tilde{\omega}_\gamma(A) \geq 0$ if $A \geq 0$, it follows that $\tilde{\omega}_\gamma$ is a state for all $\gamma \in \mathbb{T}$. (If $\mathbb{1} \notin \mathfrak{A}$, one uses an approximate identity and Proposition 2.3.11.) Now if $D \in \mathfrak{C}$ we have

$$\begin{aligned}(\Omega_\omega, \pi_\omega(A) D \Omega_\omega) &= (\Omega_\omega, F_\omega \pi_\omega(A) F_\omega D \Omega_\omega) \\ &= (\Omega_\omega, C D \Omega_\omega) \\ &= \int_{\mathbb{T}} d\mu(\gamma) \hat{C}(\gamma) \hat{D}(\gamma) = \int_{\mathbb{T}} d\mu(\gamma) \tilde{\omega}_\gamma(A) \hat{D}(\gamma) \ .\end{aligned}$$

Since $\mathfrak{C}$ is dense in $\mathfrak{M}' = \mathfrak{M}'' \cap \mathfrak{M}'$, it follows from this expression, Proposition 4.1.22, and Theorem 4.2.4, that

$$\omega(A) = \int_{\mathbb{T}} d\mu(\gamma) \tilde{\omega}_\gamma(A)$$

identifies with the central decomposition of ω, and this is just the unique extremal decomposition in this case.

Since ω is τ-invariant we find

$$\int_{\mathbb{T}} d\mu(\gamma) \tilde{\omega}_\gamma(A) \hat{D}(\gamma) = (\Omega_\omega, \pi_\omega(A) D \Omega_\omega) = \int_{\mathbb{T}} d\mu(\gamma) \tilde{\omega}_\gamma(\tau_t(A)) \hat{D}\left(\gamma + \frac{2\pi t}{T}\right)$$

and as this is true for all $\hat{D} \in C(\mathbb{T})$ it follows, by continuity, that

$$\tilde{\omega}_{\gamma + 2\pi t/T}(A) = \tilde{\omega}_\gamma(\tau_t(A))$$

for all $t \in \mathbb{R}, \gamma \in \mathbb{T}$, and $A \in \mathfrak{A}$. Thus we may define

$$\tilde{\omega} = \tilde{\omega}_0$$

and then the central (= extremal) decomposition takes the form

$$\omega(A) = \frac{1}{T} \int_0^T dt\, \tilde{\omega}(\tau_t(A)) \ .$$

Since $\tilde{\omega} \circ \alpha_t$ is pure for μ-almost all $t, \tilde{\omega}$ is pure. If $\tilde{\omega}$ were equivalent to $\tilde{\omega} \circ \alpha_t$ for some $0 < t < T$, then $\tilde{\omega} \circ \alpha_s$, would be equivalent to $\tilde{\omega} \circ \alpha_{t+s}$ for all $s \in \mathbb{R}$, and this contradicts the fact that the decomposition of ω is the central decomposition. The uniqueness statement follows from the uniqueness of the central decomposition.

Remark. Since the decomposition in Theorem 5.3.43 is the central decomposition the corresponding measure is an orthogonal measure. Moreover one concludes, *a posteriori*, that the decomposition coincides with that of Theorem 4.3.37 with $H = T\mathbb{Z}$, but the H-ergodic states $\{\tau_t^* \tilde{\omega};\ t \in H\}$ are in fact pure. Finally one can establish that the assumptions of Theorem 5.3.43 do not imply that the pair $(\mathfrak{A}, \omega)$ is H-abelian and hence the result is not a direct consequence of Theorem 4.3.37.

The important feature in Theorem 5.3.43 is the occurrence of a periodic structure. The construction used in the proof allows one to conclude a strong uniqueness statement for the decomposition of ergodic states of systems for which τ is periodic.

Corollary 5.3.44. *Let $(\mathfrak{A}, \mathbb{R}, \tau)$ be a C^*-dynamical system where τ is periodic with period T, and assume that ω is an $\mathbb{R}$-ergodic state on $\mathfrak{A}$.*

It follows that there exists a pure state $\tilde{\omega}$ such that

$$\omega(A) = \frac{1}{T}\int_0^T dt\, \tilde{\omega}(\tau_t(A))$$

for all $A \in \mathfrak{A}$, and any two translates $\tilde{\omega} \circ \tau_s$ and $\tilde{\omega} \circ \tau_t$ of $\tilde{\omega}$ are either equal or disjoint. Furthermore, $\tilde{\omega}$ is unique up to translation by τ.

Proof. The periodicity assumption on τ implies that the unitary representation U_ω is periodic with period T, and hence

$$\sigma(U_\omega) \subseteq 2\pi\mathbb{Z}/T \ .$$

If ω is pure we may set $\tilde{\omega} = \omega$, if not we use the $\tilde{\omega}$ of Theorem 5.3.43 and note that the period T of τ is an integer multiple of the period T occurring in Theorem 5.3.43.

This last result partially complements the discussion of the uniqueness of the ergodic decomposition given in Chapter 4. It should, however, be emphasized that the periodic assumption which is crucial for the uniqueness of the extremal decomposition in Corollary 5.3.44 is largely incompatible with the conditions of asymptotic abelianness which are relevant for uniqueness of ergodic decompositions. More precisely, if $(\mathfrak{A}, G, \tau)$ is a C^*-dynamical system based on a compact group G one can establish that $(\mathfrak{A}, \omega)$ is G-abelian for all $\omega \in E_{\mathfrak{A}}^G$ if and only if the fixed-point algebra $\mathfrak{A}^\tau$ is abelian. The latter situation is atypical if $\mathfrak{A}$ is simple and G is compact.

5.4. Stability and Equilibrium

5.4.1. Stability of KMS States

In the previous section we analyzed properties of individual KMS states and affine properties of the set of KMS states. But hitherto we made no attempts to justify the interpretation of KMS states as equilibrium states of quantum-mechanical systems. The purpose of this section is to remedy this omission.

We have noted several times that the finite-volume Gibbs states are the unique KMS states and that the KMS property, or at least the accompanying modular structure, has a tendency to persist in the infinite-volume limit. Thus empirical acceptance of the Gibbs formalism indicates that the KMS property is a suitable characterization of equilibrium and this motivated the foregoing analysis. Now, however, we attempt to derive the KMS condition from various general, physically motivated, properties, notably properties of ergodicity and stability. As a preliminary we analyze the stability properties of KMS states and ground states under perturbation of the dynamics.

In Section 3.1.4 we discussed perturbations of generators of C_0- and C_0^*-semigroups and we now apply this theory to groups of *-automorphisms τ of C^*- and W^*-algebras. We are particularly interested in perturbations by bounded symmetric derivations, and the algebraic structure leads to several refinements of the general theory. For example, the derivation property ensures that the perturbed group τ^P is a group of *-automorphisms and hence it is norm-preserving by Corollary 2.3.4. This strengthens one of the conclusions of Theorem 3.1.33. Next recall that every bounded symmetric derivation δ of a W^*-algebra $\mathfrak{M}$ is inner by Corollary 3.2.47, i.e., there is an $H = H^* \in \mathfrak{M}$ such that

$$\delta(A) = i[H, A]$$

for all $A \in \mathfrak{M}$. A similar result is true for representations of C^*-algebras, Corollary 3.2.48. Thus, it is natural to concentrate on inner derivations. The perturbation series for τ^P then assumes a distinctive form in terms of commutators and τ, and τ^P, are related in a simple algebraic fashion by a unitary co-cycle.

Proposition 5.4.1. *Let $(\mathfrak{A}, \tau)$ be a C^*- or W^*-dynamical system and let δ denote the infinitesimal generator of τ. Furthermore, for each $P = P^* \in \mathfrak{A}$ define the bounded derivation δ_P by $D(\delta_P) = \mathfrak{A}$ and $\delta_P(A) = i[P, A]$ for $A \in \mathfrak{A}$.*

It follows that $\delta + \delta_P$ generates a one-parameter group of *-automorphisms τ^P of $\mathfrak{A}$ given by

$$\tau_t^P(A) = \tau_t(A) + \sum_{n\geq 1} i^n \int_0^t dt_1 \int_0^{t_1} dt_2 \cdots \int_0^{t_{n-1}} dt_n [\tau_{t_n}(P), [\cdots [\tau_{t_1}(P), \tau_t(A)]]] \ .$$

Moreover, one has

$$\tau_t^P(A) = \Gamma_t^P \tau_t(A) \Gamma_t^{P*} \ ,$$

where $\Gamma_t^P \in \mathfrak{A}$ is a one-parameter family of unitary elements, determined by

$$\begin{aligned}\Gamma_t^P &= \mathbb{1} + \sum_{n\geq 1} i^n \int_0^t dt_1 \int_0^{t_1} dt_2 \cdots \int_0^{t_{n-1}} dt_n \tau_{t_n}(P) \cdots \tau_{t_1}(P) \\ &= \mathbb{1} + \sum_{n\geq 1} i^n \int_0^t dt_1 \int_0^{t_1} dt_2 \cdots \int_0^{t_{n-1}} dt_n \tau_{t_1}^P(P) \cdots \tau_{t_n}^P(P) \ ,\end{aligned}$$

which satisfies the co-cycle relation

$$\Gamma_{t+s}^P = \Gamma_t^P \tau_t(\Gamma_s^P) \ .$$

All integrals converge in the strong topology for the C^*-system and in the σ-weak topology for the W^*-system. The integrals define norm-convergent series of bounded operators and

$$\|\tau_t^P(A) - \tau_t(A)\| \leq (e^{|t|\,\|P\|} - 1)\|A\|, \qquad \|\Gamma_t^P - \mathbb{1}\| \leq (e^{|t|\|P\|} - 1) \ .$$

Proof. We give the proof for the C^*-system. The W^*-case follows by transposition from the predual as in the proof of Theorem 3.1.33.

The first statement of the proposition can be obtained from Theorem 3.1.33 by suitable replacement of X by $\mathfrak{A}$, etc. but it is most easily deduced from the proof of the latter theorem. This proof established that τ^P is the unique solution of the integral equation.

$$\tau_t^P(A) = \tau_t(A) + i \int_0^t dt_1 [\tau_{t_1}(P), \tau_{t_1} \tau_{t-t_1}^P(A)] \ .$$

Alternatively τ^P is the unique solution of the integral equation

$$\tau_t^P(A) = \tau_t(A) + i \int_0^t dt_1 \tau_{t_1}^P \tau_{-t_1}([\tau_{t_1}(P), \tau_t(A)]) \ .$$

Solution by iteration gives the perturbation expansion of τ^P. The automorphism property of τ^P follows with the aid of the derivation condition, e.g.,

$$\frac{d}{dt} \tau_{-t}^P(\tau_t^P(A)\tau_t^P(B)) = 0 \ .$$

Next consider Γ_t^P defined by the first series. The nth term in this series is well-defined and has norm less than $|t|^n \|P\|^n/n!$. Thus Γ_t^P is a norm-continuous one-parameter family of elements of $\mathfrak{A}$ with $\Gamma_0^P = \mathbb{1}$. Consequently Γ_t^P is invertible for all $t \in [-t_0, t_0]$ for some $t_0 > 0$. Next one has

$$\frac{d\Gamma_t^P}{dt} = i\Gamma_t^P \tau_t(P) \ , \qquad \frac{d\Gamma_t^{P*}}{dt} = -i\tau_t(P)\Gamma_t^{P*} \ ,$$

in the strong sense and hence

$$\frac{d(\Gamma_t^P \Gamma_t^{P*})}{dt} = 0 \ .$$

Therefore, $\Gamma_t^P \Gamma_t^{P*} = \mathbb{1}$ and Γ_t^P is unitary for $t \in [-t_0, t_0]$. Unitarity for other t will follow from the co-cycle relation. To establish this relation we first note that

$$\frac{d\Gamma_{t+s}^P}{ds} = i\Gamma_{t+s}^P \tau_{t+s}(P)$$

and $\Gamma_{t+s}^P|_{s=0} = \Gamma_t^P$. But $\tau_t(\Gamma_s^P) = \Gamma_s^{\tau_t(P)}$ and hence

$$\frac{d}{ds}\Gamma_t^P \tau_t(\Gamma_s^P) = i\Gamma_t^P \Gamma_s^{\tau_t(P)} \tau_s(\tau_t(P)) = i\Gamma_t^P \tau_t(\Gamma_s^P)\tau_{t+s}(P) \ .$$

Moreover, $\Gamma_t^P \tau_t(\Gamma_s^P)|_{s=0} = \Gamma_t^P$. Thus $s \mapsto \Gamma_{t+s}^P$ and $s \mapsto \Gamma_t^P \tau_t(\Gamma_s^P)$ satisfy the same first-order differential equation and boundary condition, for each $t \in \mathbb{R}$. Therefore, the two functions are equal and can be obtained by iteration of the integral equation

$$X_t(s) = \Gamma_t^P + i\int_0^s ds' X_t(s')\tau_{t+s'}(P) \ .$$

Next the unitarity and norm continuity of Γ^P ensure that $t \mapsto \Gamma_t^P \tau_t(A)\Gamma_t^{P*}$ defines a strongly continuous one-parameter group of *-automorphisms of $\mathfrak{A}$. Let $\tilde{\delta}$ denote the infinitesimal generator of this group and set $A = (\lambda\imath + \delta + \delta_P)^{-1}(B)$ for $\lambda \in \mathbb{R}\backslash\{0\}$. One has

$$\begin{aligned}(\lambda\imath + \tilde{\delta})(A) &= \left(\lambda\imath + \frac{d}{dt}\right)(\Gamma_t^P \tau_t(A)\Gamma_t^{P*})|_{t=0} \\ &= (\Gamma_t^P \tau_t((\lambda\imath + \delta + \delta_P)(A))\Gamma_t^{P*})|_{t=0} = B \ .\end{aligned}$$

But $(\lambda\imath + \tilde{\delta})^{-1}$ is bounded, by Proposition 3.1.6, and hence

$$A = (\lambda\imath + \tilde{\delta})^{-1}(B) = (\lambda\imath + \delta + \delta_P)^{-1}(B)$$

for all $B \in \mathfrak{A}$. It then follows from Theorem 3.1.10 that

$$\begin{aligned}\tau_t^P(B) &= \lim_{n\to\infty}\left(\imath - \frac{t}{n}(\delta + \delta_P)\right)^{-n}(B) \\ &= \lim_{n\to\infty}\left(\imath - \frac{t}{n}\tilde{\delta}\right)^{-n}(B) = \Gamma_t^P \tau_t(B)\Gamma_t^{P*}\end{aligned}$$

which gives the desired relation between τ^P and τ.

Now if one perturbs τ^P by a perturbation $-P$, then the final group of automorphisms is τ because it has the generator $(\delta + \delta_P) - \delta_P = \delta$.

Therefore, one must have

$$\tau_t(A) = \hat{\Gamma}_t^P \tau_t^P(A)\hat{\Gamma}_t^{P*} \ ,$$

where

$$\hat{\Gamma}_t^P = \mathbb{1} + \sum_{n\geq 1}(-i)^n \int_0^t dt_1 \int_0^{t_1} dt_2 \cdots \int_0^{t_{n-1}} dt_n\, \tau_{t_n}^P(P)\cdots\tau_{t_1}^P(P) \ .$$

Consequently

$$\tau_t^P = (\widehat{\Gamma}_t^P)^* \tau_t(A)(\widehat{\Gamma}_t^P) \ .$$

But then

$$\frac{d}{dt}(\widehat{\Gamma}_t^P)^* = i\tau_t^P(P)(\widehat{\Gamma}_t^P)^* = i(\widehat{\Gamma}_t^P)^*\tau_t(P) \ .$$

Thus, $(\hat{\Gamma}^P)^*$ and Γ^P satisfy the same first-order differential equation and boundary condition at $t = 0$. Therefore, $\Gamma_t^P = (\widehat{\Gamma}_t^P)^*$ which is the second identification of Γ^P.

Finally the estimates on $\tau^P - \tau$ and $\Gamma^P - \mathbb{1}$ are straightforward.

Throughout the sequel we use the notation introduced in Proposition 5.4.1 for the perturbed automorphism group τ^P and the related co-cycle Γ^P. This proposition establishes that the map $P \in \mathfrak{A} \mapsto \tau^P \in \operatorname{Aut} \mathfrak{A}$ is continuous with respect to the norm topology on $\mathfrak{A}$ and the strong topology on the automorphism groups. If $(\mathfrak{A}, \tau)$ acts on a Hilbert space and τ is unitarily implemented, one easily attains continuity properties for strong convergence. Moreover, the group τ^P is unitarily implemented and the co-cycle Γ^P has a simple identification.

Corollary 5.4.2. *Adopt the assumptions of Proposition* 5.4.1 *but also assume that* $\mathfrak{A}$ *acts on a Hilbert space* $\mathfrak{H}$ *and*

$$\tau_t(A) = U_t A U_t^* \ ,$$

where $U_t = \exp\{itH\}$ *is a strongly continuous one-parameter group of unitary operators.*

It follows that

$$\tau_t^P(A) = U_t^P A U_t^{P*} \ , \qquad \Gamma_t^P = U_t^P U_{-t} \ ,$$

where

$$U_t^P = \exp\{it(H+P)\} \ .$$

If, finally, P_n *is a sequence of selfadjoint elements of* $\mathfrak{A}$ *which converges strongly to zero, then*

$$\lim_{n\to\infty} \|(\Gamma_t^{P_n} - \Gamma_t)\psi\| = 0, \qquad \lim_{n\to\infty} \|(\tau_t^{P_n}(A) - \tau_t(A))\psi\| = 0 \, ,$$

for all $\psi \in \mathfrak{H}$ *and* $A \in \mathfrak{A}$, *uniformly for* t *in finite intervals of* $\mathbb{R}$.

Proof. If U^P is defined as in the statement of the corollary and $X_t = U_t^P U_{-t}$, then

$$\frac{dX_t}{dt} = iU_t^P P U_{-t} = iX_t\tau_t(P)$$

and $X_0 = \mathbb{1}$. Thus, X_t is the unique solution of the integral equation

$$X_t = \mathbb{1} + i\int_0^t ds\, X_s\tau_s(P) \ .$$

This solution can be obtained by iteration and one finds $X_t = \Gamma_t^P$, where Γ^P is defined as in Proposition 5.4.1. The identification of τ^P follows immediately from this proposition. Moreover

$$\|(\Gamma_t^{P_n} - \mathbb{1})\psi\| \le \int_0^{|t|} ds \|P_n U_{-s}\psi\| \ .$$

But strongly convergent sequences are uniformly bounded and hence Γ^{P_n} converges strongly to the identity, with the appropriate uniformity, by the Lebesgue-dominated convergence theorem. The convergence of τ^{P_n} to τ then follows from the representation

$$\tau_t^{P_n}(A) = \Gamma_t^{P_n}\tau_t(A)\Gamma_t^{P_n *} \ .$$

EXAMPLE 5.4.3. Let $\mathfrak{A}(\mathfrak{h})$ be the CAR algebra over the Hilbert space $\mathfrak{h}$ and τ a one-parameter group of Bogoliubov transformations such that $\tau_t(a(f)) = a(U_t f)$ with $U_t = \exp\{itH\}$. The simplest symmetric perturbations are given by quadratic elements, $a^*(f)a(f)$ or combinations of such elements, e.g.,

$$a^*(f)a(g) + a^*(g)a(f) = (a^*(f+g)a(f+g) - a^*(f-g)a(f-g))/2 \ .$$

The group τ^P resulting from a quadratic perturbation is also a group of Bogoliubov transformations because for

$$P = \sum_{j=1}^{n} \lambda_j a^*(f_j)a(f_j)$$

one has

$$\delta_P(a(f)) = i\sum_{j=1}^{n} \lambda_j(f, f_j)a(f_j) \ .$$

It follows that $\tau_t^P(a(f)) = a(U_t^P f)$ with $U_t^P = \exp\{it(H + \Sigma_{j=1}^n \lambda_j E_j)\}$ where E_j is the projection on f_j, i.e.,

$$E_j g = (f_j, g)f_j$$

for all $g \in \mathfrak{h}$.

Quadratic perturbations of Bogoliubov transformations of the CCR algebra can also be introduced for regular representations but as the creation and annihilation operators are unbounded these perturbations are only affiliated with the representation.

Next we examine stability properties of KMS states ω over a dynamical system $(\mathfrak{A}, \tau)$ and establish that each such state has a vector state ω^P which is a KMS state for the perturbed evolution τ^P. Subsequently, we deduce that the (τ, β)-KMS states and the (τ^P, β)-KMS states are in one-to-one correspondence. If the KMS states are identified as equilibrium states of a physical system, these properties correspond to stability of the pure phases, and the overall phase structure, under perturbations. These results are obtained with various perturbation series which are easily understood in the finite-dimensional situation.

Let M_n denote the C^*-algebra of $n \times n$ matrices on the n-dimensional Hilbert space $\mathfrak{H}_n$ and for $H = H^* \in M_n$ define the automorphism group τ by

$$\tau_t(A) = e^{itH}Ae^{-itH} \ .$$

The perturbed group τ^P corresponding to $P = P^* \in M_n$ is then given by

$$\tau_t^P(A) = e^{it(H+P)}Ae^{-it(H+P)} \ .$$

Moreover, by Example 5.3.31, the state

$$\omega(A) = \frac{\mathrm{Tr}_{\mathfrak{H}_n}(e^{-\beta H}A)}{\mathrm{Tr}_{\mathfrak{H}_n}(e^{-\beta H})}$$

is the unique (τ, β)-KMS state and the state

$$\omega^P(A) = \frac{\mathrm{Tr}_{\mathfrak{H}_n}(e^{-\beta(H+P)}A)}{\mathrm{Tr}_{\mathfrak{H}_n}(e^{-\beta(H+P)})}$$

is the unique (τ^P, β)-KMS state. But ω^P can be expressed in terms of ω in several ways.

First,

$$\omega^P(A) = \frac{\omega(A\Gamma^P_{i\beta})}{\omega(\Gamma^P_{i\beta})}$$

where

$$\Gamma^P_{i\beta} = e^{-\beta(H+P)}e^{\beta H} \quad ,$$

i.e., $\Gamma^P_{i\beta}$ is the analytic extension of the co-cycle Γ^P, which relates τ^P and τ, at the point $i\beta$. This identification follows simply from cyclicity of the trace. But one has

$$\Gamma^P_{i\beta} = \mathbb{1} + \sum_{n\geq 1}(-1)^n \int_0^\beta ds_1 \int_0^{s_1} ds_2 \cdots \int_0^{s_{n-1}} ds_n\, \tau_{is_n}(P)\cdots\tau_{is_1}(P)$$

and this allows ω^P to be expressed as the ratio of two perturbation series. This ratio can then be rearranged as an expansion of ω^P in terms of ω. Somewhat surprisingly, the terms of this latter expansion are integrals of truncated functions.

Similarly one finds the symmetric form for ω^P in terms of ω

$$\omega^P(A) = \frac{\omega((\Gamma^P_{i\beta/2})^*A(\Gamma^P_{i\beta/2}))}{\omega((\Gamma^P_{i\beta/2})^*(\Gamma^P_{i\beta/2}))}$$

and this yields a different set of expansions. This symmetric expression is particularly useful for the study of the associated representation because one may choose Ω_{ω^P} such that

$$\Omega_{\omega^P} = \frac{\pi_\omega(\Gamma^P_{i\beta/2})\Omega_\omega}{\|\pi_\omega(\Gamma^P_{i\beta/2})\Omega_\omega\|}$$

and then deduce an expansion of the cyclic vector.

Stability properties of general τ-KMS states can now be analyzed by exploitation of these algorithms for $\omega^P, \Omega_{\omega^P}$, etc., and the perturbation series for the Γ^P_{is} to construct τ^P-KMS states. In the finite-dimensional case the various series are evidently well-defined and uniformly convergent but in the general case this is less evident. The necessary estimations are consequences of the τ-KMS condition.

The major features of stability of KMS states are shared by C^*- and W^*-dynamical systems. Discussion of the W^*-case is however more complex because it depends upon approximations in the strong operator topology while the C^*-case can be handled by uniform approximation. We next state the common results, give the detailed proof for C^*-systems, and outline the proof for W^*-systems.

Theorem 5.4.4. *Let $(\mathfrak{A}, \tau)$ be a C^*- or a W^*-dynamical system acting on a Hilbert space $\mathfrak{H}$ such that*

$$\tau_t(A) = U_t A U_t^* \ ,$$

where $U_t = \exp\{itH\}$ is a strongly continuous one-parameter unitary group, and Ω a normalized U-invariant cyclic vector such that the associated vector state, $\omega(A) = (\Omega, A\Omega)$, is a τ-KMS state.

The following statements are valid:

(1) *If $P = P^* \in \mathfrak{A}$, then $\Omega \in D(\mathscr{P}(z))$, where*

$$\mathscr{P}(z) = \tau_{z_n}(P) \cdots \tau_{z_1}(P) = e^{iz_nH} P e^{i(z_{n-1}-z_n)H} P \cdots P e^{-iz_1H}$$

for all $z = (z_1, \ldots, z_n)$ in the tube $\mathfrak{D}^{(n)}_{-1/2}$ defined by

$$\mathfrak{D}^{(n)}_{\alpha} = \{z;\ \alpha < \operatorname{Im} z_1 < \operatorname{Im} z_2 \cdots < \operatorname{Im} z_n < 0\} \ .$$

The vector-valued function $\mathscr{P}(z)\Omega$ is holomorphic in the tube $\mathfrak{D}^{(n)}_{-1/2}$, strongly continuous and uniformly bounded on its closure $\overline{\mathfrak{D}^{(n)}_{-1/2}}$, and

$$\sup_{z \in \mathfrak{D}^{(n)}_{-1/2}} \|\mathscr{P}(z)\Omega\| \leq \|P\|^n \ .$$

(2) *If $P = P^* \in \mathfrak{A}$, then $\Omega \in D(e^{(H+P)/2})$ and the vector $\Omega^P = e^{(H+P)/2}\Omega$ has the strongly convergent perturbation expansion*

$$\Omega^P = \Omega + \sum_{n \geq 1} \int_{-1/2 \leq s_1 \leq \cdots \leq s_n \leq 0} ds_1 \cdots ds_n\, \tau_{is_n}(P) \cdots \tau_{is_1}(P)\Omega \ .$$

Moreover, the state ω^P defined by

$$\omega^P(A) = \frac{(\Omega^P, A\Omega^P)}{(\Omega^P, \Omega^P)}$$

is a τ^P-KMS state and it is the unique τ^P-KMS normal state if, and only if, $\mathfrak{A}''$ is a factor.

(3) *For each $A \in \mathfrak{A}$ and $P = P^* \in \mathfrak{A}$, the truncated function*

$$F_A(t_1, \ldots, t_n) = \omega_T(A, \tau_{t_n}(P), \ldots, \tau_{t_1}(P))$$

is the boundary value of a function $F_A(z) (= \omega_T(A, \tau_{z_n}(P), \ldots, \tau_{z_1}(P)))$ which is holomorphic in the tube $\mathfrak{D}^{(n)}_{-1}$, continuous and uniformly bounded on its closure $\overline{\mathfrak{D}^{(n)}_{-1}}$, and

$$\sup_{z \in \mathfrak{D}_{-1}^{(n)}} |F_A(z)| \leq 2^n n! \|P\|^n \|A\| \ .$$

Moreover, if $2\|P\| < 1$ *the perturbed state* ω^P *is determined by the uniformly convergent series*

$$\omega^P(A) = \omega(A) + \sum_{n \geq 1} \int_{-1 \leq s_1 \leq \cdots \leq s_n \leq 0} \times ds_1 \cdots ds_n \, \omega_T(A, \tau_{is_n}(P), \ldots, \tau_{is_1}(P))$$

and hence

$$\lim_{\alpha} \|\omega^{P_\alpha} - \omega\| = 0$$

for each net $P_\alpha = P_\alpha^* \in \mathfrak{A}$ *such that* $\|P_\alpha\| \to 0$.

Remark. The convention $\beta = -1$ which we adopt in the theorem is convenient but slightly confusing for later applications. With this convention the perturbation corresponds to the addition of the "energy" P to the Hamiltonian H, i.e., the generator of the modular unitary group. If, however, one rescales by replacing τ_t with $\tau_{-\beta t}$ and simultaneously replaces P by βP, then H is replaced by $H - P$. Thus, the perturbation corresponds to the subtraction of the "energy" P. This is most easily seen by examining the perturbation of Ω. With $\beta = -1$ one has

$$\Omega^P = e^{(H+P)/2}\Omega \ .$$

But the rescaling $\tau_t \mapsto \tau_{-\beta t}$ corresponds to the replacement $H \mapsto -\beta H$ and hence for general β one has

$$\Omega^{\beta P} = e^{(-\beta H + \beta P)/2}\Omega = e^{-\beta(H-P)/2}\Omega \ .$$

Proof. We examine first the C^*-system.

(1) First choose $P_L \in \mathfrak{A}_\tau$ such that $\|P_L\| \leq \|P\|$ and $\|P_L - P\| \to 0$. This is possible by Proposition 2.5.22 and one has

$$\|(\mathscr{P}_L(z) - \mathscr{P}_M(z))\Omega\| \leq \sum_{j=1}^{n} \|\tau_{z_n}(P_L) \cdots \tau_{z_j}(P_L - P_M) \cdots \tau_{z_1}(P_M)\Omega\| \ .$$

For $z \in \mathfrak{D}_{-1/2}^{(n)}$ the right-hand side can be estimated by repeated application of the three line theorem, Proposition 5.3.5, to the vector-valued functions

$$F(z) = \tau_{z_n}(Q_n) \cdots \tau_{z_1}(Q_1)\Omega \ ,$$

where the $Q_i \in \mathfrak{A}_\tau$ are subsequently identified with P_L, P_M, etc. Thus, the maximum value of the norm of F is attained at one of the $n+1$ points

$$s_1 = s_2 = \cdots = s_j = -\frac{1}{2}, \quad s_{j+1} = s_{j+2} = \cdots = s_n = 0 \ ,$$

where $s_i = \operatorname{Im} z_i$. But at such a point

$$\begin{aligned}
&|F(t_1 - i/2, \ldots, t_j - i/2, t_{j+1}, \ldots, t_n)|^2 \\
&\quad \leq \|Q_n\|^2 \cdots \|Q_{j+1}\|^2 \|\tau_{-i/2}(\tau_{t_j}(Q_j) \cdots \tau_{t_1}(Q_1))\Omega\|^2 \\
&\quad = \|Q_n\|^2 \cdots \|Q_{j+1}\|^2 \|\tau_{t_1}(Q_1^*) \cdots \tau_{t_j}(Q_j^*)\Omega\|^2 \leq \prod_{j=1}^{n} \|Q_j\|^2 \ .
\end{aligned}$$

The equality of the second line follows from the τ-KMS condition (at value $\beta = -1$) in the symmetric form derived in Proposition 5.3.3. Therefore, one has

$$\|(\mathscr{P}_L(z) - \mathscr{P}_M(z))\Omega\| \ \leq \ \|P_L - P_M\| \sum_{j=1}^{n} \|P_L\|^{j-1} \|P_M\|^{n-j}$$

for all $z \in \overline{\mathfrak{D}^{(n)}_{-1/2}}$. Hence $\mathscr{P}_L(z)\Omega$ is a Cauchy sequence uniformly on $\overline{\mathfrak{D}^{(n)}_{-1/2}}$. Because of the uniformity and the choice of $P_L \in \mathfrak{A}_\tau$ the limit function $\Omega(z)$ has the holomorphy and continuity properties stated for $\mathscr{P}(z)\Omega$. Moreover, by the same estimates

$$\|\Omega(z)\| \ \leq \ \lim_{L \to \infty} \|\mathscr{P}_L(z)\Omega\| \ \leq \ \|P\|^n$$

for all $z \in \overline{\mathfrak{D}^{(n)}_{-1/2}}$. It remains to identify $\Omega(z)$ and $\mathscr{P}(z)\Omega$.

It follows from Corollary 5.3.4 and Theorem 5.3.10 that $\Delta = e^H$ is the modular operator for the pair $(\mathfrak{A}'', \Omega)$ and in particular $\mathfrak{A}\Omega \subset D(\Delta^{iz})$ whenever $-\frac{1}{2} \leq \operatorname{Im} z \leq 0$. But Δ^{iz} is closed and hence

$$\Delta^{iz} P\Omega = \lim_{L \to \infty} \Delta^{iz} P_L \, \Omega \ .$$

This establishes $\Omega(z) = \mathscr{P}(z)\Omega$ for $n = 1$. Next assume the identification for $n \leq N - 1$. In particular for $z \in \mathfrak{D}^{(N)}_{-1/2}$

$$P_L \Delta^{i(z_{N-1} - z_N)} P_L \cdots \Delta^{i(z_1 - z_2)} P_L \Omega \to P \Delta^{i(z_{N-1} - z_N)} P \cdots P \Delta^{i(z_1 - z_2)} P\Omega \ .$$

But one also has

$$\Delta^{iz_N} P_L \Delta^{i(z_{N-1} - z_N)} P_L \cdots \Delta^{i(z_1 - z_2)} P_L \Omega \to \Omega(z)$$

by the previous estimates. Thus, as Δ^{iz_N} is closed, one obtains $\Omega(z) = \mathscr{P}(z)\Omega$.

The bound on $\|\mathscr{P}(z)\Omega\|$ follows by choosing $Q_L = P$ in the previous set of estimates.

(2) Assume $P \in \mathfrak{A}_\tau$ and define Γ^P_{is} by

$$\Gamma^P_{is} = \mathbb{1} + \sum_{n \geq 1} (-1)^n \int_0^s ds_1 \int_0^{s_1} ds_2 \cdots \int_0^{s_{n-1}} ds_n \tau_{is_n}(P) \cdots \tau_{is_1}(P) \ .$$

Each term in the series is well-defined because $P \in \mathfrak{A}_\tau$, the series converges uniformly, and $\Omega^P = \Gamma^P_{-i/2}\Omega$. Now calculating with convergent power series one concludes that $\Gamma^P_{is} \in \mathfrak{A}_\tau$ and

$$\tau_{is}(\Gamma^{P*}_{is} A) = \tau^P_{is}(A) \Gamma^P_{is}$$

for all $A \in \mathfrak{A}_\tau$. Therefore,

$$\begin{aligned}
(\Gamma^P_{-i/2}\Omega, \ \tau^P_{i/2}(A)\tau^P_{-i/2}(B)\Gamma^P_{-i/2}\Omega) &= (\tau_{-i/2}(\Gamma^{P*}_{-i/2}A^*)\Omega, \ \tau_{-i/2}(\Gamma^{P*}_{-i/2}B)\Omega) \\
&= (\Gamma^P_{-i/2}\Omega, \ BA\Gamma^P_{-i/2}\Omega)
\end{aligned}$$

for all $A, B \in \mathfrak{A}_\tau$, where the second step uses the symmetric form of the τ-KMS condition, Proposition 5.3.3. But Ω is separating for $\mathfrak{A}$ and hence $\Gamma^P_{-i/2}\Omega \neq 0$.

Therefore, the vector state ω^P is well-defined and is a τ^P-KMS state by Proposition 5.3.3. Next note that Γ^P is invertible.

$$(\Gamma^P_{is})^{-1} = \mathbb{1} + \sum_{n \geq 1} \int_0^s ds_1 \int_0^{s_1} ds_2 \cdots \int_0^{s_{n-1}} ds_n \tau_{is_1}(P) \cdots \tau_{is_n}(P)$$

and hence the set of vector states of ω and ω^P are identical. Thus, the equivalence of the uniqueness of ω^P, as a τ^P-KMS normal state of ω, and the factor property of ω follows from Theorem 5.3.30 or Proposition 5.3.29.

Next choose $\mathscr{P}_L \in \mathfrak{A}_\tau$ such that $\|P_L - P\| \to 0$ and define Ω^{P_L} and Ω^P by the perturbation expansion given in the theorem. It follows from the estimates of (1) that $\|\Omega^{P_L} - \Omega^P\| \to 0$. Moreover, $\|\tau_t^{P_L}(A) - \tau_t^P(A)\| \to 0$ for all $A \in \mathfrak{A}$ and $t \in \mathbb{R}$ by Proposition 5.4.1. Therefore, ω^{P_L} converges to a state ω^P and this state is a τ^P-KMS state by Proposition 5.3.25. By the same approximation procedure one concludes that the vector states of ω and ω^P are identical and the uniqueness-factoriality equivalence follows as before.

It remains to identify Ω^P and $e^{(H+P)/2}\Omega$.

First, define $\Omega^P(z)$ by

$$\Omega^P(z) = \Omega + \sum_{n \geq 1} z^n \int_{-1/2 \leq s_1 \leq \cdots \leq s_n \leq 0} ds_1 \cdots ds_n \tau_{is_n z}(P) \cdots \tau_{is_1 z}(P)\Omega \ ,$$

then $\Omega^P(z)$ is holomorphic for $\operatorname{Re} z \in \langle 0, 1\rangle$ and strongly continuous for $\operatorname{Re} z \in [0, 1]$ as a corollary of the estimates of (1). Moreover, $\Omega^P(1) = \Omega^P$. Now let D denote the union, over the intervals $I \subset \mathbb{R}$, of the ranges of $E(I)$ where E is the spectral family of $H + P$. If $\varphi \in D$ one has

$$(e^{\bar{z}(H+P)/2}\varphi, \Omega) = (\varphi, \Omega^P(z))$$

for pure imaginary z. But both sides are holomorphic for $\operatorname{Re} z \in \langle 0, 1\rangle$ and continuous for $\operatorname{Re} z \in [0, 1]$. Hence they are equal for $\operatorname{Re} z \in [0, 1]$ by the edge of the wedge theorem, Proposition 5.3.6. Since D is a core for $e^{(H+P)/2}$, one concludes that $\Omega \in D(e^{(H+P)/2})$, and

$$\Omega^P = \Omega^P(1) = e^{(H+P)/2}\Omega \ .$$

(3) Again we choose $P_L \in \mathfrak{A}_\tau$ such that $\|P_L\| \leq \|P\|$ and $\|P_L - P\| \to 0$. Setting

$$f_{A,L}(z) = \omega(A\tau_{z_n}(P_L) \cdots \tau_{z_1}(P_L))$$

one has

$$|f_{A,L}(z) - f_{A,M}(z)| \leq \sum_{j=1}^n |\omega(A\tau_{z_n}(P_L) \cdots \tau_{z_j}(P_L - P_M) \cdots \tau_{z_1}(P_M))| \ .$$

But if $Q_i \in \mathfrak{A}_\tau$, repeated application of the three-line theorem gives

$$\begin{aligned}
&\sup_{z \in \mathfrak{D}_{-1}^{(n)}} |\omega(A\tau_{z_n}(Q_n) \cdots \tau_{z_1}(Q_1))| \\
&\quad \leq \sup_{1 \leq j \leq n} \sup_{t \in \mathbb{R}^n} |\omega(A\tau_{t_n}(Q_n) \cdots \tau_{t_j - i}(Q_j) \cdots \tau_{t_1 - i}(Q_1))| \\
&\quad = \sup_{1 \leq j \leq n} \sup_{t \in \mathbb{R}^n} |\omega(\tau_{t_j}(Q_j) \cdots \tau_{t_1}(Q_1) A \tau_{t_n}(Q_n) \cdots \tau_{t_{j+1}}(Q_{j+1}))| \leq \|A\| \prod_{i=1}^n \|Q_i\|
\end{aligned}$$

where the second step uses the τ-KMS condition. Combination of these estimates establishes that $f_{A,L}$ is a Cauchy sequence uniformly on $\overline{\mathfrak{D}_{-1}^{(n)}}$ and thus the limit function f_A is holomorphic in $\overline{\mathfrak{D}_{-1}^{(n)}}$ and continuous on its closure $\overline{\mathfrak{D}_{-1}^{(n)}}$. Moreover,

$$\sup_{z \in \mathfrak{D}_{-1}^{(n)}} |f_A(z)| \leq \|A\| \, \|P\|^n \ .$$

But the truncated functions are finite linear combinations of products of the non-truncated functions and if we define F_A as the appropriate combination of the f_A, it follows that F_A has the correct holomorphy and continuity properties and the desired boundary value.

To derive the uniform bound on F_A we first take $P \in \mathfrak{A}_\tau$ and remark that

$$\begin{aligned} &\omega_T(A, \tau_{t_n}(P), \ldots, \tau_{t_{j+1}}(P), \tau_{t_j - i}(P), \ldots, \tau_{t_1 - i}(P)) \\ &\quad = \omega_T(\tau_{t_j}(P), \ldots, \tau_{t_1}(P), A, \tau_{t_n}(P), \ldots, \tau_{t_{j+1}}(P)) \ . \end{aligned}$$

This equality follows from the definition of the ω_T in terms of ω and the τ-KMS condition. It then follows as above that

$$\sup_{z \in \mathfrak{D}_{-1}^{(n)}} |F_A(z)| \leq \sup_{1 \leq j \leq n} \sup_{t \in \mathbb{R}^n} |\omega_T(\tau_{t_j}(P), \ldots, \tau_{t_1}(P), A, \tau_{t_n}(P), \ldots, \tau_{t_{j+1}}(P))| \ .$$

Now recall that a function F over the index set $\mathfrak{J}$ and its truncation F_T are related by

$$F(I) = F_T(I) + \sum_{\alpha \in J \subset I} F_T(J) F(I \backslash J) \ ,$$

where α is any point in I. Next assume that $|F(I)| \leq 1$ and $|F_T(I)| < 2^{|I|-1}(|I|-1)!$ for $|I| \leq n$ where $n \geq 2$ and $|I|$ denotes the number of points in I. For $|I| = n+1$ one obtains from the foregoing equation

$$\begin{aligned} |F_T(I)| &\leq 1 + \sum_{m=1}^{n} {}^nC_{m-1} 2^{m-1}(m-1)! \\ &= 2^n n! \left\{ (2^n n!)^{-1} + \sum_{m=1}^{n} \frac{1}{(n-m+1)!} \frac{1}{2^{n-m+1}} \right\} \\ &\leq 2^n n! \left\{ 1/8 + e^{1/2} - 1 \right\} < 2^n n! . \end{aligned}$$

We may apply this result to truncated functions $\omega_T(A_1, A_2, \ldots, A_n)$ with $\|A_i\| \leq 1$. One has $|\omega(A_1 A_2 \cdots A_n)| \leq 1$ and $|\omega_T(A_i)| \leq 1, |\omega_T(A_i, A_j)| \leq 2$. Hence

$$|\omega_T(A_1, \ldots, A_n)| \leq 2^{n-1}(n-1)!$$

for all $n \geq 1$ by induction.

Combination of the conclusions of the two preceding paragraphs immediately gives

$$\sup_{z \in \mathfrak{D}_{-1}^{(n)}} |F_A(z)| \leq 2^n n! \|P\|^n \|A\|$$

for $P \in \mathfrak{A}_\tau$ and the general result follows by uniform approximation. Thus, we have established the existence and convergence properties of the perturbation series given in the fourth statement and it remains to identify this series with ω^P when $2\|P\| < 1$.

Let $P \in \mathfrak{A}_\tau$ and define $\omega_n^P(A)$ by $\omega_0^P(A) = \omega(A)$ and

$$\omega_n^P(A) = \int_{-1 \le s_1 \le \cdots \le s_n \le 0} ds_1 \cdots ds_n \, \omega(A\tau_{is_n}(P) \cdots \tau_{is_1}(P)) \ .$$

It follows that

$$\sum_{n \ge 0} \omega_n^P(A) = \omega(A\Gamma_{-i}^P) \ .$$

But $\Gamma_{it}^P \in \mathfrak{A}_\tau$ and it satisfies the analytically continued co-cycle relations

$$\Gamma_{i(s+t)}^P = \Gamma_{it}^P \tau_{it}(\Gamma_{is}^P), \quad \tau_{it}(\Gamma_{-it}^P) = (\Gamma_{-it}^P)^*, \quad (\Gamma_{it}^P)^{-1} = (\Gamma_{-it}^P)^* .$$

Therefore,

$$\begin{aligned} \omega(A\Gamma_{-i}^P) &= \omega(A\Gamma_{-i/2}^P \, \tau_{-i/2}(\Gamma_{-i/2}^P)) \\ &= \omega(\Gamma_{-i/2}^{P*} A \Gamma_{-i/2}^P) \\ &= \omega^P(A)\omega(\Gamma_{-i/2}^{P*} \Gamma_{-i/2}^P) = \omega^P(A)\omega(\Gamma_{-i}^P) \ . \end{aligned}$$

These two identities lead to the relation

$$\sum_{n \ge 0} \lambda^n \omega_n^P(A) = \omega^{\lambda P}(A) \sum_{n \ge 0} \lambda^n \omega_n^P(\mathbb{1}) \ .$$

But it follows from the representation of ω^P given in (2) that $\lambda \in \mathbb{R} \mapsto \omega^{\lambda P}$ has a power-series expansion

$$\omega^{\lambda P}(A) = \sum_{n \ge 0} \lambda^n \hat{\omega}_n^P(A)$$

with a nonzero radius of convergence. Thus, by multiplication and term-by-term comparison of power series one obtains

$$\omega_n^P(A) = \hat{\omega}_n^P(A) + \sum_{r=1}^{n} \hat{\omega}_{n-r}^P(A)\omega_r^P(\mathbb{1}) \ . \qquad (*)$$

In particular as $\hat{\omega}_0^P(A) = \omega(A)$ one finds

$$\hat{\omega}_1^P(A) = \omega_1^P(A) - \omega(A)\omega_1^P(\mathbb{1}) = \int_{-1}^{0} ds \, \omega_T(A, \tau_{is}(P)) \ .$$

Now for $I = \{i_m, \ldots, i_1\}$ adopt the notation

$$\omega_T(A; I) = \omega_T(A, \tau_{is_{i_1}}(P), \ldots, \tau_{is_{i_m}}(P)) \ ,$$

$$\omega(A; I) = \omega(A\tau_{is_{i_1}}(P) \cdots \tau_{is_{i_m}}(P)) \ .$$

We assume that

$$\hat{\omega}_r^P(A) = \int_{-1 \le s_1 \le \cdots \le s_n \le 0} ds_1 \cdots ds_n \, \omega_T(A; \{1, 2, \ldots, r\})$$

for $r \le n-1$ and then use the relation (*) to prove that it is valid for $r = n$. First, from (*)one has

$$\omega_n^P(A) = \hat{\omega}_n^P(A) + \sum_{r=1}^{n} \int_{-1 \le s_{n-r+1} \le \dots \le s_n \le 0} ds_{n-r+1} \dots ds_n \omega_T(A; \{n-r+1, \dots, n\})$$
$$\times \int_{-1 \le s_1 \le \dots \le s_{n-r} \le 0} ds_1 \dots ds_{n-r} \omega(\mathbb{1}; \{1, \dots, n-r\}) \ .$$

But by change of integration variable one finds

$$\omega_n^P(A) = \hat{\omega}_n^P(A) + \int_{-1 \le s_1 \le \dots \le s_n \le 0} ds_1 \cdots ds_n \sum_{J \subset I} \omega_T(A; J) \omega(\mathbb{1}; I \backslash J) \ ,$$

where $I = \{1, \dots, n\}$ and the sum is over the strict subsets of I. But the general relation between a function and its truncations gives

$$\sum_{J \subset I} \omega_T(A; J) \omega(\mathbb{1}; I \backslash J) = \omega(A; I) - \omega_T(A; I)$$

and hence

$$\hat{\omega}_n^P(A) = \omega_n^P(A) - \int_{-1 \le s_1 \le \dots \le s_n \le 0} ds_1 \cdots ds_n \{\omega(A; I) - \omega_T(A; I)\}$$
$$= \int_{-1 \le s_1 \le \dots \le s_n \le 0} ds_1 \cdots ds_n \omega_T(A; I) \ .$$

This establishes the correct identification of the perturbation series for $P \in \mathfrak{A}_\tau$. For general P the series is obtained by uniform approximation.

Thus, the proof of the C^*-version of Theorem 5.4.4 is complete. The W^*-version can be established by the following variation of the above arguments.

The first statement of the theorem is established by an inductive reasoning which necessitates a multivariable version of the three-line theorem. This allows one to define Ω^P for all selfadjoint $P \in \mathfrak{A}$. Next one proves that if $P_M \to P$ in the strong operator topology, then $\Omega^{P_M} \to \Omega^P$ strongly. This is an imaginary time version of the last statement of Corollary 5.4.2 which follows from a double approximation procedure. One first introduces regularizations.

$$P_{M,\lambda} = \sqrt{\frac{\lambda}{\pi}} \int dt \ e^{-\lambda t^2} \tau_t(P_M) \ ,$$

and P_λ, of P_M and P, and then $P_{M,\lambda} \to P_M$ and $P_\lambda \to P$ strongly by Proposition 2.5.22. Next, one uses the explicit form of the regularization and a change of variables to deduce that

$$\lim_{\lambda \to \infty} \|\Delta^{z_n} P_{M,\lambda} \Delta^{z_{n-1}-z_n} P_{M,\lambda} \cdots \Delta^{z_1-z_2} P_{M,\lambda} \Omega$$
$$- \Delta^{z_n} P_M \Delta^{z_{n-1}-z_n} P_M \cdots \Delta^{z_1-z_2} P_M \Omega\| = 0$$

for all $z \in \mathfrak{D}_{-1/2}^{(n)}$, and a similar result for P_λ and P. But one can also conclude from the uniform boundedness of convergent sequences, the Lebesgue-dominated convergence theorem, and the regularization that

$$\lim_{M \to \infty} \|\Delta^{z_n} P_{M,\lambda} \Delta^{z_{n-1}-z_n} P_{M,\lambda} \cdots \Delta^{z_1-z_2} P_{M,\lambda} \Omega - \Delta^{z_n} P_\lambda \Delta^{z_{n-1}-z_n} P_\lambda \cdots \Delta^{z_1-z_2} P_\lambda \Omega\| = 0$$

for all $z \in \mathfrak{D}_{-1/2}^{(n)}$. It now follows from these two estimates and the uniform boundedness property of the first part of the theorem that

$$\lim_{M \to \infty} \|\Delta^{z_n} P_M \Delta^{z_{n-1}-z_n} P_M \cdots \Delta^{z_1-z_2} P_M \Omega - \Delta^{z_n} P \Delta^{z_{n-1}-z_n} P \cdots \Delta^{z_1-z_2} P \Omega\| = 0 \ .$$

Another application of boundedness and the Lebesgue-dominated covergence theorem finally yields the desired convergence $\Omega^{P_M} \to \Omega^P$. But the τ-analytic elements form a strongly dense subspace of $\mathfrak{A}$, by Proposition 2.5.22, and hence the continuity of Ω^P allows the further discussion to proceed through approximation with analytic elements in the same manner used for the C^*-version of the theorem.

Note that the vectors Ω^P are cyclic and separating for $\mathfrak{A}$ (or for $\mathfrak{A}''$ in the C^*-case) as a consequence of the τ-KMS condition, Corollary 5.3.9. But if $P \in \mathfrak{A}_\tau$, then $\Gamma^P_{is} \in \mathfrak{A}_\tau$ and

$$\Omega^P = \Gamma^P_{-i/2}\Omega = \Gamma^P_{-i/4}\,\tau_{-i/4}(\Gamma^P_{-i/4})\Omega$$

by use of the analytically continued co-cycle relation. Moreover,

$$\tau_{is}(\Gamma^P_{-is}) = (\Gamma^P_{-is})^* \ .$$

Therefore,

$$\begin{aligned}\Omega^P &= \Gamma^P_{-i/4}\Delta^{1/4}\Gamma^P_{-i/4}\Omega \\ &= \Gamma^P_{-i/4}\Delta^{1/2}\tau_{i/4}(\Gamma^P_{-i/4})\Omega \\ &= \Gamma^P_{-i/4}\Delta^{1/2}\Gamma^P_{-i/4}{}^*\Omega = \Gamma^P_{-i/4}J\Gamma^P_{-i/4}\Omega \ ,\end{aligned}$$

where J is the modular conjugation associated with the pair $(\mathfrak{A}, \Omega)$. This establishes that Ω^P lies in the natural cone $\mathscr{P}$ corresponding to $(\mathfrak{A}, \Omega)$, Definition 2.5.25, and this conclusion extends to all $P = P^* \in \mathfrak{A}$ by strong approximation of P by analytic elements and the continuity of $P \mapsto \Omega^P$. Thus, $\Omega^P/\|\Omega^P\|$ is the unique normalized representative of the τ^P-KMS state ω^P contained in the cone $\mathscr{P}$, Theorem 2.5.31. This allows one to readily identify the modular operator associated with ω^P. For example, if $\Delta = \exp\{H\}$ is the modular operator associated with $(\mathfrak{A}, \Omega)$ and if

$$\Delta_P = e^{H+P-JPJ} \ ,$$

then by a perturbation expansion

$$\tau^P_t(A) = \Delta_P^{it} A \Delta_P^{-it}$$

for all $A \in \mathfrak{A}$ and $t \in \mathbb{R}$, i.e., Δ_P implements the modular group of the pair $(\mathfrak{A}, \Omega^P)$. But the Trotter product formula, Corollary 3.1.31, shows that

$$\Delta_P^{it}\psi = \lim_{n\to\infty}(\Delta^{it/n}\, e^{itP/n}\, J e^{itP/n}\, J)^n \psi \ .$$

This representation demonstrates that $\Delta_P^{it}\mathscr{P} \subseteq \mathscr{P}$ and hence Δ_P is the modular operator for the pair $(\mathfrak{A}, \Omega^P)$ by Corollary 2.5.32.

The conclusions of Theorem 5.4.4 extend to (τ, β)-KMS states, for any $\beta \in \mathbb{R}$, by rescaling. Thus, for each (τ, β)-KMS state ω the theorem provides a recipe for construction of a (τ^P, β)-KMS vector state ω^P. The following corollary summarizes the properties of this map $\omega \mapsto \omega^P$.

Corollary 5.4.5. *Let* $(\mathfrak{A}, \tau)$ *be a* C^**- or* W^**-dynamical system and for* $P = P^* \in \mathfrak{A}$, $\beta \in \mathbb{R}$, *associate with each* (τ, β)*-KMS state* ω *a* (τ^P, β)*-KMS state* ω^P *by*

$$\omega^P(A) = \frac{(\Omega^P, \pi_\omega(A)\Omega^P)}{(\Omega^P, \Omega^P)}$$

and

$$\Omega^P = \Omega_\omega + \sum_{n \geq 1} (-1)^n \int_0^{\beta/2} ds_1 \int_0^{s_1} ds_2 \cdots \int_0^{s_{n-1}} ds_n \, \pi_\omega(\tau_{is_n}(P) \cdots \tau_{is_1}(P))\Omega_\omega \ .$$

It follows that the map $\gamma_\tau^P; \omega \mapsto \omega^P$ *is an isomorphism of the set of* (τ, β)*-KMS states onto the set of* (τ^P, β)*-KMS states which maps extremal points into extremal points. The inverse map is given by* $(\gamma_\tau^P)^{-1} = \gamma_{\tau^P}^{-P}$.

Proof. The map γ_τ^P is well-defined, and it maps extremal points into extremal points, by Theorems 5.4.4 and 5.3.30. Next assume that $P \in \mathfrak{A}_\tau$, then $\Omega^P = \pi_\omega(\Gamma_{i\beta/2}^P)\Omega_\omega$. But the image of ω^P under $\gamma_{\tau^P}^{-P}$ is then determined by the vector

$$\hat{\Omega}^{-P} = \pi_\omega(\Gamma_{i\beta/2}^P)\Omega_\omega + \sum_{n \geq 1} \int_0^{\beta/2} ds_1 \int_0^{s_1} ds_2 \cdots \int_0^{s_{n-1}} ds_n \pi_\omega(\tau_{is_n}^P(P) \cdots \tau_{is_1}^P(P)\Gamma_{i\beta/2}^P)\Omega_\omega \ .$$

It follows readily from the second identification of Γ^P in Proposition 5.4.1, and analytic continuation, that

$$\hat{\Omega}^{-P} = \pi_\omega((\Gamma_{i\beta/2}^P)^{-1})\pi_\omega(\Gamma_{i\beta/2}^P)\Omega_\omega = \Omega_\omega \ .$$

Thus, $\gamma_{\tau^P}^{-P}\gamma_\tau^P\omega = \omega$ and interchanging τ and τ^P one also has $\gamma_\tau^P\gamma_{\tau^P}^{-P}\omega^P = \omega^P$. This establishes that $(\gamma_\tau^P)^{-1} = \gamma_{\tau^P}^{-P}$ and γ_τ^P is an isomorphism. The result for general P follows by approximation with a sequence of analytic elements and use of the continuity property $\Omega^{P_n} \to \Omega^P$.

It should be emphasized that the map γ_τ^P is not affine.

There is a second "time-dependent" approach to the stability of KMS states which is less complete than the above but is of interest for various reasons. First, it emphasizes different physical aspects; it is dynamical rather than kinematical. Second, it plays a fundamental role in the subsequent attempts to justify the KMS condition as a characteristic of equilibrium. Third, it applies to ground states and ceiling states for which the above "time-independent" analysis has no analogue because the whole modular structure is lacking.

To illustrate the difference between the two approaches and to explain the time-dependent time-independent nomenclature we first recall the discussion of the finite-dimensional system which preceded Theorem 5.4.4. In this example the relation between the perturbed state ω^P and the unperturbed state ω arose by expansion of the ω^P density matrix in terms of the ω density matrix. But these density matrices determine the probability distribution of the various kinematic states of the system and hence this method is basically a time-independent, or kinematic, way of linking the appropriate equilibrium dis-

tributions. The second approach is distinct in that it is time-dependent and consists of attempting to identify the perturbed equilibrium state as the evolute of the unperturbed state under the perturbed dynamics. Conversely, the original state should arise by evolution of the perturbed state under the original dynamics. This latter phenomenon, which is often referred to as return to equilibrium, is not universal but depends intimately upon some form of ergodicity of the system $(\mathfrak{A}, \tau)$ and purity of the state ω. It appears that the necessary ergodicity should be some form of asymptotic abelianness. Properties of this type for the dynamical group correspond to dispersion, with time, of local disturbances. Their role in the time-dependent approach is illustrated by the following result which establishes the tendency of perturbed KMS states to return to equilibrium.

Proposition 5.4.6. *Let $(\mathfrak{A}, \tau)$ be a C^*-dynamical system, where $\mathfrak{A}$ has an identity, and τ^P the perturbed evolution corresponding to the perturbation $P = P^* \in \mathfrak{A}$. Further let ω^P be a (τ^P, β)-KMS state for $\beta \in \mathbb{R} \cup \{\pm\infty\}$ and ω a weak*-limit point of $\tau_t^* \omega^P$ as t tends to infinity.*

If $(\mathfrak{A}, \tau)$ is asymptotically abelian in the norm sense, i.e., if

$$\lim_{t \to \infty} \|[A, \ \tau_t(B)]\| = 0$$

for all $A, \ B \in \mathfrak{A}$, then ω is a $(\tau, \ \beta)$-KMS state.

Proof. If $\beta = 0$, then ω^P is a trace and ω is a trace, i.e., a $(\tau, \ 0)$-KMS state. Next assume $\beta \in \mathbb{R} \backslash \{0\}$ and let δ denote the generator of τ. The generator of τ^P is $\delta + \delta_P$ where $\delta_P(A) = i[P, \ A]$. The $(\tau, \ \beta)$-KMS condition now follows by verification of the auto-correlation lower bounds of Theorem 5.3.15. Explicitly one has

$$\begin{aligned}
\omega(A^*A) \log \frac{\omega(A^*A)}{\omega(AA^*)} &\leq \lim_{t \to \infty} \omega^P(\tau_t(A^*)\tau_t(A)) \log \frac{\omega^P(\tau_t(A^*)\tau_t(A))}{\omega^P(\tau_t(A)\tau_t(A^*))} \\
&\leq \lim_{t \to \infty} -i\beta\omega^P(\tau_t(A^*)(\delta + \delta_P)(\tau_t(A))) \\
&= -i\beta\omega(A^*\delta(A)) + \lim_{t \to \infty} \beta\omega^P(\tau_t(A^*)[P, \ \tau_t(A)]) \\
&= -i\beta\omega(A^*\delta(A)) \ .
\end{aligned}$$

The first step uses the lower semi-continuity of $u, \ v \mapsto u \ \log \ (u/v)$, the second uses the auto-correlation lower bounds for ω^P, the third relies on $\delta\tau = \tau\delta$, and the fourth follows from asymptotic abelianness. Similarly, if $\beta = +\infty$, i.e., ω^P is a τ^P ground state,

$$\begin{aligned}
-i\omega(A^*\delta(A)) &= -i \lim_{t \to \infty} \omega^P(\tau_t(A^*)\delta(\tau_t(A))) \\
&\geq -\lim_{t \to \infty} \omega^P(\tau_t(A^*)[P, \ \tau_t(A)]) = 0
\end{aligned}$$

and ω is a τ ground state. The case $\beta = -\infty$ is identical.

This proposition does not establish the existence of the limit of $\tau_t^* \omega^P$ but if there is a unique $(\tau, \ \beta)$-KMS state, this follows because all limit points must be equal. In fact, one can deduce a stronger result for $\beta \in \mathbb{R}$ by use of the time-independent theory.

Corollary 5.4.7. *Let ω^P be an extremal (τ^P, β)-KMS state for $\beta \in \mathbb{R}\backslash\{0\}$ and assume that $(\mathfrak{A}, \tau)$ is asymptotically abelian in the norm sense.*

It follows that the limit

$$\omega(A) = \lim_{t\to\infty} \omega^P(\tau_t(A))$$

exists for all $A \in \mathfrak{A}$, and ω is the unique (τ, β)-KMS vector state of ω^P.

PROOF. Corollary 5.4.5 establishes the existence of an extremal (τ, β)-KMS vector state ω, of ω^P, and ω is a factor state by Theorem 5.3.30. But it then follows from Example 4.3.24 that

$$\lim_{t\to\infty} \omega(A\tau_t(B)C) = \omega(AC)\omega(B)$$

i.e., $\pi_\omega(\tau_t(B))$ converges weakly to $\omega(B)\mathbb{1}_\omega$ for all $B \in \mathfrak{A}$. But ω^P is a vector state of ω and hence

$$\omega(A) = \lim_{t\to\infty} \omega^P(\tau_t(A)) \ .$$

Thus asymptotic abelianness and extremality imply the existence of the limit states and as the argument works equally well as $t \to -\infty$ one deduces that the two limits are equal. In fact, if one replaces the pointwise limit by a mean value one can deduce an existence result without extremality of ω^P. One exploits the mean ergodic theorem and the methods of Section 4.3. Again the mean over positive t and the mean over negative t are equal.

In order to further develop the time-dependent formalism it is useful to introduce a stronger notion of asymptotic abelianness.

Definition 5.4.8. A C^*-dynamical system $(\mathfrak{A}, \tau)$ is defined to be $L^1(\mathfrak{A}_0)$-asymptotically abelian if

$$\int_{-\infty}^{\infty} dt \|[A, \tau_t(B)]\| < +\infty$$

for all A, B in the norm-dense *-subalgebra $\mathfrak{A}_0$.

This strong form of asymptotic abelianness is useful because it implies the existence of the norm limits $\gamma_\pm$ of $\tau^P_{-t}\tau_{+t}$, as $t \to \pm\infty$, for all $P \in \mathfrak{A}_0$, Proposition 5.4.10. Thus, if ω^P is a τ^P-invariant state,

$$\lim_{t\to\pm\infty} \omega^P(\tau_t(A)) = \lim_{t\to\pm\infty} \omega^P(\tau^P_{-t}\tau_t(A)) = \omega^P(\gamma_\pm(A))$$

exists. The problem with such conditions, however, is that they are difficult to verify in particular models. This is not surprising because these conditions express a form of ergodicity. Nevertheless in the simplest example, the ideal Fermi gas, the L^1 property can be verified.

EXAMPLE 5.4.9. Let $\mathfrak{A}$ be the CAR algebra over $L^2(\mathbb{R}^\nu)$ and $\mathfrak{A}_e$ the even C^*-subalgebra, i.e., the subalgebra generated by even polynomials in the annihilation and creation operators $a(f)$ and $a^*(g)$. Next let τ denote the free evolution discussed in Section 5.2.4. Thus τ is a group of Bogoliubov transformations, $\tau_t(a(f)) = a(U_t f)$, and

$$(U_t f)(x) = (2\pi)^{-\nu/2} \int d^\nu p \hat{f}(p) e^{ipx + i(p^2-\mu)t}.$$

If $\nu \geq 3$, define $\mathfrak{A}_0$ as the *-subalgebra of $\mathfrak{A}_e$ formed by even polynomials of the $a(f)$ and $a^*(g)$ with f and g of compact support. It follows that the pair $(\mathfrak{A}_e, \tau)$ is $L^1(\mathfrak{A}_0)$-asymptotically abelian. This is established by first noting that if $A, B \in \mathfrak{A}_e$, then $\|[A, \tau_t(B)]\|$ is bounded by a sum of terms of the form

$$\text{constant} \times \left[\int_\Lambda d^\nu x \, |(U_t f)(x)|^2 \right]^{1/2} .$$

This follows from the CARs because we have chosen an even subalgebra and the compact support property. To estimate these bounds we note that

$$\begin{aligned}(U_t f)(x) &= (2\pi)^{-\nu} \int d^\nu y \, f(y) \int d^\nu p \, e^{ip(x-y)} e^{i(p^2-\mu)t} \\ &= (-4\pi i t)^{-\nu/2} \int d^\nu y \, f(y) e^{-i(x-y)^2/4t} e^{-i\mu t} ,\end{aligned}$$

where we have used the Fresnel integral

$$\int d^\nu p \, e^{itp^2} = (i\pi/t)^{\nu/2} .$$

But then

$$(U_t f)(x) = \frac{e^{-ix^2/4t} e^{-i\mu t}}{(-4\pi i t)^{\nu/2}} \int d^\nu y \, e^{-iy^2/4t} f(y) e^{ixy/2t}.$$

Therefore,

$$|(U_t f)(x)| \leq (4\pi|t|)^{-\nu/2} \int_{\Lambda'} d^\nu y \, |f(y)| \leq \frac{|\Lambda'|^{1/2}}{(4\pi|t|)^{\nu/2}} \|f\| ,$$

where $|\Lambda'|$ is the volume of the support Λ' of f. Hence,

$$\left| \int d^\nu x \, g(x)(U_t f)(x) \right| = \left| \int_{\Lambda''} d^\nu x \, g(x)(U_t f)(x) \right| \leq \|g\| \frac{(|\Lambda'| \, |\Lambda''|)^{1/2}}{(4\pi|t|)^{\nu/2}} \|f\| ,$$

where Λ'' is the support of g. Thus, the bound for $\|[A, \tau_t(B)]\|$ is integrable for all $\nu \geq 3$.

If $\nu = 1, 2$, then $(\mathfrak{A}_e, \tau)$ is not $L^1(\mathfrak{A}_0)$-asymptotically abelian with the above choice of $\mathfrak{A}_0$. If, however, one redefines $\mathfrak{A}_0$ as the algebra of even polynomials in $a(f)$ and $a^*(g)$, where f, g are in the domain $D(X^2)$ of the multiplication operator, $(X^2 f)(x) = x^2 f(x)$, and their Fourier transforms vanish in a neighborhood of the origin, the property is again valid. To see this one simply remarks that

$$\begin{aligned}t^2(g, U_t f) &= \left(\frac{1}{2i}\right)^2 \int d^\nu p \, \overline{\hat{g}(p)} \hat{f}(p) \left(\frac{1}{p_j} \frac{\partial}{\partial p_j} \right)^2 e^{i(p^2-\mu)t} \\ &= \left(\frac{i}{2}\right)^2 \int d^\nu p \left(\frac{\partial}{\partial p_j} \frac{1}{p_j} \right)^2 \overline{(\hat{g}(p)} \hat{f}(p)) e^{i(p^2-\mu)t} .\end{aligned}$$

Now the right-hand side can be bounded by the Cauchy-Schwarz inequality and use of the special properties of $\hat{f}$ and $\hat{g}$, e.g., $\hat{f}$ vanishes in a neighborhood of the origin and $\partial \hat{f}/\partial p_j, \partial^2 \hat{f}/\partial p_j^2 \in L^2(\mathbb{R}^\nu)$. Thus, one finds $|(g, U_t f)| < \text{constant} \times |t|^{-2}$ and $(\mathfrak{A}_e, \tau)$ is once more $L^1(\mathfrak{A}_0)$-asymptotically abelian.

Note that the integrability conditions arise directly from the action of U on $L^2(\mathbb{R}^\nu)$. Thus, if one considers the full CAR algebra $\mathfrak{A}$, then $(\mathfrak{A}, \tau)$ is $L^1(\mathfrak{A}_0)$-asymptotically abelian in a slightly more intricate sense. The commutator norms $\|[A, \tau(B)]\|$ are integrable whenever A, or B, is an even element of a subalgebra $\mathfrak{A}_0$ built with appropriate test functions but the anti-commutator norms $\|\{A, \tau(B)\}\|$ are integrable if A and B are both odd elements.

The motivation for the introduction of $L^1(\mathfrak{A}_0)$-asymptotic abelianness is provided by the following.

Proposition 5.4.10. *Let $(\mathfrak{A}, \tau)$ be an $L^1(\mathfrak{A}_0)$-asymptotically abelian C^*-system. It follows that the limits*

$$\gamma_\pm(A) = \lim_{t \to \pm\infty} \tau^P_{-t}\tau_t(A)$$

exist in norm for all $A \in \mathfrak{A}$ and $P = P^* \in \mathfrak{A}_0$. The $\gamma_\pm$ are norm-preserving *-morphisms of $\mathfrak{A}$ which satisfy the intertwining relations

$$\gamma_\pm \tau = \tau^P \gamma_\pm \ .$$

If $\mathfrak{A}$ has an identify, then the adjoints $\gamma^*_\pm$ are affine transformations of the states $E_{\mathfrak{A}}$ into $E_{\mathfrak{A}}$ with the following properties:

(1) *The $\gamma^*_\pm$ map τ^P-invariant states into τ-invariant states and extremal τ^P-invariant states into extremal τ-invariant states.*

(2) *The $\gamma^*_\pm$ map (τ^P, β)-KMS states into (τ, β)-KMS and extremal (τ^P, β)-KMS states into extremal (τ, β)-KMS states for all $\beta \in (\mathbb{R} \cup \{\pm\infty\}) \backslash \{0\}$.*

(3) *If $\beta \in \mathbb{R}\backslash\{0\}$ then the maps $\gamma^*_\pm$ coincide in restriction to the (τ^P, β)-KMS states.*

Proof. By differentiation and integration one obtains the estimate

$$\|\tau^P_{-t_2}\tau_{t_2}(A) - \tau^P_{-t_1}\tau_{t_1}(A)\| \leq \int_{t_1}^{t_2} ds \, \|[P, \tau_s(A)]\|$$

and hence

$$\gamma_\pm(A) = \lim_{t \to \pm\infty} \tau^P_{-t}\tau_t(A)$$

exist in norm for all $A \in \mathfrak{A}_0$ and $P = P^* \in \mathfrak{A}_0$. But as $\mathfrak{A}_0$ is norm dense and τ^P and τ are norm-preserving the limits must exist, and satisfy $\|\gamma_\pm(A)\| = \|A\|$, for all $A \in \mathfrak{A}$. As limits of *-morphisms the $\gamma_\pm$ are automatically *-morphisms and the intertwinning property follows because

$$\gamma_\pm(\tau_t(A)) = \lim_{s \to \pm\infty} \tau^P_{-s}\tau_{t+s}(A) = \lim_{s \to \pm\infty} \tau^P_t \tau^P_{-t-s}\tau_{t+s}(A) = \tau^P_t \gamma_\pm(A) \ .$$

Since the $\gamma_\pm$ are *-morphisms their adjoints are affine maps of the dual which map positive functionals into positive functionals. But $\gamma_\pm(\mathbb{1}) = (\mathbb{1})$ and hence $\gamma^*_\pm$ must map $E_{\mathfrak{A}}$ into $E_{\mathfrak{A}}$.

(1) If ω^P is τ^P-invariant, it follows that

$$(\gamma_\pm^* \omega^P)(\tau_t(A)) = \omega^P(\gamma_\pm \tau_t(A)) = \omega^P(\tau_t^P \gamma_\pm(A)) = (\gamma_\pm^* \omega^P)(A)$$

because of the intertwining property. Moreover,

$$(\gamma_\pm^* \omega^P)(A\tau_t(B)) = \omega^P(\gamma_\pm(A)\tau_t^P(\gamma_\pm(B))) \ .$$

Thus, if ω^P is extremal τ^P-invariant and M is an invariant mean over $\mathbb{R}$, then

$$\begin{aligned} M((\gamma_\pm^* \omega^P)(A\tau(B))) &= M(\omega^P(\gamma_\pm(A)\tau^P(\gamma_\pm(B)))) \ . \\ &= (\omega^P(\gamma_\pm(A))\omega^P(\gamma_\pm(B)) = (\gamma_\pm^* \omega^P)(A)(\gamma_\pm^* \omega^P)(B) \ , \end{aligned}$$

where the second step follows from the mean ergodic theorem and the criteria for extremality given by Theorems 4.3.17 and 4.3.22. But $(\mathfrak{A}, \tau)$ is asymptotically abelian and hence this cluster property is equivalent to extremality of $\gamma_\pm^* \omega$ by the same theorems.

(2) If ω^P is (τ^P, β)-KMS

$$(\gamma_\pm^* \omega^P)(A) = \lim_{t \to \pm\infty} \omega^P(\tau_{-t}^P \tau_t(A)) = \lim_{t \to \pm\infty} \omega^P(\tau_t(A))$$

and $\gamma_\pm^* \omega^P$ is (τ, β)-KMS by Proposition 5.4.6. If ω^P is extremal ω is extremal, by Corollary 5.4.7, for all $\beta \in \mathbb{R}\backslash\{0\}$. Now if $\beta = +\infty$ and ω^P is an extremal (τ^P, β)-KMS state, i.e., an extremal τ^P ground state, then ω^P is pure by Theorem 5.3.37 and τ^P-invariant by Proposition 5.3.19. In particular, ω^P is extremal τ^P-invariant and $\gamma_\pm^* \omega^P$ is extremal τ-invariant by the first statement above. But $\gamma_\pm^* \omega^P$ is a τ ground state by Proposition 5.4.6 and hence it is an extremal τ ground state by Theorem 5.3.37. The argument for $\beta = -\infty$ is identical.

(3) If ω^P is an extremal (τ^P, β)-KMS state for $\beta \in \mathbb{R}$, then $\gamma_+^* \omega^P = \omega = \gamma_-^* \omega^P$, where ω is the unique (τ, β)-KMS vector state of ω^P, by Corollary 5.4.7. Therefore, the maps $\gamma_\pm^*$ coincide on the extremal points of the (τ^P, β)-KMS states and because they are affine they must coincide on the convex closure of these extremal points. But this is exactly the set of (τ^P, β)-KMS states by the Krein-Milman theorem.

The *-morphisms $\gamma_\pm$ are algebraic analogues of the wave operators, or Møller matrices, which occur in quantum-mechanical scattering theory and hence we refer to them as *Møller morphisms*. They provide a global comparison of the two evolutions τ and τ^P. These morphisms are not necessarily *-automorphisms because they may not be invertible. Their kernels are zero but their ranges may be strict subalgebras of $\mathfrak{A}$. In scattering theory the formation of bound states is a typical phenomenon which signals the lack of invertibility of the Møller matrices and in statistical mechanics lack of invertibility of the Møller morphisms $\gamma_\pm$ certainly occurs if the perturbation P isolates finite subsystems. The formation of bound states, or the isolation of subsystems, is indicated by the appearance of a point spectrum for the perturbed evolution. But if γ_+ or γ_- is invertible, the intertwining relations give

$$\gamma_\pm \tau \gamma_\pm^{-1} = \tau^P$$

and hence the point spectra of τ and τ^P are identical. Conversely, if the point spectra differ the $\gamma_\pm$ are not invertible.

Although the ranges of the $\gamma_\pm$ are not automatically equal to $\mathfrak{A}$ the morphism and isometric properties imply that they are C^*-subalgebras $\mathfrak{A}_\pm$ and the intertwining property shows that these algebras are τ^P-invariant. It is then interesting to note that if $(\mathfrak{A}, \tau)$ is asymptotically abelian in the norm sense, the $(\mathfrak{A}_\pm, \tau^P)$ are asymptotically abelian in the same sense, e.g.,

$$\|[\gamma_\pm(A), \tau_t^P(\gamma_\pm(B))]\| = \|\gamma_\pm([A, \tau_t(B)])\| = \|[A, \tau_t(B)]\| \ .$$

Similarly if the pair $(\mathfrak{A}, \tau)$ is $L^1(\mathfrak{A}_0)$-asymptotically abelian the $(\mathfrak{A}_\pm, \tau^P)$ are $L^1(\gamma_\pm(\mathfrak{A}_0))$-asymptotically abelian. Thus, stability of the various forms of asymptotic abelianness under perturbations of the group is directly related to the invertibility of the corresponding Møller morphisms. In fact, stability of the L^1-condition is essentially equivalent to invertibility of $\gamma_\pm$. (Assume $(\mathfrak{A}, \tau)$, is $L^1(\mathfrak{A}_0)$-asymptotically abelian in order that $\gamma_\pm$ exist. If the $\gamma_\pm$ are invertible, $\mathfrak{A}_\pm = \mathfrak{A}$ and $(\mathfrak{A}, \tau^P)$ is $L^1(\gamma_\pm(\mathfrak{A}_0))$-asymptotically abelian. Conversely, if $(\mathfrak{A}, \tau^P)$ is $L^1(\gamma_\pm(\mathfrak{A}_0))$-asymptotically abelian, the limits

$$\beta_\pm(A) = \lim_{t \to \pm\infty} \tau_{-t}\, \tau_t^P(A)$$

exist for all $A \in \mathfrak{A}$ and $P = P^* \in \gamma_\pm(\mathfrak{A}_0)$ and for those $P \in \mathfrak{A}_0 \cap \gamma_\pm(\mathfrak{A}_0)$ one has $\beta_\pm = \gamma_\pm^{-1}$.)

EXAMPLE 5.4.11. Let $\mathfrak{A}$ be the CAR algebra over $L^2(\mathbb{R}^\nu)$ and τ the free evolution given in Example 5.4.9, with $\mu = 0$. Let $P = a^*(f)a(f)$ be the quadratic perturbation of Example 5.4.3 and then τ and $\tau^{\lambda P}$ are both Bogoliubov transformations $\tau_t(a(f)) = a(U_t f)$ and $\tau_t^{\lambda P}(a(f)) = a(U_t^{\lambda P} f)$. The groups U and $U^{\lambda P}$ have infinitesimal generators $-\nabla^2$ and $-\nabla^2 + \lambda E$ where E is the projection on f. It is a standard result of scattering theory (see Notes and Remarks) that the strong limits

$$W_\pm g = \lim_{t \to \pm\infty} U_{-t}^{\lambda P}\, U_t g$$

exist on $L^2(\mathbb{R}^\nu)$. Thus the Møller morphisms $\gamma_\pm$ exist on $\mathfrak{A}$ and $\gamma_\pm(a(f)) = a(W_\pm f)$. Moreover, the $W_\pm$ are given by

$$(\widehat{W_\pm g})(p) = \int d^\nu q\, W_\pm(p, q)\hat{g}(q) \ ,$$

where

$$W_\pm(p, q) = \delta(p - q) - \frac{\lambda \hat{f}(p)\overline{\hat{f}(q)}}{p^2 - q^2 \pm i\varepsilon} \frac{1}{\Delta_\pm(q^2)}$$

and

$$\Delta_\pm(q^2) = 1 - \lambda \int d^\nu p \frac{|\hat{f}(p)|^2}{q^2 - p^2 \pm i\varepsilon} \ .$$

If $\Delta_\pm(0) > 0$, the $W_\pm$ are unitary and the $\gamma_\pm$ are invertible. If, however, $\Delta_\pm(0) \leq 0$, i.e., if

$$\lambda \int d^\nu p \frac{|\hat{f}(p)|^2}{p^2} \leq -1 \ ,$$

the $W_\pm$ are isometric but not unitary. In this case $-\nabla^2 + \lambda E$ has an eigenfunction f_λ and the ranges of the $W_\pm$ are exactly the orthogonal complement of f_λ.

These results extend to more general quadratic perturbations and, for example, if $P = -(a^*(\nabla^2 f)a(f) + a^*(f)a(\nabla^2 f))$, then

$$\tau_t^P(a(f)) = e^{-it(f,\nabla^2 f)}a(f) \ .$$

One of the most significant features of the time-dependent formalism is the set of "stability" conditions necessary for consistency with the time-independent formalism. The origin and nature of these conditions, which we intend to derive below, is readily understood by examination of an extremal τ-KMS state ω from the two different points of view. The time-independent formalism expresses ω as a vector state of a unique τ^P-KMS state ω^P which is related to ω by the convergent perturbation expansion of Theorem 5.4.4. After rescaling this assumes the form

$$\omega^P(A) = \omega(A) + \sum_{n\geq 1}(-1)^n \int_0^\beta ds_1 \int_0^{s_1} ds_2 \cdots \int_0^{s_n - 1} ds_n\, \omega_T(A, \tau_{is_n}(P), \ldots, \tau_{is_1}(P)) \ .$$

Now consider the orbit of ω under the perturbed evolution τ^P. The time-dependent formalism indicates that under certain general ergodicity hypotheses ω evolves into a τ^P-KMS state. It is natural to define the system as stable if the evolved state is the unique τ^P-KMS vector state of ω, namely, ω^P. Explicitly this definition of stability requires that

$$\omega^P(A) = \lim_{t\to\pm\infty} \omega(\tau_t^P(A)) \ .$$

It then follows from the τ-invariance of ω and the definition of τ^P given in Proposition 5.4.1 that

$$\begin{aligned}\omega^P(A) &= \lim_{t\to\pm\infty} \omega(\tau_{-t}\,\tau_t^P(A)) \\ &= \omega(A) + \lim_{t\to\pm\infty} \sum_{n\geq 1} i^n \int_{-t}^0 dt_1 \int_{-t}^{t_1} dt_2 \cdots \int_{-t}^{t_n - 1} dt_n\, \omega([\tau_{t_n}(P), [\cdots [\tau_{t_1}(P), A]]]) \ .\end{aligned}$$

Thus one obtains two seemingly different series expansions for ω^P and the identity of these series, term by term, yields the stability conditions. The simplest and most important is the first-order condition.

Theorem 5.4.12. *Let ω be a (τ, β)-KMS state over the C^*- or W^*-dynamical system $(\mathfrak{A}, \tau)$ and assume that ω is strongly clustering, i.e.,*

$$\lim_{t\to\pm\infty} \omega^P(A\tau_t(B)) = \omega(A)\omega(B)$$

for all $A, B \in \mathfrak{A}$.

It follows that

$$\lim_{T\to\pm\infty} \int_0^T dt\, \omega([A, \tau_t(B)]) = i \int_0^\beta ds\, \omega_T(A, \tau_{is}(B))$$

and hence

$$\lim_{T\to\infty}\int_{-T}^{T} dt\,\omega([A,\tau_t(B)]) = 0$$

for all $A, B \in \mathfrak{A}$.

PROOF. For each $A, B \in \mathfrak{A}$ the function $t \mapsto \omega(A\tau_t(B))$ is the boundary value of a function, which we denote by $z \mapsto \omega(A\tau_z(B))$, analytic in the strip $\mathfrak{D}_\beta; 0 < \operatorname{Im} z < \beta$ (or $\beta < \operatorname{Im} z < 0$ if $\beta < 0$), continuous on the boundary of the strip, such that

$$\sup_{z\in\overline{\mathfrak{D}}_\beta} |\omega(A\tau_z(B))| \le \|A\|\|B\| \ .$$

Now the (τ,β)-KMS condition gives

$$\omega(A\tau_{i\beta}(B)) = \omega(BA)$$

and therefore

$$\begin{aligned}\int_0^T dt\,\omega(A\tau_t(B) - \tau_t(B)A) &= \int_0^T dt\,\omega(A\tau_t(B) - A\tau_{t+i\beta}(B)) \\ &= i\int_0^\beta ds\,\omega(A\tau_{is}(B) - A\tau_{T+is}(B)) \ .\end{aligned}$$

The second identity follows because the integral of $z \mapsto \omega(A\tau_z(B))$ around the parallelepiped with corners at $(0,0), (T,0), (T,\beta)$, and $(0,\beta)$ is zero. But

$$\omega(A\tau_{T+is}(B)) = (U_\omega(is/2)\pi_\omega(A^*)\Omega_\omega,\ U_\omega(T)U_\omega(is/2)\pi_\omega(B)\Omega_\omega)$$

and the strong clustering condition is equivalent to the weak convergence of $U_\omega(T)$ to the projection on Ω_ω as $T \to \pm\infty$. Therefore,

$$\lim_{T\to\pm\infty} \omega(A\tau_{T+is}(B)) = \omega(A)\omega(B) = \omega(A)\omega(\tau_{is}(B)).$$

It then follows from the Lebesgue-dominated convergence theorem that

$$\lim_{T\to\pm\infty}\int_0^\beta ds\,\omega(A\tau_{T+is}(B)) = \int_0^\beta ds\,\omega(A)\omega(\tau_{is}(B)) \ .$$

Combination of these results gives the first statement of the theorem and the second follows by subtracting the two cases $T \to \pm\infty$.

The stability condition

$$\lim_{T\to\infty}\int_{-T}^{T} dt\,\omega([A,\tau_t(B)]) = 0$$

will be of special significance in Section 5.4.2 where we demonstrate that under suitable ergodicity hypotheses it is equivalent to the KMS condition for $\beta \in \mathbb{R}\cup\{\pm\infty\}$.

Comparison of the two perturbation formalisms also gives higher-order stability properties for KMS states.

Proposition 5.4.13. *Let ω be a (τ,β)-KMS state over the C^*- or W^*-dynamical system $(\mathfrak{A},\tau)$ with $\beta \in \mathbb{R}$ and assume that ω is strongly clustering.*

It follows that

$$\lim_{T_1 \to \pm\infty} \cdots \lim_{T_n \to \pm\infty} \int_0^{T_1} dt_1 \cdots \int_{t_{n-1}}^{T_n} dt_n\, \omega([\tau_{t_n}(B),\, [\cdots [\tau_{t_1}(B),\, A]]])$$
$$= (-i)^n \int_0^{\beta} ds_1 \int_0^{s_1} ds_2 \cdots \int_0^{s_{n-1}} ds_n\, \omega_T(A, \tau_{is_n}(B), \ldots, \tau_{is_1}(B))$$

for all $A,\ B \in \mathfrak{A}$.

PROOF. Let $B \in \mathfrak{A}_\tau$ and introduce $B(s_1, \ldots, s_j) = \tau_{is_j}(B) \cdots \tau_{is_1}(B)$. We first argue that

$$\int_{t_j}^{T_{j+1}} dt_{j+1} \int_0^{\beta} ds_1 \cdots \int_0^{s_{j-1}} ds_j\, \omega([\tau_{t_{j+1}}(B),\, C]\tau_{t_{j+1}}(B(s_1, \ldots, s_j))$$
$$= -i \int_0^{\beta} ds_1 \cdots \int_0^{s_j} ds_{j+1}\, \omega(C\tau_{t_j}(B(s_1, \ldots, s_{j+1})) - C\tau_{T_{j+1}}(B(s_1, \ldots, s_{j+1})))$$

for all $C \in \mathfrak{A}$. This follows by an application of the KMS condition and contour integration as in the proof of Theorem 5.4.12. The KMS condition allows one to reexpress the left-hand side as the difference of two terms L_1 and L_2, where

$$L_1 = \int_{t_j}^{Tj+1} dt_{j+1} \int_0^{\beta} ds_1 \cdots \int_0^{s_{j-1}} ds_j\, \omega(C\tau_{t_{j+1}}(B(\beta, s_1, \ldots, s_j)))\ ,$$
$$L_2 = \int_{t_j}^{T_{j+1}} dt_{j+1} \int_0^{\beta} ds_1 \cdots \int_0^{s_{j-1}} ds_j\, \omega(C\tau_{t_{j+1}}(B(s_1, \ldots, s_j, 0)))\ .$$

Next by a change of variables $s'_k = s_{k+1} - s_k + \beta$, $k = 1, \ldots, j-1$, and $s'_j = \beta - s_1$ and a subsequent shift of the contour of integration one finds

$$L_2 = \int_{t_j}^{T_{j+1}} dt_{j+1} \int_0^{\beta} ds_1 \ldots \int_0^{s_{j-1}} ds_j\, \omega(C\tau_{t_{j+1}}(B(\beta - s_j, s_1 - s_j, \ldots, s_{j-1} - s_j, 0)))$$
$$= L_1 + i \int_0^{\beta} ds_1 \ldots \int_0^{s_j} ds_{j+1}$$
$$\times \{\omega(C\tau_{t_j}(B(\beta - s_j + s_{j+1}, \ldots, s_{j-1} - s_j + s_{j+1}, s_{j+1})))$$
$$- \omega(C\tau_{T_{j+1}}(B(\beta - s_j + s_{j+1}, \ldots, s_{j-1} - s_j + s_{j+1}, s_{j+1})))\}\ .$$

Another change of variable gives the desired identification of $L_1 - L_2$. A similar identity is valid for a general $B \in \mathfrak{A}$ by approximation with analytic elements as in the proof of Theorem 5.4.4.

Next define C and X by

$$C(t_1, \ldots, t_n) = [\tau_{t_n}(B), [\ldots [\tau_{t_1}(B),\, A]]]\ ,$$
$$X(T_1, \ldots, T_n) = \int_0^{T_1} dt_1 \int_{t_1}^{T_2} dt_2 \ldots \int_{t_{n-1}}^{T_n} dt_n\, \omega(C(t_1, \ldots, t_n))\ .$$

Application of the above identity and strong clustering gives

$$\begin{aligned}
&\lim_{T_1,\ldots,T_n\to\pm\infty} X(T_1,\ldots,T_n)\\
&\quad=\sum_{j=1}^{n-1} -(-i)^{n-j} \lim_{T_1,\ldots,T_j\to\pm\infty} \int_0^{T_1} dt_1 \ldots \int_{t_{j-1}}^{T_j} dt_j\, \omega(C(t_1,\ldots,t_j))\\
&\qquad\times \int_0^{\beta} ds_1 \cdots \int_0^{s_{n-j-1}} ds_{n-j}\, \omega(B(s_1,\ldots,s_{n-j}))\\
&\qquad+(-i)^n \int_0^{\beta} ds_1 \cdots \int_0^{s_{n-1}} ds_n\, \omega(AB(s_1,\ldots,s_n))
\end{aligned}$$

for $n \geq 2$ and for $n = 1$ one obtains the result of Theorem 5.4.12.

The proof is conducted by induction. Theorem 5.4.12 gives the $n=1$ case and we now suppose the result is true for $j = 1, 2, \ldots, n-1$. The above identity then gives

$$\begin{aligned}
&\lim_{T_1,\ldots,T_n\to\pm\infty} X(T_1,\ldots,T_n)\\
&\quad=-(-i)^n \sum_{j=1}^{n-1} \int_0^{\beta} ds_1 \cdots \int_0^{s_{n-j-1}} ds_{n-j}\, \omega(\tau_{is_{n-j}}(B)\ldots\tau_{is_1}(B))\\
&\qquad\times \int_0^{\beta} ds_{n-j+1} \cdots \int_0^{s_{n-1}} ds_n\, \omega_T(A, \tau_{is_n}(B),\ldots,\tau_{is_{n-j+1}}(B))\\
&\qquad+(-i)^n \int_0^{\beta} ds_1 \cdots \int_0^{s_{n-1}} ds_n\, \omega(A\tau_{is_n}(B)\ldots\tau_{is_1}(B))\\
&\quad=(-i)^n \int_0^{\beta} ds_1 \cdots \int_0^{s_{n-1}} ds_n\, \omega_T(A, \tau_{is_n}(B),\ldots,\tau_{is_1}(B)) \ ,
\end{aligned}$$

where we have changed the integration variables and used the general relation between a function and its truncations. (For a similar argument see the conclusion of the proof of Theorem 5.4.4.) This completes the induction and the proof.

To conclude the discussion of stability of KMS states we examine various properties of ground states, i.e., KMS states at the value $+\infty$. All our comments apply equally well to ceiling states.

The principal difference between ground states and τ-KMS states, in the present context, is that the ground states have a tendency to be less stable. There exist C^*-systems $(\mathfrak{A}, \tau)$ and perturbations P such that $(\mathfrak{A}, \tau)$ and $(\mathfrak{A}, \tau^P)$ have unique ground states which are disjoint. Thus these states, which are automatically pure by Theorem 5.3.37, generate unitarily inequivalent irreducible representations (see Example 5.4.15).

We begin with a positive result concerning existence of ground states of perturbed C^*-systems.

Proposition 5.4.14. *Let $(\mathfrak{A}, \tau)$ be a C^*-dynamical system with a ground state ω and assume $\mathfrak{A}$ has an identity.*

It follows, for each $P = P^* \in \mathfrak{A}$, that the perturbed system $(\mathfrak{A}, \tau^P)$ has a ground state.

PROOF. The ground state ω is τ-invariant, the corresponding unitary representation $U_\omega(t) = \exp\{itH_\omega\} \in \pi_\omega(\mathfrak{A})''$, and $H_\omega \geq 0$, by Proposition 5.3.19. Moreover Corollary 5.4.2 establishes that τ^P is unitarily implemented by the operators

$$U_\omega^P(t) = e^{it(H_\omega + \pi_\omega(P))} \ .$$

But $H_\omega + \pi_\omega(P)$ is lower semi-bounded and hence one may find a $\lambda \in \mathbb{R}$ and a sequence of unit vectors $\psi_n \in \mathfrak{H}_\omega$ such that $H_\omega + \pi_\omega(P) \geq \lambda \mathbb{1}_\omega$ but

$$\lim_{n \to \infty} \|(H_\omega + \pi_\omega(P) - \lambda \mathbb{1}_\omega)\psi_n\| = 0 \ .$$

Now let ω_n be the sequence of vector states associated with the ψ_n and ω^P a limit point of this sequence in the weak* topology. It follows from the estimate

$$(\psi_n, \pi_\omega(A^*)[H_\omega + \pi_\omega(P) - \lambda \mathbb{1}_\omega, \pi_\omega(A)]\psi_n) \geq -\|A\|^2 \|(H_\omega + \pi_\omega(P) - \lambda \mathbb{1}_\omega)\psi_n\|$$

that ω^P is a ground state of $(\mathfrak{A}, \tau^P)$.

The following example shows that ω^P is not necessarily π_ω-normal.

EXAMPLE 5.4.15. Let $\mathfrak{A}$ be the CAR algebra over $L^2(\mathbb{R}^\nu)$, τ the free evolution, and $P = a^*(f)a(f)$ the perturbation discussed in Example 5.4.11. It follows from Example 5.3.20 that $(\mathfrak{A}, \tau)$ has a unique ground state ω_0, the gauge-invariant quasi-free state with the two-point function

$$\omega_0(a^*(g_1)a(g_2)) = (g_2, \ Tg_1) \ ,$$

where

$$\begin{aligned} (\widehat{Tg})(p) &= \hat{g}(p), \qquad \text{if } p^2 \leq \mu \\ &= 0, \qquad \text{if } p^2 > \mu \ . \end{aligned}$$

But Example 5.4.11 establishes that the Møller morphisms $\gamma_\pm$ corresponding to the perturbation λP exist for all $\lambda \in \mathbb{R}$ and are invertible if

$$|\lambda| < \left\{ \int d^\nu p \, p^{-2} |\hat{f}(p)|^2 \right\}^{-1} \ .$$

Therefore, the τ and $\tau^{\lambda P}$ ground states are in one-to-one correspondence, by Proposition 5.4.10, for small λ, i.e., there exists a unique $\tau^{\lambda P}$ ground state. This ground state is given by $\omega_0^{\lambda P} = \gamma_\pm^{\lambda *} \omega_0$ and it is the gauge-invariant quasi-free state with two-point function

$$\omega_0^{\lambda P}(a^*(g_1)a(g_2)) = (W_+ g_2, TW_+ g_1) = (g_2, \ W_+^* T W_+ g_1) \ ,$$

where W_+ is the Møller matrix of Example 5.4.11.

There are various possibilities for $\omega_0^{\lambda P}$ which depend upon the support properties of the Fourier transform $\hat{f}$ of f. If supp $\hat{f} \subseteq \{p^2 \leq \mu\}$, then ω_0 is $\tau^{\lambda P}$-invariant and $\omega^{\lambda P} = \omega_0$. If supp $\hat{f} \not\subseteq \{p^2 < \mu\}$, the states are distinct but two cases occur which can be differentiated by examination of the particle density.

The state ω_0 has finite particle density because

$$N_\Lambda(\omega_0) = \sum_{n \geq 1} \omega_0(a^*(f_n)a(f_n)) = \frac{|\Lambda|}{(2\pi)^\nu} \int_{p^2 < \mu} d^\nu p$$

for any orthonormal basis $\{f_n\}_{n \geq 1}$ of $L^2(\Lambda)$. Hence, ω_0 is locally normal with respect to the Fock representation. The particle density of $\omega^{\lambda P}$ is given by

$$N_\Lambda(\omega^{\lambda P}) = (2\pi)^{-\nu} \int d^\nu p\, d^\nu q\, \hat{\chi}_\Lambda(p-q) \int_{r^2<\mu} d^\nu r\, W_+(p,r) W_+(r,q) \ ,$$

where

$$\hat{\chi}_\Lambda(p) = \int_\Lambda d^\nu x\, e^{ipx}$$

and $W_+(\cdot,\cdot)$ is the integral kernel of the Møller matrix W_+ given in Example 5.4.11. Now if supp $\hat{f} \cap \{p^2 = \mu\} = \varnothing$, then $N_\Lambda(\omega^{\lambda P}) < +\infty$ by explicit calculation. On the other hand, if supp $\hat{f} \cap \{p^2 = \mu\} \neq \varnothing$, the integral for $N_\Lambda(\omega^{\lambda P})$ can diverge because of the sharp cutoff in the r-integral. But it follows from the special structure of quasi-free states (see Notes and Remarks) that $\omega^{\lambda P}$ is locally normal if, and only if, it has finite particle density. Thus, $\omega^{\lambda P}$ is not locally normal and hence the two pure states ω and $\omega^{\lambda P}$ must generate unitarily inequivalent representations.

The foregoing example demonstrates that ground states are less stable than KMS states at finite values of β. There exist τ ground states which do not have τ^P ground states as normal states. The phenomenon which occurs in this example and destroys the normality is quite general and is usually called an *infrared divergence*. The energy difference between the perturbed and unperturbed systems is finite because P is bounded, but this energy is shared by an infinite number of particles each with an infinitesimally small energy. A similar situation occurs for the ideal Bose gas. All particles in the ground state have zero energy but a bounded perturbation can introduce an infinite number of infra-particles.

Another aspect of instability of ground states is given by examination of the condition

$$\lim_{T\to\infty} \int_{-T}^{T} dt\, \omega([A,\ \tau_t(B)]) = 0 \ .$$

In Theorem 5.4.12 we showed that each strongly clustering (τ, β)-KMS state ω satisfies this condition for all $A, B \in \mathfrak{A}$ but for ground states this condition can fail for certain A and B; in particular for those A and B which give emphasis to low-energy excitations. If ω is a strongly clustering τ ground state, the Fourier transform of

$$t \in \mathbb{R} \mapsto (\psi,\ U_\omega(t)\psi) - (\psi,\ \Omega_\omega)(\Omega_\omega, \psi) \ ,$$

where U_ω is the unitary group implementing τ on $\mathfrak{H}_\omega$ and $\psi \in \mathfrak{H}_\omega$, measures the energy distribution in the vector state ψ. The next result demonstrates that the stability condition is satisfied if, and only if, these measures give zero weight to the origin, i.e., if, and only if, infra-particles are absent.

Theorem 5.4.16. *Let $(\mathfrak{A},\ \tau)$ be a C^*- or W^*-dynamical system, ω a strongly clustering τ ground state, and $U_\omega(t) = \exp\{itH_\omega\}$ the unitary group which implements τ in the cyclic representation $(\mathfrak{H}_\omega,\ \pi_\omega,\ \Omega_\omega)$.*

The following conditions are equivalent:

(1) $$\lim_{T \to \infty} \int_{-T}^{T} dt\, \omega([A, \tau_t(B)]) = 0$$

for all $A, B \in \mathfrak{A}$.

(2) $$\lim_{T \to \infty} \int_{-T}^{T} dt \{\omega(A\tau_t(B)) - \omega(A)\omega(B)\} = 0$$

for all $A, B \in \mathfrak{A}$.

(3) $$\lim_{T \to \infty} \int_{-T}^{T} dt \{(\psi, U_\omega(t)\psi) - (\psi, \Omega_\omega)(\Omega_\omega, \psi)\} = 0$$

for all $\psi \in \mathfrak{H}_\omega$.

(4) *There exists an* $\varepsilon > 0$ *such that*

$$\sigma(H_\omega) \subseteq \{0\} \cup [\varepsilon, \infty\rangle$$

where $\sigma(H_\omega)$ *denotes the spectrum of* H_ω.

Proof. The state ω is automatically τ-invariant, Proposition 5.3.19, and hence

$$\begin{aligned}\omega(A\tau_t(B)) - \omega(A)\omega(B) = {} & (\pi_\omega(A^*)\Omega_\omega, U_\omega(t)\pi_\omega(B)\Omega_\omega) \\ & - (\pi_\omega(A^*)\Omega_\omega, \Omega_\omega)(\Omega_\omega, \pi_\omega(B)\Omega_\omega) \ .\end{aligned}$$

Therefore (3) $\Rightarrow$ (2). But (2) $\Rightarrow$ (1) trivially. To prove (1) $\Rightarrow$ (3) it suffices to consider ψ such that $(\psi, \Omega_\omega) = 0$. Now ω is pure by Theorem 5.3.37 and hence $(\mathfrak{H}_\omega, \pi_\omega)$ is irreducible. Therefore, it follows by an application of the Kadison transitivity theorem identical to the application in Example 4.3.24 that one may find $A \in \mathfrak{A}$ such that $\pi_\omega(A)\Omega_\omega = \psi$ and $\pi_\omega(A^*)\Omega_\omega = 0$. Therefore,

$$\lim_{T \to \infty} \int_{-T}^{T} dt\, (\psi, U_\omega(t)\psi) = \lim_{T \to \infty} \int_{-T}^{T} dt\, \omega([A^*, \tau_t(A)]) = 0 \ .$$

It remains to prove (3) $\Leftrightarrow$ (4).

(3) $\Rightarrow$ (4): Let H be the restriction of H_ω to a closed, separable, U_ω -invariant subspace $\mathfrak{K}$ of $\mathfrak{H}_\omega \ominus \mathbb{C}\,\Omega_\omega$,

$$H = \int_0^\infty dE(p)\, p$$

the spectral decomposition of H, and dv the measure in the corresponding spectral representation. Then

$$\int_{-T}^{T} dt\, (\psi, e^{\mathrm{i}t\mathrm{H}}\varphi) = \int_0^\infty d(\psi, E(p)\varphi)\; 2p^{-1} \sin pT$$

for all $\varphi, \psi \in \mathfrak{K}$. Hence condition (3) implies that

$$\lim_{T \to \infty} \int_0^\infty dv(p)\, g(p)\, 2p^{-1} \sin pT = 0$$

for all $g \in L^1(dv)$. But the uniform boundedness theorem then implies that the functions $p \to 2p^{-1} \sin pT_n$ are uniformly bounded in $L^\infty(dv)$ for all sequences T_n such that $T_n \to \infty$. It follows immediately that $v([0, \varepsilon\rangle) = 0$ for some $\varepsilon > 0$, i.e.,

$$\sigma(H) \subseteq [\varepsilon, \infty\rangle \ .$$

In principle, ε could depend upon $\mathfrak{K}$ but as the closed subspace generated by a countable number of such $\mathfrak{K}$ is still separable and U_ω-invariant it follows by an *ad absurdum* argument that we may choose ε independent of the subspace.

(4) $\Rightarrow$ (3): Adopt the above notation. The strong clustering assumption means that

$$\lim_{T \to \pm\infty} \int dv(p) f(p) e^{iTp} = 0$$

for all $f \in L^1(dv)$. But if $g \in L^1(dv)$, then the function f defined by $f(p) = g(p)/p$ is also in $L^1(dv)$ because $\varepsilon > 0$. Hence,

$$\lim_{T \to \infty} \int dv(p)\, g(p)\, 2p^{-1} \sin pT = 0 \ .$$

Therefore,

$$\lim_{T \to \infty} \int_{-T}^{T} dt\, (\psi, \ e^{itH_\omega} \varphi) = 0$$

for all $\varphi, \psi \in \mathfrak{H}_\omega \ominus \mathbb{C}\Omega_\omega$.

The existence of an energy gap in the excitation spectrum, i.e., the spectrum of H_ω, is not generally expected for ground states of nonrelativistic systems. Infra-particles are usually present because of a mechanism referred to as Goldstone's theorem. Thus the stability condition, condition (1) of Theorem 5.4.16, is not generally expected for strongly clustering ground states. Nevertheless, this condition is satisfied for those $A, B \in \mathfrak{A}$ which give no weight to zero energy, e.g., if $A, B \in \mathfrak{A}_0^\tau(\mathbb{R} \setminus [-\varepsilon, \varepsilon])$ for some $\varepsilon > 0$, where $\mathfrak{A}_0^\tau$ denotes the spectral subspace of Definition 3.2.37, then

$$\lim_{T \to \infty} \int_{-T}^{T} dt\ \omega(A\tau_t(B)) = 0 \ .$$

This follows by noting that $t \mapsto \omega(A\tau_t(B))$ is the boundary value of a function which is analytic in the upper half plane and the choice of A and B ensures that this function decreases like $\exp\{-\varepsilon \operatorname{Im} z\}$.

Although the stability criterion for ground states is not valid on the whole C^*-algebra when infra-particles are present, it is possible that it holds on a dense C^*-subalgebra. This is the situation if $(\mathfrak{A}, \tau)$ is $L_1(\mathfrak{A}_0)$-asymptotically abelian, Definition 5.4.8, as we next demonstrate. Subsequently we discuss the stability of such systems with the aid of Møller morphisms.

Theorem 5.4.17. *Let* $(\mathfrak{A}, \tau)$ *be an* $L^1(\mathfrak{A}_0)$*-asymptotically abelian* C^**-dynamical system.*

It follows that

$$\int_{-\infty}^{\infty} dt\, \omega([A,\ \tau_t(B)]) = 0$$

for all $A,\ B \in \mathfrak{A}_0$, *and for all* $(\tau,\ \beta)$*-KMS states* ω *with* $\beta \in \mathbb{R} \cup \{\pm\infty\}$.

PROOF. First adjoin an identity, if necessary, and extend τ to $\widetilde{\mathfrak{A}} = \mathbb{C}\mathbb{1} + \mathfrak{A}$ by setting $\tilde{\tau}_t((\alpha,\ A)) = (\alpha,\ \tau_t(A))$. We have already noted, in the discussion preceding Theorem 5.3.30, that there is a one-to-one correspondence between the $(\tau,\ \beta)$-KMS states of $(\mathfrak{A}, \tau)$ and the $(\tilde{\tau}, \beta)$-KMS states $\tilde{\omega}$ of $(\widetilde{\mathfrak{A}},\ \tilde{\tau})$ with $\|\tilde{\omega}|_{\mathfrak{A}}\| = 1$. Thus we can assume that $\mathfrak{A}$ has an identity.

Next assume $\beta \in \mathbb{R}$ and that ω is an extremal $(\tau,\ \beta)$-KMS state. Therefore, by Theorem 5.3.30, ω is a factor state. But the L^1-asymptotic abelianness, and the continuity of τ, imply that $(\mathfrak{A},\ \tau)$ is asymptotically abelian in the norm sense. Therefore, ω is strongly clustering by Example 4.3.24. Thus, the stability condition follows from Theorem 5.4.12. This condition immediately extends to finite convex combinations of extremal $(\tau,\ \beta)$-KMS states. Using $L^1(\mathfrak{A}_0)$-asymptotic abelianness the condition may be expressed as

$$\omega\left(\int_{-\infty}^{\infty} dt\, [A,\ \tau_t(B)]\right) = 0$$

and this relation extends to any $(\tau,\ \beta)$-KMS state by the Krein-Milman theorem.

Finally, consider the cases $\beta = \pm\infty$. As they are similar we assume that $\beta = +\infty$.

First for $\varepsilon > 0$ define $\hat{\chi}_\varepsilon$ by $\hat{\chi}_\varepsilon(\lambda) = (2\pi)^{1/2}/\varepsilon$ for $\lambda \in [\varepsilon,\ 2\varepsilon]$ and $\hat{\chi}_\varepsilon(\lambda) = 0$ otherwise.

By Fourier transformation one has

$$\chi_\varepsilon(t) = \varepsilon^{-1} \int_{\varepsilon}^{2\varepsilon} d\lambda\, e^{i\lambda t} = e^{3i\varepsilon t/2}(\sin \varepsilon t/2)/(\varepsilon t/2)$$

and hence

$$\lim_{\varepsilon \to 0} \chi_\varepsilon(t) = 1\ .$$

Thus, another application of the Lebesgue-dominated convergence theorem, $L^1(\mathfrak{A}_0)$-asymptotic abelianness, and Fourier transformation gives

$$\begin{aligned}\int_{-\infty}^{\infty} dt\, \omega([A, \tau_t(A^*)]) &= \lim_{\varepsilon \to 0} \int_{-\infty}^{\infty} dt\, \chi_\varepsilon(t)\omega([A, \tau_t(A^*)]) \\ &= \lim_{\varepsilon \to 0} \frac{1}{\varepsilon} \int_{\varepsilon}^{2\varepsilon} d(\pi_\omega(A^*)\Omega_\omega,\ E_\omega(\lambda)\pi_\omega(A^*)\Omega_\omega) \geq 0\end{aligned}$$

for all $A \in \mathfrak{A}_0$. We have used E_ω to denote the spectral measure associated with the unitary group U_ω which implements τ and the second step follows from the ground state condition, i.e., the support of E_ω is in $[0, \infty\rangle$. An identical argument with $\hat{\chi}_\varepsilon(\lambda)$ chosen to have support in $[-2\varepsilon, -\varepsilon]$ gives however

$$\int_{-\infty}^{\infty} dt\, \omega([A, \tau_t(A^*)]) = -\lim_{\varepsilon \to 0} \frac{1}{\varepsilon} \int_{-2\varepsilon}^{-\varepsilon} d(\pi_\omega(A)\Omega_\omega,\ E_\omega(\lambda)\pi_\omega(A)\Omega_\omega) \leq 0\ .$$

Therefore,

$$\int_{-\infty}^{\infty} dt\, \omega([A, \tau_t(A^*)]) = 0$$

for all $A \in \mathfrak{A}_0$. The general result follows by polarization.

We conclude this section with a discussion of a different type of stability condition which is expressed in terms of perturbed states and is often valid if the system $(\mathfrak{A}, \tau)$ satisfies a condition of asymptotic abelianness.

Let $(\mathfrak{A}, \tau)$ be a C^*-system which is asymptotically abelian in the norm sense, and let ω be an extremal (τ, β)–KMS state for some $\beta \in \mathbb{R}$. (If $\beta = 0$, we adopt the convention that ω is an extremal invariant trace.) It follows from Theorem 5.4.4 and Corollary 5.4.7 that there exist perturbed states ω^P of $\mathfrak{A}$ for all $P = P^* \in \mathfrak{A}$ such that:

(1) $\omega^{\lambda P}$ is $\tau^{\lambda P}$-invariant for $P = P^* \in \mathfrak{A}$ and λ sufficiently small.

(2) $\lambda \mapsto \omega^{\lambda P}$ is continuous at $\lambda = 0$ in the sense

$$\lim_{\lambda \to 0} \omega^{\lambda P}(A) = \omega(A)$$

for all $A \in \mathfrak{A}$, and all $P = P^* \in \mathfrak{A}$.

(3) The stability properties

$$\lim_{t \to \pm \infty} \omega^{\lambda P}(\tau_t(A)) = \omega(A)$$

hold for all $A \in \mathfrak{A}$, $P = P^* \in \mathfrak{A}$, and λ sufficiently small.

In fact, the $\omega^{\lambda P}$ exist for all $\lambda \in \mathbb{R}$ and are π_ω-normal for $\beta \in \mathbb{R}$. (If $\beta = 0$, one may choose $\omega^{\lambda P} = \omega$ for $\lambda \in \mathbb{R}$ and $P = P^* \in \mathfrak{A}$, the asymptotic abelianness is irrelevant, and property (1) follows because τ^P and τ are related by an inner co-cycle Γ^P, Proposition 5.4.1.)

In the introduction to the next subsection we show that the existence of a family of states with properties (1)–(3) is a stronger stability condition than the condition

$$\int_{-\infty}^{\infty} dt\, \omega([A,\ \tau_t(B)]) = 0$$

occurring in Theorem 5.4.17. It is not known if a version of Theorem 5.4.17 is valid with the stability properties (1)–(3) but some special cases can be handled. If ω is an extremal τ-KMS state at value $\beta \in \mathbb{R}$ and ω^P is the τ^P–KMS state given by Theorem 5.4.4, and $(\mathfrak{A}, \tau)$ is asymptotically abelian, then it follows from Theorem 5.4.4 and Corollary 5.4.7 that the stability properties (1)–(3) are valid.

If ω is a ground state with an energy gap, i.e., the condition $\sigma(H_\omega) \subseteq \{0\} \cup [\varepsilon, \infty\rangle$ of Theorem 5.4.16 is fulfilled, then it follows easily from resolvent identities that $H_\omega + \lambda\pi_\omega(P)$ has a unique (up to a phase) normalized eigenvector $\psi^{\lambda P}$ of minimum energy for λ small enough. One may verify that the corresponding vector states $\omega^{\lambda P}$ satisfy properties (1)–(3) and in this case the $\omega^{\lambda P}$ are still π_ω-normal. There do, however, exist ground states ω where properties (1)–(3) are valid but the $\omega^{\lambda P}$ are not π_ω-normal. This is a consequence of the following proposition applied to the free Fermi gas.

Proposition 5.4.18. *Let $(\mathfrak{A}, \tau)$ be an $L^1(\mathfrak{A}_0)$-asymptotically abelian system, and assume that $(\mathfrak{A}, \tau)$ has a unique ground state ω.*

It follows that for each $P = P^* \in \mathfrak{A}_0$ there exists a ground state ω^P for $(\mathfrak{A}, \tau^P)$. If $\{\omega^P\}$ is an arbitrary family of such ground states, then

$$\lim_{\lambda \to 0} \omega^{\lambda P}(A) = \omega(A)$$

and

$$\lim_{t \to \pm\infty} \omega^P(\tau_t(A)) = \omega(A)$$

for all $A \in \mathfrak{A}$, $P = P^* \in \mathfrak{A}_0$.

Proof. The existence of ground states of $(\mathfrak{A}, \tau^P)$ follows from Proposition 5.4.14 and we let ω^P be an arbitrary ground state of the system. The assumed asymptotic abelianness ensures that the Møller morphisms

$$\gamma_\pm^P(A) = \lim_{t \to \pm\infty} \tau_{-t}^P \tau_t(A)$$

exist for all $P = P^* \in \mathfrak{A}_0$, Proposition 5.4.10, and the $\gamma_\pm^P$ define *-isomorphisms between $\mathfrak{A}$ and $\gamma_\pm^P(\mathfrak{A})$. These *-isomorphisms also satisfy the intertwining relations

$$\gamma_\pm^P \tau_t = \tau_t^P \gamma_\pm^P$$

for all $t \in \mathbb{R}$. Hence, the C^*-dynamical systems $(\gamma_\pm^P(\mathfrak{A}), \tau^P)$ have unique ground states $\omega_\pm^P$ which are defined by $\omega_\pm^P \circ \gamma_\pm^P = \omega$. Since $\omega^P|_{\gamma_\pm^P(\mathfrak{A})}$ is a ground state, it follows that

$$\omega^P \circ \gamma_\pm^P = \omega$$

and hence

$$\omega(A) = \omega^P(\gamma_\pm^P(A)) = \lim_{t \to \pm\infty} \omega^P(\tau_t(A)) \ .$$

Now by the estimate

$$\|\gamma_+^{\lambda P}(A) - A\| \ \leq \ |\lambda| \int_0^\infty dt \|[P, \tau_t(A)]\|$$

which is valid for $A \in \mathfrak{A}_0$ it follows that

$$\lim_{\lambda \to 0} \|\gamma_+^{\lambda P}(A) - A\| = 0$$

for all $A \in \mathfrak{A}$. Combining this with

$$\omega^{\lambda P}(\gamma_+^{\lambda P}(A)) = \omega(A)$$

one concludes that

$$\lim_{\lambda \to 0} \omega^{\lambda P}(A) = \omega(A) \ .$$

Thus properties (1)–(3) are valid.

Note that the discussion of the preceding paragraph is applicable to the free Fermi gas if one works with the even C^*-algebra $\mathfrak{A}_e$ over $L^2(\mathbb{R}^\nu)$ (uniqueness of the ground state follows from Example 5.3.20) and hence properties (1)–(3) are valid for this model. Nevertheless, Example 5.4.15 demonstrates that the

corresponding ω^P are not π_ω-normal, and the absence of an energy gap in the spectrum of H_ω implies that the ground state cannot satisfy the stability properties of Theorem 5.4.16. The latter fact can also be shown by an explicit calculation on elements $A = a^*(f)a^*(g)$, $B = a(f)a(g)$ where $\hat{f}$ and $\hat{g}$ are sufficiently singular at the Fermi surface $p^2 = \mu$.

5.4.2. Stability and the KMS Condition

In the previous subsection we studied various stability properties of KMS states and our next aim is to establish that stability of a state can imply that the state is a KMS state. Roughly one deduces that all extremal τ-invariant states of asymptotically abelian dynamical systems which are stable under local perturbations of the dynamics are necessarily KMS states at some value $\beta \in \mathbb{R} \cup \{\pm\infty\}$. In fact, no completely satisfactory result of this kind occurs unless one has L^1-asymptotic abelianness. We will, however, prove two theorems in this direction. The first presupposes stronger clustering properties than are implied by extremality but relatively weak requirements of asymptotic abelianness. The second theorem is proved under weak clustering assumptions but with L^1-asymptotic abelianness of $(\mathfrak{A}, \tau)$.

Let us begin with a description of the stability properties which are central to both results. These properties arise from a reconciliation of two distinct ways of envisaging perturbations of a system, the time independent and the time dependent, in a manner already partially described in Section 5.4.1. First, assume that ω is to describe a state of equilibrium of the system $(\mathfrak{A}, \tau)$ then it is physically reasonable to postulate that ω is τ-invariant, i.e., the values of observations are stationary in time. Now consider a local perturbation P of the dynamical group. One could well expect the perturbed system to have a τ^P-invariant equilibrium state ω^P, which differs from ω in a substantial way only in the immediate neighborhood of the localization region of P, and such that the set of states $\omega^{\lambda P}$ for $\lambda \in [-\varepsilon, \varepsilon]$ approximate ω in the sense $\omega^{\lambda P}(A) \to \omega(A)$ as $|\lambda| \to 0$ for all $A \in \mathfrak{A}$. This is the time-independent point of view. Second, envisage the evolution of the perturbed states $\omega^{\lambda P}$ under the dynamical group τ. If the group τ is sufficiently ergodic, then one would expect the spatial effects of redistribution caused by the perturbation P to gradually disperse and the states $\omega^{\lambda P}$ should evolve to the state ω, i.e., one should have

$$\lim_{|t| \to \infty} \omega^{\lambda P}(\tau_t(A)) = \omega(A)$$

for all $A \in \mathfrak{A}$. This is the time-dependent point of view. But then differentiating and integrating one obtains

$$\begin{aligned}\lim_{T \to \infty} \int_{-T}^{T} dt\, \omega^{\lambda P}([P, \tau_t(A)]) &= \lim_{T \to \infty} \int_{-T}^{T} dt \frac{i}{\lambda} \frac{d}{dt} \omega^{\lambda P}(\tau_{-t}^{\lambda p} \tau_t(A)) \\ &= \lim_{T \to \infty} i\{\omega^{\lambda P}(\tau_T(A)) - \omega^{\lambda P}(\tau_{-T}(A))\}/\lambda = 0\end{aligned}$$

by use of the $\tau^{\lambda P}$-invariance of $\omega^{\lambda P}$ and the time-dependent postulate. Formally, one then finds

$$\int_{-\infty}^{\infty} dt\, \omega([P, \tau_t(A)]) = \lim_{\lambda \to 0} \int_{-\infty}^{\infty} dt\, \omega^{\lambda P}([P, \tau_t(A)]) = 0$$

by the time-independent postulate, and the exchange of limit and integral would, for example, be justified for $P, A \in \mathfrak{A}_0$ if $(\mathfrak{A}, \tau)$ is $L^1(\mathfrak{A}_0)$-asymptotically abelian. Thus, one concludes that the equilibrium state ω of the dynamical system $(\mathfrak{A}, \tau)$ should satisfy the stability requirement

$$\int_{-\infty}^{\infty} dt\, \omega([P,\ \tau_t(A)]) = 0$$

for all $P, A \in \mathfrak{A}$, or at least for a sufficiently large subset of P and A, e.g., strictly local elements of a quasi-local algebra.

The foregoing heuristic discussion relies upon a property of ergodicity of $(\mathfrak{A}, \tau)$, or of $(\mathfrak{A}, \tau, \omega)$, which we did not specify exactly. We postulated that the system was sufficiently dispersive, or mixing, to ensure that the perturbed states return to equilibrium. This problem has already been discussed in Section 5.4.1 and Propositions 5.4.6 and 5.4.10, and some form of asymptotic abelianness is certainly sufficient. But it also appears necessary to postulate that ω is relatively pure in order to ensure uniqueness of the limits of $\omega^{\lambda P}(\tau_t(A))$ as $t \to \pm\infty$. Therefore, this discussion of the behavior of equilibrium states ω is based on four types of postulates:

(1) τ-invariance, i.e., stationarity in time,
(2) ergodicity of $(\mathfrak{A},\ \tau)$, e.g., asymptotic abelianness,
(3) relative purity of ω, e.g., extremality of ω among the τ-invariant states,
(4) stability under perturbations.

These four postulates lead to the quantitative expression

$$\lim_{T \to \infty} \int_{-T}^{T} dt\, \omega([A, \tau_t(B)]) = 0$$

for $A, B \in \mathfrak{A}$, of stability and our aim is to show that they also imply that ω is a KMS state. (The relation between stability and the KMS property is in fact not so suprising when one remarks that the above stability condition reexpresses the KMS condition at zero energy in the form given in Proposition 5.3.14.)

The first result of this type is the following.

Theorem 5.4.19. *Let $(\mathfrak{A}, \tau)$ be a C^*- or W^*-dynamical system and ω a state over $\mathfrak{A}$. Assume that*

$$\lim_{|t| \to \infty} \|\pi_\omega([\tau_t(A),\ B])\psi\| = 0$$

for all, A, $B \in \mathfrak{A}$, and all $\psi \in \mathfrak{H}_\omega$. Furthermore, assume that ω satisfies the following conditions:

(a) *ω is τ-invariant.*

(b) *The functions*

$$t \mapsto |\omega(P\tau_t(A)) - \omega(P)\omega(A)| \ ,$$
$$t \mapsto \sup_{s\in\mathbb{R}} |\omega(P_1\tau_s(P_2)\tau_t(A_1\tau_s(A_2))) - \omega(P_1\tau_s(P_2))\omega(A_1\tau_s(A_2))|$$

*are L^1-functions for all A_1, P_1, A_2, and P_2 in a norm dense (σ-weakly dense) τ-invariant *-subalgebra $\mathfrak{A}_0$.*

(c) *ω is stable in the sense*

$$\lim_{T\to\infty} \int_{-T}^{T} dt\ \omega([A, \tau_t(B)]) = 0$$

for all A, $B \in \mathfrak{A}_0$.

It follows that ω is a (τ, β)–KMS state for some $\beta \in \mathbb{R}\cup\{\pm\infty\}$.

PROOF. By elementary reasoning one may assume that $\mathfrak{A}_0$ is invariant under regularization with L^1-functions. The cluster properties of ω adopted in the hypotheses of the theorem are preserved under this regularization since the convolution of two L^1-functions is an L^1-function. For example, the stability condition gives

$$\begin{aligned}\int dt\ \omega([A\tau_f(B), \tau_t(C)]) &= \iint dt\ ds f(s)\omega([A\tau_s(B), \tau_t(C)]) \\ &= \int ds\ f(s) \int dt\ \omega([A\tau_s(B), \tau_t(C)]) = 0\end{aligned}$$

if A, B, $C \in \mathfrak{A}_0$ and $f \in L^1(\mathbb{R})$.

Next, for P_i, $A_i \in \mathfrak{A}_0$ and $i = 1, 2$ define F_{A_i, P_i} and G_{A_i, P_i} by

$$F_{A_i, P_i}(t) = \omega(P_i\tau_t(A_i)) - \omega(P_i)\omega(A_i) \ ,$$
$$G_{A_i, P_i}(t) = \omega(\tau_t(A_i)P_i) - \omega(A_i)\omega(P_i)$$

for $t \in \mathbb{R}$. The τ–KMS condition can be reexpressed in terms of the Fourier transforms of these functions as in Proposition 5.3.14. We derive the condition from a series of observations concerning these functions.

OBSERVATION 1. $t \mapsto F_{A_1, P_1}(t)F_{A_2, P_2}(t) - G_{A_1, P_2}(t)G_{A_2, P_2}(t)$ is an L^1-function and

$$\int dt\{F_{A_1, P_1}(t)F_{A_2, P_2}(t) - G_{A_1, P_1}(t)G_{A_2, P_2}(t)\} = 0$$

PROOF. By the stability condition one has

$$\begin{aligned}0 &= \int_{-\infty}^{\infty} dt\ \omega([P_1\tau_s(P_2), \tau_t(A_1\tau_s(A_2))]) \\ &= \int_{-\infty}^{\infty} dt\{F_{A_1\tau_s(A_2), P_1\tau_s(P_2)}(t) - G_{A_1\tau_s(A_2), P_1\tau_s(P_2)}(t)\} \ .\end{aligned}$$

But it follows from the second clustering assumption and the τ-invariance of ω that the integrand is dominated by an L^1-function uniformly in s. Now from the first clustering assumption

$$\lim_{s\to\infty} \omega(P\tau_s(A)) = \omega(P)\omega(A)$$

for $A, P \in \mathfrak{A}_0$. But using the asymptotic abelianness one also has

$$\begin{aligned}\lim_{s\to\infty} \omega(P_1\tau_s(P_2)\tau_t(A_1\tau_s(A_2))) &= \lim_{s\to\infty} \omega(P_1[\tau_s(P_2), \tau_t(A_1)]\tau_{t+s}(A_2)) \\ &\quad + \lim_{s\to\infty} \omega(P_1\tau_t(A_1)\tau_s(P_2\tau_t(A_2))) \\ &= \omega(P_1\tau_t(A_1))\omega(P_2\tau_t(A_2)) \ .\end{aligned}$$

From this and similar relations and the Lebesgue-dominated convergence theorem applied to the above integral in the limit $s \to \infty$, it follows that

$$\begin{aligned}0 &= \int_{-\infty}^{\infty} dt\{\omega(P_1\tau_t(A_1))\omega(P_2\tau_t(A_2)) - \omega(\tau_t(A_1)P_1)\omega(\tau_t(A_2)P_2)\} \\ &= \int_{-\infty}^{\infty} dt\{F_{A_1,P_1}(t)F_{A_2,P_2}(t) - G_{A_1,P_1}(t)G_{A_2,P_2}(t)\} \\ &\quad + \omega(P_2)\omega(A_2)\int_{-\infty}^{\infty} dt(F_{A_1,P_1}(t) - G_{A_1,P_1}(t)) \\ &\quad + \omega(P_1)\omega(A_1)\int_{-\infty}^{\infty} dt(F_{A_2,P_2}(t) - G_{A_2,P_2}(t)) \\ &= \int_{-\infty}^{\infty} dt\{F_{A_1,P_1}(t)F_{A_2,P_2}(t) - G_{A_1,P_1}(t)G_{A_2,P_2}(t)\} \ .\end{aligned}$$

Now, all the functions F_{A_i,P_i} and G_{A_i,P_i} are L^1-functions, by assumption, and hence their Fourier transforms $\widehat{F}_{A_i,P_i}$ and $\widehat{G}_{A_i,P_i}$ exist as continuous functions vanishing at infinity.

OBSERVATION 2

$$\widehat{F}_{A_1,P_1}(p)\widehat{F}_{A_2,P_2}(-p) = \widehat{G}_{A_1,P_1}(p)\widehat{G}_{A_2,P_2}(-p)$$

for all $p \in \widehat{\mathbb{R}} = \mathbb{R}$ and all $A_i, P_i \in \mathfrak{A}_0$.

Proof. Since $F_{A_i,P_i}, G_{A_i,P_i} \in L^1 \cap L^\infty \subseteq L^2$, it follows by Parseval's theorem and Observation 1 that

$$\int_{-\infty}^{\infty} dp\ \widehat{F}_{A_1,P_1}(p)\widehat{F}_{A_2,P_2}(-p) = \int_{-\infty}^{\infty} dp\ \widehat{G}_{A_1,P_1}(p)\widehat{G}_{A_2,P_2}(-p) \ .$$

If f is an L^1-function, one computes that

$$\begin{aligned}F_{\tau_f(A_2),P_2}(t) &= \omega\Big(P_2 \int ds\ f(s)\tau_{t+s}(A_2)\Big) - \int ds\ f(s)\omega(A_2)\omega(P_2) \\ &= \int ds\ f(s)F_{A_2,P_2}(s+t) \ .\end{aligned}$$

Taking the Fourier transform of this convolution one obtains

$$\widehat{F}_{\tau_f(A_2),P_2}(p) = \widehat{F}_{A_2,P_2}(p)\hat{f}(-p) \ .$$

Similarly, one derives

$$\widehat{G}_{\tau_f(A_2),P_2}(p) = \widehat{G}_{A_2,P_2}(p)\hat{f}(-p) \ .$$

Inserting these relations in the earlier relation, with A_2 replaced by $\tau_f(A_2)$, one obtains

$$\int_{-\infty}^{\infty} dp\ \widehat{F}_{A_1,P_1}(p)\widehat{F}_{A_2,P_2}(-p)\hat{f}(p) = \int_{-\infty}^{\infty} dp\ \widehat{G}_{A_1,P_1}(p)\widehat{G}_{A_2,P_2}(-p)\hat{f}(p)\ .$$

As $\widehat{F}_{A_i,P_i}$ and $\widehat{G}_{A_i,P_i}$ are continuous in p it follows by letting $\hat{f}$ converge to the point measure δ_p that

$$\widehat{F}_{A_1,P_1}(p)\widehat{F}_{A_2,P_2}(-p) = \widehat{G}_{A_1,P_1}(p)\widehat{G}_{A_2,P_2}(-p)\ .$$

Now, introduce the unitary group

$$U_\omega(t) = e^{itH_\omega} = \int e^{itp}\ dE_\omega(p)$$

implementing τ in the cyclic representation $(\mathfrak{H}_\omega, \pi_\omega, \Omega_\omega)$ associated with ω.

OBSERVATION 3. If the spectrum of H_ω is not contained in $[0,+\infty\rangle$ or in $\langle-\infty,0]$, then for any $p \in \mathbb{R}$ there exists a pair A, $P \in \mathfrak{A}_0$ such that

$$\widehat{F}_{A,P}(p) \neq 0\ .$$

PROOF. Let $\mathscr{U} \subseteq \mathbb{R}$ be the set of $p \in \mathbb{R}$ such that $\widehat{F}_{A,P}(p) \neq 0$ for some A, $P \in \mathfrak{A}_0$.

By asymptotic abelianness and two-point clustering, one has

$$\lim_{T\to\infty} \frac{1}{2T}\int_{-T}^{T} dt\, \omega(A\tau_t(B)C) = \omega(AC)\omega(B)\ .$$

for all $A, B, C \in \mathfrak{A}_0$. Hence, it follows essentially as in Theorem 4.3.33 that the spectrum $\sigma(U_\omega)$ is additive,

$$\sigma(U_\omega) + \sigma(U_\omega) \subseteq \sigma(U_\omega)\ .$$

Now $E_\omega = E_\omega(\{0\})$ is the projection onto $\mathbb{C}\Omega_\omega$ and hence

$$\widehat{F}_{A,P}(p)dp = d(\pi_\omega(P^*)\Omega_\omega, E_\omega(p)\pi_\omega(A)\Omega_\omega) - (\pi_\omega(P^*)\Omega_\omega, E_\omega\pi_\omega(A)\Omega_\omega)\delta(p)dp\ .$$

The continuity of $\widehat{F}_{A,P}$ then implies that $\sigma(U_\omega)$ cannot contain isolated points. Hence,

$$\sigma(U_\omega) = \mathbb{R}$$

by Example 4.3.34. But it follows from this, and Proposition 3.2.40, that $\mathscr{U}$ is dense in $\mathbb{R}$. We argue that $\mathscr{U} = \mathbb{R}$ by contradiction. Assume that $p_0 \notin \mathscr{U}$, i.e.,

$$\int dt\ F_{A,P}(t)e^{-ip_0t} = 0$$

for all $A, P \in \mathfrak{A}_0$. Next set $A = A_1\tau_s(A_2)$ and $P = P_1\tau_s(P_2)$ in this relation and take the limit $s \to \infty$. It follows from the clustering assumption and the Lebesgue-dominated covergence theorem that

$$\begin{aligned} 0 = &\int dt\ e^{-ip_0t}F_{A_1,P_1}(t)F_{A_2,P_2}(t) \\ &+ \omega(A_2)\omega(P_2)\int dt\ e^{-ip_0t}F_{A_1,P_1}(t) \\ &+ \omega(A_1)\omega(P_1)\int dt\ e^{-ip_0t}F_{A_2,P_2}(t) = \int dt\ e^{-ip_0t}F_{A_1,P_1}(t)F_{A_2,P_2}(t)\ . \end{aligned}$$

Replacement of A_1 by $\tau_{-s}(A_1)$ gives

$$\int dt\, e^{-ip_0t} F_{A_1,P_1}(-s+t) F_{A_2,P_2}(t) = 0$$

for all $s \in \mathbb{R}$. But by Fourier transformation in s one then obtains

$$\widehat{F}_{A_1,P_1}(-p)\widehat{F}_{A_2,P_2}(p_0+p) = 0$$

for all $p \in \mathbb{R}$. Now, if $p + p_0 \in \mathscr{U}$ we can find A_2 and P_2, such that $\widehat{F}_{A_2,P_2}(p_0+p) \neq 0$, and hence

$$\widehat{F}_{A_1,P_1}(p) = 0$$

for all $p \in p_0 - \mathscr{U}$. But the latter set is dense and $\widehat{F}_{A_1,P_1}$ is continuous; hence $\widehat{F}_{A_1,P_1}$ is zero everywhere and we conclude that

$$\omega(P\tau_t(A)) = \omega(P)\omega(A)$$

for all $P, A \in \mathfrak{A}_0$ and $t \in \mathbb{R}$. This implies that ω is a τ-invariant character. In particular, $\dim \mathfrak{H}_\omega = 1$ and $U_\omega(t) = \mathbb{1}$ for all t. This contradicts the assumption that the spectrum of U_ω is not one sided. (Incidentally, ω is a τ-KMS state for all $\beta \in \mathbb{R} \cup \{\pm\infty\}$ in this case.)

OBSERVATION 4. If $\sigma(H_\omega)$ is not one sided, then there exists a unique continuous positive function Φ on $\mathbb{R}$ such that

$$\widehat{F}_{A,P}(p) = \Phi(p)\widehat{G}_{A,P}(p)$$

for all $p \in \mathbb{R}$.

PROOF. If $p \in \mathbb{R}$ is fixed, there exist, by Observation 3, elements $A_1, P_1 \in \mathfrak{A}_0$ such that $\widehat{F}_{A_1,P_1}(-p) \neq 0$. Define

$$\Phi(p) = \frac{\widehat{G}_{A_1,P_1}(-p)}{\widehat{F}_{A_1,P_1}(-p)} \ .$$

Then

$$\widehat{F}_{A,P}(p) = \Phi(p)\widehat{G}_{A,P}(p)$$

for all $A, P \in \mathfrak{A}_0$ by Observation 2. One can show as in Observation 3 that $\widehat{G}_{A,P}(p) \neq 0$ for some $A, P \in \mathfrak{A}$ and hence Φ is uniquely determined by the last relation. Furthermore, as $\widehat{F}_{A_1,P_1}$ is continuous we can use $\widehat{F}_{A_1,P_1}$ and $\widehat{G}_{A_1,P_1}$ to define Φ in a neighborhood of p, and hence Φ is continuous.

It follows immediately from the definition of $F_{A,P}$ and $G_{A,P}$ that

$$\overline{F_{A,P}(t)} = F_{P^*,A^*}(-t) = G_{A^*,P^*}(t) \ .$$

Hence, $\widehat{F}_{A,A^*}$ and $\widehat{G}_{A,A^*}$ are real for $A \in \mathfrak{A}_0$ and

$$\widehat{F}_{A,P}(-p) = \widehat{G}_{P,A}(p) \ .$$

Therefore, Φ is real and satisfies the relation

$$\Phi(-p) = \Phi(p)^{-1}.$$

But $\Phi(0) = 1$ by a direct application of the stability condition. Thus Φ is positive.

We are now prepared for the end of the proof of Theorem 5.4.19.

If $\sigma(U_\omega)$ is one sided, ω is a KMS state at $\pm\infty$ by Proposition 5.3.19. Thus we assume from now on that $\sigma(U_\omega)$ is not one sided. If $H_\omega = \int p\, dE_\omega(p)$ is the spectral decomposition of H_ω and E_ω is the projection onto $\mathbb{C}\Omega_\omega$, then

$$F_{A,P}(t) = \int e^{itp}(P^*\Omega_\omega, (dE_\omega(p) - E_\omega\delta(p)dp)A\Omega_\omega) \ ,$$

$$G_{A,P}(t) = \int e^{itp}(A^*\Omega_\omega, (dE_\omega(-p) - E_\omega\delta(p)dp)P\Omega_\omega)$$

for $A, P \in \mathfrak{A}_0$. Here, and in the sequel, we identify $\mathfrak{A}$ and $\pi_\omega(\mathfrak{A})$. Observation 4 then implies that the spectral measures are absolutely continuous with respect to Lebesgue measure, and

$$(P^*\Omega_\omega, (dE_\omega(p) - E_\omega\delta(p)dp)A\Omega_\omega) = \Phi(p)(A^*\Omega_\omega, (dE_\omega(-p) - E_\omega\delta(p)dp)P\Omega_\omega) \ .$$

Since Φ is positive with $\Phi(0) = 1$, it follows that

$$(P^*\Omega_\omega, dE_\omega(p)A\Omega_\omega) = (\Phi(p)^{1/2}A^*\Omega_\omega, dE_\omega(-p)\Phi(p)^{1/2}P\Omega_\omega) \ .$$

Hence, $\mathfrak{A}_0\Omega_\omega \subseteq D(\Phi(-H_\omega)^{1/2})$ and

$$(P^*\Omega_\omega, A\Omega_\omega) = (\Phi(-H_\omega)^{1/2}A^*\Omega_\omega, \Phi(-H_\omega)^{1/2}P\Omega_\omega) \ .$$

Now $\pi_\omega(\mathfrak{A}_0)$ is strongly* dense in $\mathfrak{M}_\omega = \pi_\omega(\mathfrak{A})''$, by Theorem 2.4.11, and as $\Phi(-H_\omega)^{1/2}$ is a closed operator it follows from the above relation that

$$\mathfrak{M}_\omega\Omega_\omega \subseteq D(\Phi(-H_\omega)^{1/2})$$

and by continuity

$$(B\Omega_\omega, A\Omega_\omega) = (\Phi(-H_\omega)^{1/2}A^*\Omega_\omega, \Phi(-H_\omega)^{1/2}B^*\Omega_\omega)$$

for all A, $B \in \mathfrak{M}_\omega$. From this it follows that

$$A\Omega_\omega = 0 \Rightarrow A^*\Omega_\omega = 0$$

for all $A \in \mathfrak{M}_\omega$. Hence Ω_ω is separating for $\mathfrak{M}_\omega$ by Lemma 5.3.8. Since $\mathfrak{M}_\omega\Omega_\omega$ is a dense, U_ω-invariant, subset of $\mathfrak{H}_\omega$ which is closed under regularization with functions in L^1, it follows by the reasoning used in the proof of Theorem 5.3.10 that $\mathfrak{M}_\omega\Omega_\omega$ is a core for $\Phi(-H_\omega)^{1/2}$. But $\mathfrak{M}_\omega\Omega_\omega$ is also a core of $\Delta^{1/2}$, where Δ is the modular operator associated with the pair $(\mathfrak{M}_\omega, \Omega_\omega)$. Moreover, as

$$(\Phi(-H_\omega)^{1/2}A\Omega_\omega, \Phi(-H_\omega)^{1/2}B\Omega_\omega) = (B^*\Omega_\omega, A^*\Omega_\omega) = (\Delta^{1/2}A\Omega_\omega, \Delta^{1/2}B\Omega_\omega)$$

for all A, $B \in \mathfrak{M}_\omega$, it follows from the remarks before Lemma 5.2.13 that

$$\Phi(-H_\omega)^{1/2} = \Delta^{1/2} \ .$$

Now identify τ with its normal extension to $\mathfrak{M}_\omega$, and let

$$\sigma_t(A) = \Delta^{it}A\Delta^{-it}$$

be the modular automorphism group. As ω is τ-invariant, it follows from Proposition 5.3.33 that

$$\tau_t\sigma_s = \sigma_s\tau_t$$

for all $t, s \in \mathbb{R}$. But as ω is separating for $\mathfrak{M}_\omega$ one has

$$\inf_{B' \in Co(\tau_{\mathbb{R}}(B))} |\omega(AB'C) - \omega(B)\omega(AC)| = 0$$

for all A, B, $C \in \mathfrak{M}_\omega$ by Theorem 4.3.23. Now Theorem 4.3.33 and the subsequent remark imply that the joint spectrum of H_ω and $\log \Delta$ is additive. Since

$$\log \Phi(-H_\omega) = \log \Delta$$

and $\sigma(H_\omega) = \mathbb{R}$ by Observation 3, it follows that the function $p \mapsto \log \Phi(p)$ is linear, and there exists, a $\beta \in \mathbb{R}$ such that

$$\Phi(p) = e^{-\beta p} \ .$$

But then

$$e^{-\beta H_\omega} = \Delta \ .$$

Hence ω is a τ-KMS state at value β as a consequence of Theorem 5.3.10.

Remark. Instead of the clustering conditions imposed on ω in Theorem 5.4.19, one could require that the truncated n-point functions $\omega_T^{(n)}$ satisfy strong clustering properties for $n = 2, 3, 4$, i.e., if $A_1, \cdots, A_n \in \mathfrak{A}_0$ there exists a non-negative, nonincreasing, integrable, function $g_{A_1} \cdots A_n$ on $\mathbb{R}_+$ such that

$$|\omega_T^{(n)}(\tau_{t_1}(A_1), \ldots, \tau_{t_n}(A_n))| \leq g_{A_1 \ldots A_n}\Big(\sup_{i,j} |t_i - t_j|\Big)$$

for $n = 2, 3, 4$ and $t_i \in \mathbb{R}$.

We now show that the clustering properties of the state imposed in Theorem 5.4.19 can be weakened if one imposes a stronger form of asymptotic abelianness. In fact, the following theorem essentially characterizes extremal (τ, β)-KMS states of L^1-asymptotically abelian systems as stable factor states. The only discrepancy in this characterization occurs if $\beta = 0$ because the extremal $(\tau, 0)$–KMS states, i.e., the extremal traces, are not necessarily factor states. Of course, this discrepancy is absent if $\mathfrak{A}$ has a unique trace-state.

Theorem 5.4.20. *Let $(\mathfrak{A}, \tau)$ be a C^*-dynamical system which is $L^1(\mathfrak{A}_0)$-asymptotically abelian in the sense of Definition* 5.4.8, and *ω a τ-invariant state over $\mathfrak{A}$. Assume that*

(1) *Either*

$$\lim_{\inf_{i \neq j} |t_i - t_j| \to \infty} \omega(\tau_{t_1}(A_1)\tau_{t_2}(A_2)\tau_{t_3}(A_3)) = \omega(A_1)\omega(A_2)\omega(A_3)$$

for all A_1, A_2, $A_3 \in \mathfrak{A}$, or ω is a factor state.

(2) *ω satisfies the stability requirement*

$$\int_{-\infty}^{\infty} dt\ \omega([P, \tau_t(A)]) = 0$$

for all A, $P \in \mathfrak{A}_0$.

It follows that ω is an extremal (τ, β)-KMS state for some $\beta \in \mathbb{R} \cup \{\pm\infty\}$.

PROOF. As $t \mapsto \tau_t(B)$ is uniformly continuous for each $B \in \mathfrak{A}_0$, it follows from the $L^1(\mathfrak{A})$-asymptotic abelianness that

$$\lim_{t \to \pm\infty} \|[A, \tau_t(B)]\| = 0$$

for all $A, B \in \mathfrak{A}_0$, and hence for all $A, B \in \mathfrak{A}$. Thus if ω is a factor state it follows from Example 4.3.34 that

$$\lim_{\inf_{i \neq j} |t_i - t_j| \to \infty} \omega(\tau_{t_1}(A_1) \cdots \tau_{t_n}(A_n)) = \omega(A_1) \cdots \omega(A_n)$$

for all $n \in \mathbb{Z}_+$ and $A_i \in \mathfrak{A}$. Therefore, it suffices to prove the theorem under the three-point clustering assumption.

If $\{E_\alpha\}$ is an approximate identity on $\mathfrak{A}$, it follows from Proposition 2.3.11 that

$$\lim_\alpha \pi_\omega(E_\alpha)\Omega_\omega = \Omega_\omega$$

and using this one easily proves the two-point cluster property

$$\lim_{t \to \pm\infty} \omega(A\tau_t(B)) = \omega(A)\omega(B)$$

from the corresponding three-point property. Also, as in the proof of Theorem 5.4.19, we may assume that $\mathfrak{A}_0$ is closed under regularization by L^1-functions.

Let us define

$$F_i(t) = F_{A_i, P_i}(t) = \omega(P_i \tau_t(A_i)) - \omega(P_i)\omega(A_i) \ ,$$
$$G_i(t) = G_{A_i, P_i}(t) = \omega(\tau_t(A_i)P_i) - \omega(A_i)\omega(P_i) \ ,$$

for $A_i, P_i \in \mathfrak{A}_0$.

OBSERVATION 1. $t \mapsto F_1(t)F_2(t) - G_1(t)G_2(t)$ is an L^1-function, and

$$\int_{-\infty}^{\infty} dt \{F_1(t)F_2(t) - G_1(t)G_2(t)\} = 0 \ .$$

PROOF. By the stability requirement we have

$$0 = \int_{-\infty}^{\infty} dt \ \omega([P_1 \tau_s(P_2), \tau_t(A_1 \tau_s(A_2))]) = I_1(s) + I_2(s) + I_3(s) + I_4(s) \ ,$$

where

$$I_1(s) = \int_{-\infty}^{\infty} dt \ \omega(P_1[\tau_s(P_2), \tau_t(A_1)]\tau_{t+s}(A_2)) \ ,$$

$$I_2(s) = \int_{-\infty}^{\infty} dt \ \omega(P_1 \tau_t(A_1)[\tau_s(P_2), \tau_{s+t}(A_2)]) \ ,$$

$$I_3(s) = \int_{-\infty}^{\infty} dt \ \omega([P_1, \tau_t(A_1)]\tau_{t+s}(A_2)\tau_s(P_2)) \ ,$$

$$I_4(s) = \int_{-\infty}^{\infty} dt \ \omega(\tau_t(A_1)[P_1, \tau_{t+s}(A_2)]\tau_s(P_2)) \ .$$

The integrands of I_2 and I_3 are dominated by L^1-functions which are independent of s, and using the two-point clustering and the Lebesgue-dominated convergence theorem we obtain

$$\begin{aligned}\lim_{s\to\infty}\{I_2(s)+I_3(s)\} &= \int_{-\infty}^{\infty} dt\ \omega(P_1\tau_t(A_1))\omega([P_2,\ \tau_t(A_2)]) \\ &\quad + \int_{-\infty}^{\infty} dt\ \omega([P_1,\tau_t(A_1)])\omega(\tau_t(A_2)P_2) \\ &= \int_{-\infty}^{\infty} dt\{F_{A_1,P_1}(t)F_{A_2,P_2}(t) - G_{A_1,P_1}(t)G_{A_2,P_2}(t)\}\ ,\end{aligned}$$

where the last step uses the stability condition. Hence it is enough for Observation 1 to show that

$$\lim_{s\to\infty} I_1(s) = \lim_{s\to\infty} I_4(s) = 0\ .$$

But, by a change of variable,

$$I_1(s) = \int_{-\infty}^{\infty} dt\ \omega(\tau_{-s}(P_1)[P_2,\tau_t(A_1)]\tau_{t+s}(A_2))\ .$$

Again the integrand is dominated by the L^1-function $t \mapsto \|P_1\|\ \|[P_2,\tau_t(A_1)]\|\ \|A_2\|$, which is independent of s, and the limit of the integrand as $s \to \infty$ is

$$\omega(P_1)\omega([P_2,\tau_t(A_1)])\omega(A_2)$$

by the three-point cluster property. Thus, by the Lebesgue-dominated convergence theorem,

$$\lim_{s\to\infty} I_1(s) = \omega(P_1)\omega(A_2)\int_{-\infty}^{\infty} dt\ \omega([P_2,\tau_t(A_1)]) = 0\ .$$

One shows that $\lim_{s\to\infty} I_4(s) = 0$ by a similar reasoning, and this ends the proof of Observation 1.

Now, from the relations

$$F_{A,P}(t) = G_{P,A}(-t), \quad F_{t_s(A),P}(t) = F_{A,P}(t+s)\ ,$$

and Observation 1 it follows that

$$\int dt\{F_1(t)G_2(s-t) - G_1(t)F_2(s-t)\} = 0\ .$$

Define $H_{A,P} = F_{A,P} - G_{A,P}$ and set $H_1 = H_{A_1,P_1}$ so

$$H_1(t) = F_1(t) - G_1(t)\ .$$

Then H_1 is an L^1-function, and from the relation above we obtain

$$\int dt\{H_1(t)G_2(s-t) - G_1(t)H_2(s-t)\} = 0\ .$$

and

$$\int dt\{F_1(t)H_2(s-t) - H_1(t)F_2(s-t)\} = 0\ .$$

If $U_\omega(t) = \int e^{ipt}\,dE_\omega(p)$ is the spectral decomposition of U_ω, let

$$\mu_i = \mu_{A_i,P_i}, \quad \nu_i = \nu_{A_i,P_i}$$

be the measures defined by

$$d\mu_i(p) = (P_i^*\Omega_\omega,\, dE_\omega(p)A_i\Omega_\omega) - \omega(P_i)\omega(A_i)\delta(p)dp \ ,$$
$$d\nu_i(p) = (A_i^*\Omega_\omega, dE_\omega(-p)P_i\Omega_\omega) - \omega(A_i)\omega(P_i)\delta(p)dp \ .$$

Then

$$F_i(t) = \int e^{itp}d\mu_i(p), \quad G_i(t) = \int e^{itp}d\nu_i(p) \quad ,$$

and thus

$$d\mu_i(p) - d\nu_i(p) = \widehat{H}_i(p)dp \ ,$$

where $\widehat{H}_i$ is the Fourier transform of H_i. From the convolution relations above we now obtain

OBSERVATION 2

$$\widehat{H}_2(p)d\nu_1(p) = \widehat{H}_1(p)d\nu_2(p) \ ,$$
$$\widehat{H}_2(p)d\mu_1(p) = \widehat{H}_1(p)d\mu_2(p) \ ,$$

for all $A_i, P_i \in \mathfrak{A}_0$.

Next, define a subset $S \subseteq \mathbb{R}$ by

$$S = \{p \in \mathbb{R};\, \widehat{H}_{A,P}(p) \neq 0 \quad \text{for some } A, P \in \mathfrak{A}_0\} \ .$$

OBSERVATION 3. S is an open set, $S = -S$ and $0 \notin S$.

PROOF. S is open since each $\widehat{H}_{A,P}$ is the Fourier transform of an L^1-function, and thus is continuous. The symmetry follows from the relation

$$\begin{aligned} dp\,\widehat{H}_{A,P}(p) &= (P^*\Omega_\omega, dE\omega(p)A\Omega_\omega) - (A^*\Omega_\omega, dE_\omega(-p)P\Omega_\omega) \\ &= -dp\,\widehat{H}_{P,A}(-p) \ , \end{aligned}$$

and $\widehat{H}_{A,P}(0) = 0$ by this same relation (or stability).

OBSERVATION 4. There exists a well-defined pair μ, ν of σ-finite measures on S such that

$$d\mu_{A,P}(p) = \widehat{H}_{A,P}(p)d\mu(p), \quad d\nu_{A,P}(p) = \widehat{H}_{A,P}(p)d\nu(p)$$

for $p \in S$, and, furthermore

$$d\mu(p) = -d\nu(-p) \ .$$

PROOF. Since S is open, S is the union of an increasing sequence of compact sets, and as each $\widehat{H}_{A,P}$ is continuous, it follows that there exists a countable partition $\{S_1, S_2, \cdots\}$ of S into Borel sets, and elements $A_i, P_i \in \mathfrak{A}_0$ such that

$$|\widehat{H}_{A_i P_i}(p)| \geq 1$$

for $p \in S_i$. Now, define

$$d\mu(p) = \frac{d\mu_{A_i,\,P_i}(p)}{\widehat{H}_{A_i,\,P_i}(p)}, \quad d\nu(p) = \frac{d\nu_{A_i,\,P_i}(p)}{\widehat{H}_{A_i,\,P_i}(p)}$$

for $p \in S_i$, $i = 1, 2, \cdots$ Then μ and ν are well-defined σ-finite Borel measures on S, and Observation 2 implies that

$$d\mu_{A,\,P}(p) = \widehat{H}_{A,\,P}(p)d\mu(p), \quad d\nu_{A,\,P}(p) = \widehat{H}_{A,\,P}(p)d\nu(p)$$

for all A, $P \in \mathfrak{A}_0$ and all $p \in S$. Finally,

$$d\mu(p) = \frac{d\mu_{A_i,\,P_i}(p)}{\widehat{H}_{A_i,\,P_i}(p)} = \frac{d\nu_{P_i,\,A_i}(-p)}{-\widehat{H}_{P_i,\,A_i}(-p)} = -d\nu(-p) \ .$$

Now, the Radon-Nikodym theorem implies that there exist $|\mu| + |\nu|$-measurable functions ψ_i on S such that

$$d\mu(p) = \psi_1(p)d(|\mu| + |\nu|)(p), \quad d\nu(p) = \psi_2(p)d(|\mu| + |\nu|)(p) \ .$$

Since $d\mu(-p) = -d\nu(p)$ we have $d(|\mu| + |\nu|)(p) = d(|\mu| + |\nu|)(-p)$ and $\psi_1(-p) = -\psi_2(p)$. Define subsets S_0, S_∞, and S_f of $\mathbb{R}$ by

$$S_0 = \{p \in S; \psi_1(p) = 0\}, \quad S_\infty = \{p \in S; \psi_2(p) = 0\} \ ,$$
$$S_f = \mathbb{R}\backslash(S_0 \cup S_\infty) \ .$$

Since $\psi_1(p) = 0$ if, and only if, $\psi_2(-p) = 0$, we deduce immediately

OBSERVATION 5

$$S_0 = -S_\infty, \quad S_f = -S_f$$

in the sense that the sets differ only on a set of $|\mu| + |\nu|$-measure zero.

Define a Borel function φ on $\mathbb{R}\backslash S_\infty$ by

$$\varphi(p) = \begin{cases} \frac{\psi_1(p)}{\psi_2(p)}, & \text{on } S\backslash S_\infty \\ 1, & \text{on } \mathbb{R}\backslash S \ . \end{cases}$$

OBSERVATION 6

$$d\mu_{A,P}(p) = \varphi(p)d\nu_{A,P}(p)$$

on $\mathbb{R}\backslash S_\infty$. Furthermore, $\varphi(p) > 0$ and $\varphi(-p) = \varphi(p)^{-1}$ on S_f (except for a set of $|\mu| + |\nu|$-measure zero).

PROOF. It follows from Observation 4 that

$$d\mu_{A,P}(p) = \psi_1(p)\widehat{H}_{A,P}(p)d(|\mu| + |\nu|)(p) \ ,$$
$$d\nu_{A,P}(p) = \psi_2(p)\widehat{H}_{A,P}(p)d(|\mu| + |\nu|)(p) \ ,$$

for $p \in S$, while

$$d\mu_{A,P}(p) - d\nu_{A,P}(p) = \widehat{H}_{A,P}(p)dp = 0 \ .$$

for $p \in S^c$. As $d\mu_{A^*,A}(p) \geq 0$ and $d\nu_{A^*,A}(p) \geq 0$ for all $p \neq 0$ and all $A \in \mathfrak{A}_0$, it follows that $\varphi(p) \geq 0$ and since $\varphi(p) \neq 0$ for $p \in S_f$, one has $\varphi(p) > 0$ for $p \in S_f$. Thus $\varphi(p) = \varphi(-p)^{-1}$ is a consequence of $\psi_1(p) = -\psi_2(-p)$.

OBSERVATION 7. If E_ω is the projection-valued measure corresponding to H_ω, then

$$E_\omega(S_0) = 0$$

and, consequently,

$$E_\omega(S_\infty \cup S_f) = \mathbb{1} \ .$$

PROOF. From the relation

$$d\mu_{A,P}(p) = \psi_1(p)\widehat{H}_{A,P}(p)d(|\mu| + |\nu|)(p)$$

it follows that

$$\mu_{A,P}(S_0) = 0$$

and hence, as $0 \notin S_0$ by Observation 3,

$$(P^*\Omega_\omega, E_\omega(S_0)A\Omega_\omega) = \mu_{A,P}(S_0) = 0$$

for all $A, P \in \mathfrak{A}_0$.

OBSERVATION 8

$$(P^*\Omega_\omega, E_\omega(S_f)A\Omega_\omega) = (\varphi(-H_\omega)^{1/2}A^*\Omega_\omega,\ \varphi(-H_\omega)^{1/2}P\Omega_\omega)$$

for all $A, P \in \mathfrak{M}_\omega = \pi_\omega(\mathfrak{A})''$.

PROOF. By Observation 6, one has

$$\begin{aligned}(P^*\Omega_\omega,\ dE_\omega(p)A\Omega_\omega) &= d\mu_{A,P}(p) + \omega(P)\omega(A)\delta(p)dp \\ &= \varphi(p)d\nu_{A,P}(p) + \omega(P)\omega(A)\delta(p)dp \\ &= (\varphi(p)^{1/2}A^*\Omega_\omega, dE_\omega(-p)\varphi(p)^{1/2}P\Omega_\omega)\end{aligned}$$

for $p \in \mathbb{R}\backslash S_\infty$, and $A, P \in \mathfrak{A}_0$, where we have identified $\mathfrak{A}$ and $\pi_\omega(\mathfrak{A})$. Integrating over $\mathbb{R}\backslash S_\infty = S_f \cup S_0$, we obtain from spectral theory that

$$\mathfrak{A}_0\Omega_\omega \subseteq D(\varphi(-H_\omega)^{1/2}E_\omega(-(S_f \cup S_0)))$$

and

$$\begin{aligned}(P^*\Omega_\omega,\ E_\omega(S_f)A\Omega_\omega) &= (P^*\Omega_\omega, E_\omega(S_f \cup S_0)A\Omega_\omega) \\ &= (\varphi(-H_\omega)^{1/2}A^*\Omega_\omega,\ \varphi(-H_\omega)^{1/2}P\Omega_\omega)\end{aligned}$$

where we have used the relations $E_\omega(S_0)$ and $E_\omega(-(S_f \cup S_0)) = E_\omega(S_f \cup S_\infty)$ which follow from Observations 5 and 7.

Since $\mathfrak{A}_0$ is strongly* dense in $\mathfrak{M}_\omega$ by Corollary 2.4.15, this last equation extends to all $A, P \in \mathfrak{M}_\omega$.

Next define

$$E_f = [\mathfrak{M}'_\omega\Omega_\omega] \ .$$

Then $E_f \in \mathfrak{M}_\omega$.

OBSERVATION 9

$$E_\omega(S_f) = E_\omega(S_f)E_f = E_f E_\omega(S_f) \ .$$

PROOF. Since

$$e^{itH_\omega}\mathfrak{M}'_\omega e^{-itH_\omega} = \mathfrak{M}'_\omega$$

for all $t \in \mathbb{R}$, it follows that E_f commutes with e^{itH_ω}, and hence

$$E_\omega(S_f)E_f = E_f E_\omega(S_f) \ .$$

By Observation 8, one has

$$\begin{aligned}(E_\omega(S_f)(\mathbb{1} - E_f)\, P^*\Omega_\omega, E_\omega(S_f)(\mathbb{1} - E_f)A\Omega_\omega)\\ = (\varphi(-H_\omega)^{1/2}A^*(\mathbb{1} - E_f)\Omega_\omega, \varphi(-H_\omega)^{1/2}P(\mathbb{1} - E_f)\Omega_\omega) = 0\end{aligned}$$

for all $A, P \in \mathfrak{M}_\omega$, and hence

$$E_\omega(S_f)(\mathbb{1} - E_f) = 0 \ .$$

Now, Ω_ω is cyclic and separating for the von Neumann algebra $\mathfrak{M}_E = E_f\mathfrak{M}_\omega E_f$ on $\mathfrak{H}_E = E_f\mathfrak{H}_\omega$ by Lemma 4.3.13. Define $H_E = H_\omega E_f = E_f H_\omega$ and let Δ and J be the modular operator and modular conjugation associated with the pair $(\mathfrak{M}_E, \Omega)$. Then

$$H_E = \int p\ dE_E(p) = \int p\ dE_\omega(p)E_f$$

is the spectral decomposition of H_E. As e^{itH_E} leaves Ω_ω invariant and defines an automorphism group of $\mathfrak{M}_E$, it follows as in the proof of (3) $\Rightarrow$ (2) in Theorem 3.2.61 that

$$JH_E J = -H_E$$

and hence

$$JE_E(B)J = E_E(-B)$$

for all Borel sets $B \subseteq \mathbb{R}$. In particular, it follows from Observation 7 that

$$E_f = JE_f J = JE_E(S_f \cup S_\infty)J = E_E(-(S_f \cup S_\infty)) \ .$$

But

$$E_E(-S_\infty) = E_E(S_0) = 0$$

by Observations 5 and 7. Thus,

$$E_f = E_E(-S_f) = E_\omega(S_f)E_f$$

and Observation 9 implies:

OBSERVATION 10

$$E_f = E_\omega(S_f) \ .$$

Now, Theorem 4.3.22 implies that $E_\omega = E_\omega(\{0\})$ is a one-dimensional projection, and as Ω_ω is separating for $\mathfrak{M}_E$ it follows from Theorem 4.3.23 that

$$\inf_{B' \in Co(\tau_{\mathbb{R}}(B))} |\omega(AB'C) - \omega(B)\omega(AC)| = 0$$

for all $A, B, C \in \mathfrak{M}_E$. As H_E and Δ commute strongly by Proposition 5.3.33, (2), it follows from Theorem 4.3.33 and the subsequent remark that the joint spectrum Σ of $(\log \Delta, H_E)$ is a closed additive subset of $\mathbb{R}^2$. But since Ω_ω is separating for $\mathfrak{M}_E$, Lemma 3.2.42, (2), implies that Σ is symmetric, and we conclude

OBSERVATION 11. The joint spectrum Σ of $(\log \Delta, H_E)$ is a closed subgroup of $\mathbb{R}^2$.

We next show

OBSERVATION 12. $E_\omega(S_f)$ is not one-dimensional, then S_f is dense in $\mathbb{R}$ and $\sigma(H_E) = \mathbb{R}$.

PROOF. $\sigma(H_E)$ is a group by the remarks before Observation 11, and as 0 is a simple eigenvalue of H_ω it follows from the assumption and $E_\omega(S_f) = E_f$ that $\sigma(H_E) \neq \{0\}$. But $\sigma(H_E)$ cannot have any nonzero isolated points because this would imply that H_ω has a nonzero eigenvalue λ with a corresponding eigenvector ψ such that

$$U_\omega(t)\psi = e^{i\lambda t}\psi \ .$$

But then

$$(\psi, \pi_\omega(\tau_t(B))\Omega) = (U_\omega(-t)\psi, \pi_\omega(B)\Omega_\omega) = e^{i\lambda t}(\psi, \pi_\omega(B)\Omega_\omega)$$

for all $B \in \mathfrak{A}$. Therefore, choosing B such that

$$(\psi, \pi_\omega(B)\Omega_\omega) \neq 0$$

this contradicts the fact that

$$\lim_{t\to\infty} \pi_\omega(\tau_t(B)) = \omega(B)\mathbb{1}$$

in the weak topology. It follows from Example 4.3.34 that

$$\sigma(H_E) = \mathbb{R} \ .$$

OBSERVATION 13

$$\sigma(H_E) + \sigma(H_{\mathbb{1}-E}) \subseteq \sigma(H_{\mathbb{1}-E}) \ .$$

PROOF. This is demonstrated as in the last part of the proof of Theorem 5.3.22.

OBSERVATION 14. The restrictions of the measures $d\mu_{A,P}$ and $d\nu_{A,P}$ to $S_0 \cup S_\infty$ are absolutely continuous with respect to Lebesgue measure, and

$$d\mu_{A,P}(p) = \begin{cases} 0, & p \in S_0 \\ \widehat{H}_{A,P}(p)dp, & p \in S_\infty \end{cases} ,$$

$$d\nu_{A,P}(p) = \begin{cases} -\widehat{H}_{A,P}(p)dp, & p \in S_0 \\ 0, & p \in S_\infty \end{cases} .$$

PROOF. This follows from the relation

$$d\mu_{A,P}(p) - d\nu_{A,P}(P) = \widehat{H}_{A,P}(p)dp$$

together with the equations

$$d\mu_{A,P}(p) = 0, \ p \in S_0, \qquad d\nu_{A,P}(p) = 0, \ p \in S_\infty \ .$$

Next, define subsets $S_\pm \subseteq \mathbb{R}$ by

$$S_+ = \bigcap_{A \in \mathfrak{A}_0} \{p; \widehat{H}_{A,A^*}(p) \geq 0\}, \qquad S_- = \bigcap_{A \in \mathfrak{A}_0} \{p; \widehat{H}_{A,A^*}(p) \leq 0\} \ .$$

Then $S_\pm$ are closed sets, and since

$$S = \bigcup_{A \in \mathfrak{A}_0} \{p; \widehat{H}_{A,A^*}(p) \neq 0\} \ .$$

by polarization, it follows that

$$S_+ \cap S_- \cap S = \varnothing \ .$$

But the measures $d\mu_{A,A^*}(p)$ and $d\nu_{A,A^*}(p)$ are non-negative for $p \neq 0$, and hence it follows from Observation 14 that

$$S_\infty \subseteq S_+, \qquad S_0 \subseteq S_-$$

except for sets of spectral measure zero. By subtracting the latter sets from S_∞ and S_0 we may assume that the inclusions are strict and hence

$$\overline{S_\infty} \subseteq S_+, \qquad \overline{S_0} \subseteq S_- \ ,$$

where the bar denotes closure. Therefore, one has

OBSERVATION 15

$$\overline{S_\infty} \cap \overline{S_0} \cap S \subseteq S_+ \cap S_- \cap S = \varnothing \ .$$

Now, by Observations 7 and 10, one has

$$E_\omega(S_\infty) = \mathbb{1} - E_f$$

and thus

OBSERVATION 16

$$\sigma(H_{\mathbb{1}-E}) \subseteq \overline{S_\infty} \ .$$

We now finish the proof of Theorem 5.4.20. We consider two cases:

Case 1. $E_\omega(S_f)$ is not one-dimensional. In this case $\sigma(H_E) = \mathbb{R}$ by Observation 12. We show, *ad absurdum,* that $E_f = \mathbb{1}$. If not, $\sigma(H_{\mathbb{1}-E}) = \mathbb{R}$ by Observation 13 and hence $\overline{S_\infty} = \mathbb{R}$ by Observation 16. But then $\overline{S_0} = \overline{-S_\infty} = \mathbb{R}$ by Observation 5, and hence $\overline{S_\infty} \cap \overline{S_0} \cap S = S$. But $S \neq \varnothing$ since $S_\infty \subseteq S$, and hence this contradicts Observation 15. It follows that $E_f = \mathbb{1}$. Now $E_\omega(S_f) = \mathbb{1}$ by Observation 10, thus $E_\omega(S_\infty) = 0$, and we may assume that $S_\infty = S_0 = \varnothing$ by modifying ψ_1, ψ_2 on sets of $|\mu| + |\nu|$-measure zero.

It follows from Observation 8 that

$$\begin{aligned}(\Delta^{1/2}A^*\Omega_\omega, \Delta^{1/2}P\Omega_\omega) &= (P^*\Omega_\omega, A\Omega_\omega) \\ &= (\varphi(-H_\omega)^{1/2}A^*\Omega_\omega, \varphi(-H_\omega)^{1/2}P\Omega_\omega)\end{aligned}$$

for all $A, P \in \mathfrak{M}_\omega$. As $\mathfrak{M}_\omega\Omega$ is a core for $\Delta^{1/2}$, and H_ω and $\Delta^{1/2}$ commute strongly, by Proposition 5.3.33, (2), it follows from this relation and a joint spectral representation of H_ω and Δ that

$$\Delta = \varphi(-H_\omega) \ .$$

It follows that

$$\Sigma \subseteq \overline{\{(\log(\varphi(-p)), p); p \in \mathbb{R}\}} \ .$$

Now, Σ cannot have any isolated points by the reasoning used in Observation 12, and Σ is a closed subgroup of $\mathbb{R}^2$ by Observation 11. As $\sigma(H_\omega) = \mathbb{R}$ it follows that Σ must have one of the forms:

(1) $\Sigma = \mathbb{R}^2$,

(2) Σ is an array of equidistant straight lines, not parallel with the log Δ axis, one of which contains the orgin.

(3) Σ is a straight line through the origin not coinciding with the log Δ axis.

In case 3, there exists a $\beta \in \mathbb{R}$ such that $\Sigma = \{(-\beta p, p);\ p \in \mathbb{R}\}$ and thus log $\Delta = -\beta H_\omega$, or

$$\Delta = e^{-\beta H_\omega} \ .$$

But Theorem 5.3.10 then implies that ω is a τ-KMS state at value β. Hence to complete the treatment of Case 1, we must eliminate possibilities (1) and (2) above. There are now two possibilities:

Case 1a. $H_{A,A^*} = 0$ for all $A \in \mathfrak{A}_0$. In this case

$$\begin{aligned}\omega(AA^*) &= F_{A,A^*}(0) + \omega(A)\omega(A^*)\\ &= G_{A,A^*}(0) + \omega(A)\omega(A^*) = \omega(A^*A)\end{aligned}$$

for all $A \in \mathfrak{A}_0$, and hence ω is a trace, i.e., ω is a $(\tau, 0)$-KMS state.

Case 1b. $\widehat{H}_{A,A^*}(p_0) \neq 0$ for some $A \in \mathfrak{A}_0$ and $p_0 \in \mathbb{R}$. Since $\widehat{H}_{A,A^*}$ is continuous, we may assume that $p_0 \neq 0$ and that $\widehat{H}_{A,A^*}(p) \neq 0$ for all $p \in (p_0 - \varepsilon, p_0 + \varepsilon)$, where ε is some positive number. From Observation 6 and the relation

$$d\mu_{A,A^*}(p) - d\nu_{A,A^*}(p) = \widehat{H}_{A,A^*}(p)dp \ ,$$

we deduce that

$$\begin{aligned}(\varphi(p) - 1)d\nu_{A,A^*}(p) &= \widehat{H}_{A,A^*}(p)dp \ ,\\ (1 - \varphi(p)^{-1})d\mu_{A,A^*}(p) &= \widehat{H}_{A,A^*}(p)dp \ .\end{aligned}$$

As $\widehat{H}_{A,A^*}$ is a real function we have two possibilities: $\widehat{H}_{A,A^*}(p_0) \gtrless 0$. If $\widehat{H}_{A,A^*}(p_0) > 0$, then $\widehat{H}_{A,A^*}(p) > 0$ for $p \in (p_0 - \varepsilon, p_0 + \varepsilon)$. We now deduce from the relation

$$d\nu_{A,A^*}(p) = \widehat{H}_{A,A^*}(p)d\nu(p)$$

that ν is a positive measure on $(p_0 - \varepsilon, p_0 + \varepsilon)$ and

$$(\varphi(p) - 1)d\nu(p) = dp$$

on this interval. It follows that $\varphi(p) \geq 1$ for $p \in (p_0 - \varepsilon, p_0 + \varepsilon)$ except for a set of $|\nu|$-measure zero. But $d\mu(p) = \varphi(p)d\nu(p)$ and so $\varphi(p) \geq 1$ for $p \in (p_0 - \varepsilon, p_0 + \varepsilon)$ except for a set of μ-measure, and hence spectral measure, zero. Thus we may choose φ such that $\varphi(p) \geq 1$ on $(p_0 - \varepsilon, p_0 + \varepsilon)$. But this means that the set

$$\overline{\{(\log(\varphi(-p)), p); p \in \mathbb{R}\}}$$

does not contain any point of the form (d, p), where $d < 0$ and $-p \in (p_0 - \varepsilon, p_0 + \varepsilon)$. As ε is contained in this set, this excludes possibilities (1) and (2).

The case $\widehat{H}_{A,A^*}(p_0) < 0$ is treated by noting that $\widehat{H}_{A,A^*}(-p_0) = -\widehat{H}_{A,A^*}(p_0)$.

Case 2. $E_\omega(S_f)$ is one-dimensional. If $E_\omega(S_f) = \mathbb{1}$ in this case, it follows that ω is a τ-invariant character, and hence ω is a KMS state at all values $\beta \in \mathbb{R} \cup \{\pm\infty\}$. If $E_\omega(S_f) \neq \mathbb{1}$, then $E_\omega(S_\infty) = \mathbb{1} - E_\omega(S_f) \neq 0$ and $S \neq \varnothing$ because $S_\infty \subseteq S$. We argue, *ad absurdum*, that $S_\infty \neq \mathbb{R}$. If not, then $\overline{S_0} = \overline{-S_\infty} = \mathbb{R}$ and hence $\overline{S_\infty} \cap \overline{S_0} \cap S = S \neq \varnothing$ in contradiction with Observation 15. Thus $\overline{S_\infty} \neq \mathbb{R}$, and by Observation 16

$$\sigma(H_\omega) \subseteq \overline{S_\infty} \cup \{0\} \neq \mathbb{R} \ .$$

But since $\sigma(H_\omega)$ has no isolated points, it follows from Example 4.3.34 that $\sigma(H_\omega)$ is contained in one of the sets $\pm[0, +\infty\rangle$, and thus ω is a ground state or a ceiling state, i.e., ω is KMS state at value $+\infty$ or $-\infty$.

By summarizing the results of the last two subsections, we obtain an almost completely satisfactory theory for the connection between stability and the KMS condition for C^*-dynamical systems $(\mathfrak{A}, \tau)$ which are $L^1(\mathfrak{A}_0)$-asymptotically abelian in the sense of Definition 5.4.8. Assume that $\mathfrak{A}$ has an identity $\mathbb{1}$, and let ω be a τ-stationary state on $\mathfrak{A}$. If $P = P^* \in \mathfrak{A}_0$, it follows from Proposition 5.4.10 that the Møller morphisms

$$\gamma_\pm^{\lambda P} = \lim_{t \to \pm\infty} \tau_{-t}^{\lambda P} \tau_t$$

exist strongly for $\lambda \in \mathbb{R}$. Furthermore, one has the intertwining relations

$$\gamma_\pm^{\lambda P} \tau_t = \tau_t^{\lambda P} \gamma_\pm^{\lambda P}$$

and

$$\lim_{\lambda \to 0} \gamma_\pm^{\lambda P}(A) = A$$

for all $A \in \mathfrak{A}$ by the estimate

$$\|\gamma_\pm^{\lambda P}(A) - A\| \leq |\lambda| \int_0^{\pm\infty} d|s| \ \|[P, \tau_s(A)]\|$$

which is valid for $A \in \mathfrak{A}_0$.

Now, there exists a unique state $\omega^{\lambda p}$ on $\gamma_-^{\lambda P}(\mathfrak{A})$ satisfying

$$\omega^{\lambda P}(\gamma_-^{\lambda P}(A)) = \omega(A)$$

and $\omega^{\lambda P}$ is $\tau^{\lambda P}$-stationary by the intertwining relations. But $\omega^{\lambda P}$ extends to a state of $\mathfrak{A}$ by Proposition 2.3.24, and applying an invariant mean to this extension composed with $\tau^{\lambda P}$ we obtain a state $\omega^{\lambda P}$ on $\mathfrak{A}$ such that the relation above remains valid, and

(1) *$\omega^{\lambda P}$ is $\tau^{\lambda P}$-stationary.*

Next, it follows from the estimate

$$|\omega^{\lambda P}(A) - \omega(A)| = |\omega^{\lambda P}(A - \gamma_-^{\lambda P}(A))| \leq \|A - \gamma_-^{\lambda P}(A)\|$$

that

(2) *$\lambda \mapsto \omega^{\lambda P}$ is continuous at $\lambda = 0$ in the sense*

$$\lim_{\lambda \to 0} \omega^{\lambda P}(A) = \omega(A)$$

for all $A \in \mathfrak{A}$.

Now, define a state $\omega_+^{\lambda P}$ on $\mathfrak{A}$ by

$$\omega_+^{\lambda P}(A) = \omega^{\lambda P}(\gamma_+^{\lambda P}(A)) \ .$$

From the relation

$$\omega^{\lambda P}(\tau_t(A)) = \omega^{\lambda P}(\tau_{-t}^{\lambda P}\tau_t(A))$$

it follows that

(3) *The limits $\lim_{t \to \pm\infty} \omega^{\lambda P}(\tau_t(A))$ exist for all $A \in \mathfrak{A}$, and*

$$\lim_{t \to -\infty} \omega^{\lambda P}(\tau_t(A)) = \omega(A), \qquad \lim_{t \to +\infty} \omega^{\lambda P}(\tau_t(A)) = \omega_+^{\lambda P}(A) \ .$$

We call any family $\{\omega^{\lambda P};\ P = P^* \in \mathfrak{A}_0, |\lambda| < \varepsilon_p\}$ of states satisfying requirements (1)–(3) (including the existence of $\omega_+^{\lambda P}$) *a family of perturbed states of ω.*

Corollary 5.4.21. *Let $(\mathfrak{A}, \tau)$ be an $L^1(\mathfrak{A}_0)$-asymptotically abelian C^*-dynamical system, and assume that $\mathfrak{A}$ has an identity. Let ω be a τ-stationary state of $\mathfrak{A}$, and let $\{\omega^{\lambda P};\ P = P^* \in \mathfrak{A}_0, |\lambda| < \varepsilon_p\}$ be a family of perturbed states of ω. Consider the following conditions:*

(1_β) *ω is an extremal τ-KMS state at value β.*

(2) (a) *ω has the three-point cluster property*

$$\lim_{\substack{\inf \\ i \neq j}} {}_{|t_i - t_j| \to \infty} \omega(\tau_{t_1}(A_1)\tau_{t_2}(A_2)\tau_{t_3}(A_3)) = \omega(A_1)\omega(A_2)\omega(A_3)$$

(b) *ω satisfies the stability property*

$$\lim_{\lambda \to 0} |\omega_+^{\lambda P}(A) - \omega(A)|/\lambda = 0$$

for all $A \in \mathfrak{A}$.

It follows that (2) *implies* (1_β) *for some $\beta \in \mathbb{R} \cup \{\pm\infty\}$. Conversely* ($1_\beta$) *for $\beta \in (\mathbb{R} \cup \{\pm\infty\})\backslash\{0\}$ implies* (2) *and* (1_β) *for $\beta = 0$ implies* (2) *when* (2)(a) *is replaced by the weaker cluster property*

$$M(\omega(A\tau(B))) = \omega(A)\omega(B)$$

for all $A, B \in \mathfrak{A}$, and any invariant mean M on $\mathbb{R}$.

In particular, (1_β) *for some $\beta \in \mathbb{R} \cup \{\pm\infty\}$ and* (2) *are equivalent if ω is a factor state or if $\mathfrak{A}$ has a unique trace-state.*

Furthermore, the family of perturbations $\{\omega^{\lambda P}\}$ can be chosen such that $\omega_+^{\lambda P} = \omega$ in the following cases:

(A) *if* (1) *holds with $\beta \in \mathbb{R}$*

(B) *if* (1) *holds with $\beta = +\infty$ and there exists an $\varepsilon > 0$ such that*

$$\sigma(H_\omega) \subseteq \{0\} \cup [\varepsilon, +\infty\rangle$$

(C) *if* (1) *holds with* $\beta = +\infty$, *and* $(\mathfrak{A}, \tau)$ *has a unique ground state. In these cases* $\omega^{\lambda P}$ *can even be taken to be a* $\tau^{\lambda P}$*-KMS state at value* β.

PROOF. We first show that the stability condition (2)(b) is equivalent to the by now familiar condition

$$\int_{-\infty}^{\infty} dt\, \omega([P, \tau_t(A)]) = 0 \tag{$*$}$$

for all $A, P \in \mathfrak{A}_0$. But this is a consequence of the relation

$$\tau_{-t}^{\lambda P}\tau_t(A) = A - i\lambda \int_0^t ds\, \tau_{-s}^{\lambda P}([P, \tau_s(A)])$$

which gives

$$\omega(A) = \omega^{\lambda P}(\gamma_-^{\lambda P}(A)) = \omega^{\lambda P}(A) - i\lambda \int_0^{-\infty} ds\, \omega^{\lambda P}([P, \tau_s(A)])$$
$$\omega_+^{\lambda P}(A) = \omega^{\lambda P}(\gamma_+^{\lambda P}(A)) = \omega^{\lambda P}(A) - i\lambda \int_0^{\infty} ds\, \omega^{\lambda P}([P, \tau_s(A)])$$

and hence

$$(\omega_+^{\lambda P}(A) - \omega(A))/\lambda = -i \int_{-\infty}^{\infty} ds\, \omega^{\lambda P}([P, \tau_s(A)]) \ .$$

The Lebesgue-dominated convergence theorem and requirement (2) on the family $\{\omega^{\lambda P}\}$ now immediately imply that the two stability conditions are equivalent. Thus, it follows from Theorem 5.4.20 that (2) implies (1_β) for some $\beta \in \mathbb{R} \cup \{\pm\infty\}$. But (1_β) for $\beta \in \mathbb{R} \cup \{\pm\infty\}$ implies $(*)$ by Theorem 5.4.17.

Now, (1_β) for $\beta \in \mathbb{R}\backslash\{0\}$ implies that ω is a factor state by Theorem 5.3.30 (3) and if (1_β) is true for $\beta \in \{\pm\infty\}$, then ω is pure by Theorem 5.3.37. Thus, ω is a factor state in both cases, and it follows from Example 4.3.34 and the asymptotic abelianness that

$$\lim_{\substack{\inf |t_i - t_j| \to \infty \\ i \neq j}} \omega(\tau_{t_1}(A_1) \cdots \tau_{t_n}(A_n)) = \omega(A_1) \cdots \omega(A_n)$$

for all $n \in \mathbb{Z}_+$ and all $A_i \in \mathfrak{A}$.

If (1_β) holds for $\beta = 0$, i.e., ω is an extremal invariant trace, then ω is an extremal invariant state by asymptotic abelianness, and thus

$$M\omega(A\tau(B)) = \omega(A)\omega(B)$$

by Theorems 4.3.17 and 4.3.22.

If ω is assumed to be a factor state, one derives n-point clustering as above, and hence (2) and (1_β), for some $\beta \in \mathbb{R} \cup \{\pm\infty\}$, are completely equivalent.

But if $\mathfrak{A}$ has a unique trace-state, then every extremal (τ, β)-KMS state ω must be a factor state. For $\beta \neq 0$ this follows from Theorem 5.3.30. (If $\beta = 0$, then ω is the unique trace and is automatically a factor state.) The equivalence and (2) and (1_β), for some $\beta \in \mathbb{R} \cup \{\pm\infty\}$, follows once again.

The last statement of the corollary follows from Corollary 5.4.7 and Theorem 5.4.4 in case A, Proposition 5.4.18 in case C, and the remarks preceding this proposition in case B.

A slightly annoying feature of the stability requirement (2b) of Corollary 5.4.21 is the small order in λ behavior required for $\omega_+^{\lambda P}(A) - \omega(A)$. One may avoid this by assuming stability in norm of the limits $\lim_{t\to\pm\infty} \omega \circ \tau_t^{\lambda P}$. To be more precise, assume that τ satisfies a uniform L^1-asymptotic abelian property in the sense that

$$t \mapsto \|[P, \tau_t^{\lambda P}(A)]\|$$

is an L^1-function for all A, $P = P^* \in \mathfrak{A}_0$ and λ sufficiently small. Proposition 5.4.10 and its subsequent remark then imply that the Møller morphisms

$$\gamma_\pm^{\lambda P} = \lim_{t\to\pm\infty} \tau_{-t}^{\lambda P}\tau_t$$

exist strongly and are *-automorphisms of $\mathfrak{A}$. Furthermore,

$$\gamma_\pm^{\lambda P}\tau_t = \tau_t^{\lambda P}\gamma_\pm^{\lambda P} \ .$$

Define states $\omega_\pm^{\lambda P}$ by

$$\omega_\pm^{\lambda P}(A) = \omega((\gamma_\pm^{\lambda P})^{-1}(A)) = \lim_{t\to\pm\infty} \omega(\tau_t^{\lambda P}(A))$$

and then $\omega_\pm^{\lambda P}$ are $\tau^{\lambda P}$-stationary states. Now the stability condition

$$\lim_{\lambda\to 0} \|\omega_\pm^{\lambda P} - \omega\| = 0$$

implies that ω is a τ-KMS state for some value $\beta \in \mathbb{R} \cup \{\pm\infty\}$. This is seen as follows. First, note that the states $\omega_\pm^{\lambda P}$ have a property of return to equilibrium, i.e.,

$$\lim_{t\to+\infty} \omega_+^{\lambda P}(\tau_t(A)) = \lim_{t\to+\infty} \omega_+^{\lambda P}(\tau_{-t}^{\lambda P}\tau_t(A)) = \omega_+^{\lambda P}(\gamma_+^{\lambda P}(A)) = \omega(A)$$

and

$$\lim_{t\to-\infty} \omega_-^{\lambda P}(\tau_t(A)) = \omega(A) \ .$$

Thus, letting $T \to \infty$ and $S \to -\infty$ in the relations

$$\omega_+^{\lambda P}(\tau_T(A) - A)/\lambda = -i\int_0^T dt\, \omega_+^{\lambda P}([P, \tau_t(A)]) \ ,$$

$$\omega_-^{\lambda P}(A - \tau_S(A))/\lambda = -i\int_S^0 dt\, \omega_-^{\lambda P}([P, \tau_t(A)]) \ ,$$

we obtain

$$(\omega_-^{\lambda P} - \omega_+^{\lambda P})(A)/\lambda = -i\int_{-\infty}^{\infty} dt\, \omega_{\operatorname{sign} t}^{\lambda P}([P, \tau_t(A)]) \ . \qquad (*)$$

Theorem 4.3.17 implies that the two states $\omega_\pm^{\lambda P} = \omega \circ (\gamma_\pm^{\lambda P})^{-1}$ are centrally ergodic with respect to the action $\tau_t^{\lambda P} = \gamma_\pm^{\lambda P}\tau_t(\gamma_\pm^{\lambda P})^{-1}$ and hence it follows from

Theorem 4.3.19 that the $\omega_{\pm}^{\lambda P}$ are either equal or disjoint. But $\|\omega_{+}^{\lambda P} - \omega_{-}^{\lambda P}\| < 2$ for small λ by the stability requirement, and $\omega_{+}^{\lambda P}$ and $\omega_{-}^{\lambda P}$ cannot be disjoint by a straightforward extension of the argument used to prove Corollary 2.6.11. It follows that

$$\omega_{+}^{\lambda P} = \omega_{-}^{\lambda P}$$

for small λ. Hence, letting $\lambda \to 0$ in $(*)$ we find the standard stability condition

$$\int_{-\infty}^{\infty} dt\, \omega([P, \tau_t(A)]) = 0$$

and ω is a τ-KMS state at some value $\beta \in \mathbb{R} \cup \{\pm\infty\}$.

The stability required for the state in Corollary 5.4.21 could be viewed as a stability against contamination of the system. The perturbation of the Hamiltonian represents the introduction of an impurity into the system. One could alternatively envisage another kind of stability, namely, that the system $(\mathfrak{A}, \tau)$ in the state ω is stable in coexistence with another system $(\mathfrak{A}', \tau')$ in a state ω', i.e., the joint system $(\mathfrak{A} \otimes \mathfrak{A}', \tau \otimes \tau')$ is stable in the sense of condition (2) of Corollary 5.4.21. One then has directly

$$\int dt\, (F(t)F'(t) - G(t)G'(t)) = 0 \ ,$$

where F, F', G, and G' are defined as before Observation 1 of Theorem 5.4.19. If ω' has strong clustering properties and is a τ'-KMS state at value $\beta \in \mathbb{R}$, one can now proceed as in the proof of Theorem 5.4.19 to show that ω is a τ-KMS state at the same value β, without assuming any purity of ω. Assuming purity of ω, it is enough that ω' is not a ground, or ceiling, state to reach the same conclusion.

5.4.3. Gauge Groups and the Chemical Potential

In the previous subsection we described how the inverse temperature β enters the formalism of thermodynamic equilibrium from requirements of stability. But in the description of equilibrium states of the ideal Fermi and Bose gas in Sections 5.2.4 and 5.2.5, these states were also characterized by a second parameter μ, the chemical potential. Equilibrium states φ were considered to be states which are $\tau\gamma_\mu$-KMS states at value β, where $t \mapsto \gamma_{\mu t}$ is the group of gauge automorphisms of the algebra, i.e., $t \mapsto \gamma_t$ is the group of Bogoliubov automorphisms induced by the unitary group $t \mapsto e^{it}\mathbb{1}$ on the one-particle space.

In order to see how the chemical potential enters one has to examine the role of gauge invariance more closely. The setting of the problem is described by the following definition.

Definition 5.4.22. A *field system* is a sextuple $(\mathfrak{F}, \mathfrak{A}, G, \tau, \gamma, \sigma)$ where $\mathfrak{F}$ is a C^*-algebra with identity, called the *field algebra, G* is a compact group, called

the *gauge group*, and $g \in G \mapsto \gamma_g$ is a continuous, faithful, representation of G into the *-automorphism group of $\mathfrak{F}$. Further $\mathfrak{A} = \mathfrak{F}^\gamma$, the fixed-point algebra under the action of G, is called the *observable algebra* and $t \mapsto \tau_t$ is a continuous one-parameter group of *-automorphisms of $\mathfrak{F}$, called the *time-translation group*. Finally, σ is a fixed *-automorphism of $\mathfrak{F}$ such that

$$\sigma^2 = \iota\,, \quad \sigma \in \{\gamma_g; g \in G\}\ .$$

The groups τ, γ, and σ are interrelated by

$$\sigma\tau_t = \tau_t\sigma\,, \quad \sigma\gamma_g = \gamma_g\sigma\,, \quad \tau_t\gamma_g = \gamma_g\tau_t\ ,$$

for all $t \in \mathbb{R}, g \in G$.

Define the even and odd subalgebras of $\mathfrak{F}$ by

$$\mathfrak{F}_+ = \{A \in \mathfrak{F}; \sigma(A) = A\}, \quad \mathfrak{F}_- = \{A \in \mathfrak{F}; \sigma(A) = -A\}\ .$$

Then $\mathfrak{F}$ is assumed to have the following asymptotic commutation property with respect to τ:

$$\lim_{|t|\to\infty} \|[A, \tau_t(B)]\| = 0$$

if $A \in \mathfrak{F}, B \in \mathfrak{F}_+$, and

$$\lim_{|t|\to\infty} \|\{A, \tau_t(B)\}\| = 0$$

if $A, B \in \mathfrak{F}_-$.

In typical applications the field algebra, or the algebra of quasi-local operations, is the algebra generated by creation and annihilation operators $a_i^*(f)$ and $a_i(f)$, where the index i denotes the different particle types and their transformation properties under internal symmetries. The group of these symmetries constitutes the gauge group G. In an example of scalar particles the index i would range over $1, 2, \ldots, n$, for some $n \in \mathbb{N}$ and G would be the n-dimensional torus $\mathbb{T}^n$. An element $g \in G$ is parametrized by n angles $0 \le \varphi_i \le 2\pi$ in this case, and the action of the corresponding automorphism γ_g is explicitly given by

$$\gamma_g(a_i^*(f)) = e^{i\varphi_i} a_i^*(f)\,, \quad \gamma_g(a_i(f)) = e^{-i\varphi_i} a_i(f)\ .$$

As G represents inner symmetries of individual particles one expects γ to commute with time translation τ, and one also expects γ-dependent quantities to be macroscopically unobservable. Hence the name observable algebra for $\mathfrak{A} = \mathfrak{F}^\gamma$. The other concepts occurring in Definition 5.4.22 have been explained earlier (see, for example, Definition 2.6.3).

Since τ and γ commute, it follows that $\mathfrak{A}$ is globally τ-invariant. Moreover, as $\sigma \in \gamma_G$ one has $\mathfrak{A} \subseteq \mathfrak{F}_+$, and hence $\mathfrak{A}$ is asymptotically abelian with respect to τ. The results of the previous section then justify the KMS condition as a criterion for a state ω of $\mathfrak{A}$ to be an equilibrium state. But in Sections 5.2.4 and 5.2.5 the equilibrium states φ of the ideal Fermi and Bose gases were defined to be KMS states at value β for some group of automorphisms of the form

$t \in \mathbb{R} \mapsto \tau_t \gamma_{\xi_t}$ where $t \mapsto \xi_t$ is a one-parameter subgroup of G given by the chemical potential. Conversely, $t \mapsto \xi_t$ determines the chemical potential. But the restriction of $t \mapsto \tau_t \gamma_{\xi_t}$ to $\mathfrak{A}$ is just $\tau|_{\mathfrak{A}}$, and hence $\omega = \varphi|_{\mathfrak{A}}$ satisfies the τ-KMS condition at value β.

The aim of this section is to show that knowledge of the state $\omega = \varphi|_{\mathfrak{A}}$ is enough to determine the chemical potential under quite general circumstances. This is achieved in two steps:

(1) If ω is an extremal τ-invariant state of $\mathfrak{A}$, then ω has an extremal τ-invariant extension φ to $\mathfrak{F}$, and any two such extensions φ_1 and φ_2, are related by

$$\varphi_1 = \varphi_2 \circ \gamma_g$$

for some $g \in G$.

(2) If, in the situation described by (1), π_ω is a faithful representation of $\mathfrak{A}$ and ω is a τ-KMS state at value $\beta \in \mathbb{R}\backslash\{0\}$, then there exists a continuous one-parameter subgroup $t \mapsto \xi_t$ of G such that φ is a $t \mapsto \tau_t \gamma_{\xi_t}$-KMS state at value β.

We first prove these two results, and subsequently make several remarks pertaining to variants, the case $\beta = 0$, etc.

Before the actual proof of these theorems, we characterize the extremal invariant states of field systems by cluster properties. In the case that the system is asymptotically abelian, i.e., $\sigma = \iota$, these properties follow already from Theorem 4.3.17 and Example 4.3.5. For general σ we use a method of proof which is similar to that used to characterize states with trivial even algebra at infinity in Theorem 2.6.5.

Proposition 5.4.23. *Let $(\mathfrak{F}, \mathfrak{A}, G, \tau, \gamma, \sigma)$ be a field system, and φ a τ-invariant state of $\mathfrak{F}$. Then $\varphi \circ \sigma = \varphi$, i.e., $\varphi|_{\mathfrak{F}_-} = 0$. The following conditions are equivalent:*

(1) *φ is τ-ergodic.*

(2) *φ has the clustering property*

$$\lim_{T-S\to\infty} \frac{1}{T-S} \int_S^T dt\, \varphi(A\tau_t(B)) = \varphi(A)\varphi(B) \ .$$

Furthermore, in this situation one has

$$\varphi(A)\mathbb{1} = \lim_{T-S\to\infty} \frac{1}{T-S} \int_S^T dt\, \pi_\varphi(\tau_t(A))$$

where the limit exists in the strong operator topology. Finally,

$$\lim_{T-S\to\infty} \frac{1}{T-S} \int_S^T dt\, \varphi(A\tau_t(A')\gamma_g(B\tau_t(B'))) = \varepsilon_{A',B}\varphi(A\gamma_g(B))\varphi(A'\gamma_g(B'))$$

for all A, A', B, $B' \in \mathfrak{F}_\pm$, $g \in G$, where the convergence is uniform in g, and $\varepsilon_{A',B} = -1$ if A', $B \in \mathfrak{F}_-$ and $\varepsilon_{A',B} = +1$ otherwise.

PROOF. Let φ be a τ-invariant state on $\mathfrak{F}$. If U_φ is the unitary group which implements τ on $\mathfrak{H}_\varphi$, and E_φ is the projection onto the U_φ-invariant vectors, it follows from Example 4.3.5 that

$$\begin{aligned}\lim_{T-S\to\infty} \frac{1}{T-S}\int_S^T dt\, \pi_\varphi(\tau_t(A))\Omega_\varphi &= \lim_{T-S\to\infty} \frac{1}{T-S}\int_S^T dt\, U_\varphi(t)\pi_\varphi(A)\Omega_\varphi \\ &= E_\varphi \pi_\varphi(A)\Omega_\varphi\end{aligned}$$

for all $A \in \mathfrak{F}$.

The last assumption of Definition 5.4.22 and the relation above imply that the following limits exist

$$\begin{aligned}&\lim_{T-S\to\infty} \frac{1}{T-S}\int_S^T dt\, \pi_\varphi(\tau_t(A))\pi_\varphi(B)\Omega_\varphi \\ &\quad = \varepsilon_{A,B}\pi_\varphi(B)\left(\lim_{T-S\to\infty} \frac{1}{T-S}\int_S^T dt\, \pi_\varphi(\tau_t(A))\Omega_\varphi\right) \\ &\quad = \varepsilon_{A,B}\pi_\varphi(B)E_\varphi\pi_\varphi(A)\Omega_\varphi\end{aligned}$$

and, by uniform boundedness, the limits

$$M(A) = \lim_{T-S\to\infty} \frac{1}{T-S}\int_S^T dt\, \pi_\varphi(\tau_t(A))$$

exist in the strong topology. Now, if $A \in \mathfrak{F}_+$, then $M(A)$ commutes with $\pi_\varphi(\mathfrak{F})$ and $M(A)$ is τ-invariant, hence

$$M(A) \in \{\pi_\varphi(\mathfrak{F}) \cup U_\varphi(\mathbb{R})\}' \ , \tag{*}$$

for $A \in \mathfrak{F}_+$.

If $A \in \mathfrak{F}_-$, then $A^* \in \mathfrak{F}_-$, and we have

$$\begin{aligned}(\Omega_\varphi, \pi_\varphi(A)^* E_\varphi \pi_\varphi(A)\Omega_\varphi) &= \lim_{T-S\to\infty} \frac{1}{T-S}\int_S^T dt\, \varphi(A^*\tau_t(A)) \\ &= -\lim_{T-S\to\infty} \frac{1}{T-S}\int_S^T dt\, \varphi(\tau_t(A)A^*) \\ &= -(\Omega_\varphi, \pi_\varphi(A)E_\varphi\pi_\varphi(A)^*\Omega_\varphi) \ ,\end{aligned}$$

and hence, applying this on $(A + A^*)/2$ and $(A - A^*)/2i$,

$$E_\varphi \pi_\varphi(A)\Omega_\varphi = 0 \ .$$

In particular, $\varphi(A) = 0$ for all $A \in \mathfrak{F}_-$ and this implies that

$$\varphi \circ \sigma = \varphi \ .$$

Let $U_\varphi(\sigma)$ be the unitary implementing σ on $\mathfrak{H}_\varphi$. Then $M(A)U_\varphi(\sigma)$ commutes with $\pi_\varphi(\mathfrak{F})$, and it is also τ-invariant, hence

$$M(A)U_\varphi(\sigma) \in \{\pi_\varphi(\mathfrak{F}) \cup U_\varphi(\mathbb{R})\}' \tag{**}$$

for $A \in \mathfrak{F}_-$.

We now prove (1) $\Rightarrow$ (2). Ergodicity of φ is equivalent to

$$\{\pi_\varphi(\mathfrak{F}) \cup U_\varphi(\mathbb{R})\}' = \mathbb{C}\mathbb{1}$$

by Theorem 4.3.17. If $A \in \mathfrak{F}_+$, it follows from (*) that

$$M(A) = (\Omega_\varphi, M(A)\Omega_\varphi)\mathbb{1} = \varphi(A)\mathbb{1} \ .$$

If $A \in \mathfrak{F}_-$ (**) implies

$$\begin{aligned} M(A)U_\varphi(\sigma) &= (\Omega_\varphi, M(A)U_\varphi(\sigma)\Omega_\varphi)\mathbb{1} \\ &= (\Omega_\varphi, M(A)\Omega_\varphi)\mathbb{1} = \varphi(A)\mathbb{1} = 0 \ , \end{aligned}$$

where the last relation follows from the first part of the proposition. Hence

$$M(A) = 0 = \varphi(A)\mathbb{1}$$

for $A \in \mathfrak{F}_-$, and by linearity

$$M(A) = \varphi(A)\mathbb{1}$$

for all $A \in \mathfrak{F}$. Thus

$$\lim_{T-S\to\infty} \frac{1}{T-S}\int_S^T dt\, \varphi(A\tau_t(B)) = (\Omega_\varphi, \pi_\varphi(A)M(B)\Omega_\varphi) = \varphi(A)\varphi(B) \ .$$

Conversely, (2) $\Rightarrow$ (1) is an immediate consequence of Theorems 4.3.22 and 4.3.17. It remains to establish that

$$\lim_{T-S\to\infty} \frac{1}{T-S}\int_S^T dt\, \varphi(A\tau_t(A')\gamma_g(B\tau_t(B'))) = \varepsilon_{A',B}\varphi(A\gamma_g(B))\varphi(A'\gamma_g(B'))$$

for A, A', B, $B' \in \mathfrak{F}_\pm$, uniformly for $g \in G$. Since G is compact and $g \mapsto \gamma_g(B)$ and $g \mapsto \gamma_g(B')$ are continuous, it follows that

$$g \mapsto \varphi(A\tau_t(A')\gamma_g(B\tau_t(B')))$$

is equicontinuous in g when t ranges over $\mathbb{R}$. Hence, the uniformity of the convergence in g follows once we can show pointwise convergence. But this follows immediately from the two-point cluster properties of φ and the asymptotic commutation property

$$\lim_{|t|\to\infty} \|\tau_t(A')B - \varepsilon_{A',B}B\tau_t(A')\| = 0$$

together with the fact that $\gamma_g(\mathfrak{F}_\pm) = \mathfrak{F}_\pm$ for all $g \in G$, as a consequence of $\sigma\gamma_g = \gamma_g\sigma$.

We now state the first main theorem of this section.

Theorem 5.4.24. *Let $(\mathfrak{F}, \mathfrak{A}, G, \tau, \gamma, \sigma)$ be a field system, and ω an extremal τ-invariant state on $\mathfrak{A}$.*

It follows that ω possesses an extremal τ-invariant extension φ to the field algebra $\mathfrak{F}$. Moreover, two such extensions φ_1 and φ_2 are related by

$$\varphi_2 = \varphi_2 \circ \gamma_g$$

for some $g \in G$.

Proof. We first prove the existence of φ by a method analogous to that used to prove Proposition 2.3.24. This proposition implies that ω has an extension to a state of $\mathfrak{F}$ and, by applying an invariant mean to this state composed with τ, we deduce that the set E_ω^τ of τ-invariant extensions of ω to states of $\mathfrak{F}$ is nonempty. But E_ω^τ is

clearly convex and weak* compact, and thus it contains an extremal element φ by the Krein-Milman theorem. If $\varphi = \lambda\varphi_1 + (1-\lambda)\varphi_2$, $0 < \lambda < 1$, where φ_1 and φ_2 are τ-invariant states of $\mathfrak{F}$, one has $\omega = \varphi|_{\mathfrak{A}} = \lambda\varphi_1|_{\mathfrak{A}} + (1-\lambda)\varphi_2|_{\mathfrak{A}}$ and hence $\varphi_1|_{\mathfrak{A}} = \varphi_2|_{\mathfrak{A}} = \omega$, by the extremality of ω. It follows that $\varphi_1 = \varphi_2 = \varphi$ since φ is extremal in E^{τ}_{ω}.

To prove uniqueness of φ up to gauge transformations, fix an extremal τ-invariant extension φ of ω and define

$$G_{\varphi} = \{g \in G; \varphi \circ \gamma_g = \varphi\} \ .$$

In the sequel we denote by $C(X)$ the C^*-algebra of continuous functions on the compact set X, and for $f \in C(G)$ and $g \in G$ we define

$$(\rho(g)f)(s) = f(sg), \quad (\lambda(g)f)(s) = f(g^{-1}s) \ ,$$

for $s \in G$.

OBSERVATION 1. The norm closure of

$$C^1_{\varphi}(G) = \{\varphi^{(A)} : g \in G \mapsto \varphi(\gamma_g(A)); A \in \mathfrak{F}\}$$

in the continuous functions $C(G)$ on G coincides with $C(G_{\varphi}\backslash G)$.

PROOF. Indeed $\overline{C^1_{\varphi}(G)}$ is selfadjoint since $\overline{\varphi^{(A)}} = \varphi^{(A^*)}$ for $A \in \mathfrak{F}$, and multiplicative since by Proposition 5.4.23,

$$\lim_{T-S\to\infty} \frac{1}{T-S}\int_S^T dt\, \varphi^{(A\tau_t(B))}(g) \ = \ \varphi^{(A)}(g)\varphi^{(B)}(g)$$

for $A, B \in \mathfrak{F}$, uniformly for $g \in G$.

Define an equivalence relation $\sim$ on G by $g_1 \sim g_2$ if, and only if, $f(g_1) = f(g_2)$ for all $f \in \overline{C^1_{\varphi}(G)}$. It follows by the Stone-Weierstrass theorem that

$$\overline{C^1_{\varphi}(G)} = \{f \in C(G); g_1 \sim g_2 \Rightarrow f(g_1) = f(g_2)\} \cong C(G/\sim) \ .$$

But $G/\sim = G_{\varphi}\backslash G$ because

$$\begin{aligned} g_1 \sim g_2 &\Leftrightarrow \varphi(\gamma_{g_1}(A)) = \varphi(\gamma_{g_2}(A)) \text{ for all } A \in \mathfrak{F} \\ &\Leftrightarrow \varphi(A) = \varphi(\gamma_{g_2 g_1^{-1}}(A)) \text{ for all } A \in \mathfrak{F} \\ &\Leftrightarrow g_2 g_1^{-1} \in G_{\varphi} \Leftrightarrow g_2 \in G_{\varphi} g_1 \ . \end{aligned}$$

Hence

$$\overline{C^1_{\varphi}(G)} = C(G_{\varphi}\backslash G) \ .$$

OBSERVATION 2. Let $K_i, i = 1, 2$, be closed subgroups of the compact group G, and identify $C(K_i\backslash G)$ with the space consisting of the functions in $C(G)$ which are invariant under all left translations $\lambda(k_i), k_i \in K_i, i = 1, 2$. It follows that each *-isomorphism of $C(K_1\backslash G)$ into $C(K_2\backslash G)$ which commutes with the right translations $\rho(g), g \in G$, is of the form $\lambda(h)$ for some $h \in G$ such that $K_2 = hK_1h^{-1}$.

PROOF. The transposed map σ^* of σ maps the pure states $K_2\backslash G$ of $C(K_2\backslash G)$ continuously onto the pure states $K_1\backslash G$ of $C(K_1\backslash G)$ and hence defines a

homeomorphism $\sigma^*: K_2\backslash G \mapsto K_1\backslash G$ which commutes with right translations by $g \in G$.

Thus

$$\sigma^*(K_2 g) = \sigma^*(K_2 eg) = \sigma^*(K_2)g = (K_1 h^{-1})g$$

for all $g \in G$, where $h \in G$ is any element such that $\sigma^*(K_2) = K_1 h^{-1}$. By transposition we obtain $\sigma = \lambda(h)$. Since $\sigma f, f \in C(K_1\backslash G)$, has to be invariant under all $\lambda(k_2), k_2 \in K_2$, we must have

$$f(h^{-1}k_2^{-1}g) = (\sigma f)(k_2^{-1}g) = \lambda(k_2)(\sigma f)(g) = \sigma f(g) = f(h^{-1}g)$$

for all $k_2 \in K_2, f \in C(K_1\backslash G)$, and hence $h^{-1}k_2^{-1} \in K_1 h^{-1}$ or $K_2 \subseteq hK_1h^{-1}$. A similar argument with σ replaced σ^{-1} shows the reverse inclusion, and

$$K_2 = hK_1h^{-1} \ .$$

We now resume the proof of the uniqueness part of Theorem 5.4.24. Let φ_1 and φ_2 be two extremal τ-invariant extensions of ω to $\mathfrak{F}$, and $K_i = G_{\varphi_i}$ the corresponding stabilizers in G. Now the element

$$\int_G dg\, \gamma_g(A^*\tau_t(B))$$

belongs to $\mathfrak{A}$ for all $A, B \in \mathfrak{F}$, and thus gives the same value of φ_1 and φ_2. It follows that

$$\begin{aligned}
(\varphi_1^{(A)}, \varphi_1^{(B)})_{L^2(K_1\backslash G)} &= \int dg\, \varphi_1^{(A^*)}(g)\varphi_1^{(B)}(g) \\
&= \lim_{T-S\to\infty} \frac{1}{T-S}\int_S^T dt\, \varphi_1\left(\int_G dg\, \gamma_g(A^*\tau_t(B))\right) \\
&= \lim_{T-S\to\infty} \frac{1}{T-S}\int_S^T dt\, \varphi_2\left(\int_G dg\, \gamma_g(A^*\tau_t(B))\right) \\
&= (\varphi_2^{(A)}, \varphi_2^{(B)})_{L^2(K_2\backslash G)} \ ,
\end{aligned}$$

where we used Proposition 5.4.23. It follows that there exists a linear isometry V from $L^2(K_1\backslash G)$ onto $L^2(K_2\backslash G)$ defined by

$$V\varphi_1^{(A)} = \varphi_2^{(A)} \ ,$$

for $A \in \mathfrak{F}$. Since

$$\lim_{T-S\to\infty} \frac{1}{T-S}\int_S^T dt\, \varphi^{(A\tau_t(B))}(g) = \varphi^{(A)}(g)\varphi^{(B)}(g)$$

uniformly in $g \in G$, it follows that

$$V(\varphi_1^{(A)}\varphi_1^{(B)}) = \varphi_2^{(A)}\varphi_2^{(B)}$$

for $A, B \in \mathfrak{F}$. If T_i is the representation of $C(K_i\backslash G)$ on $L^2(K_i\backslash G)$ obtained from pointwise multiplication, one then has

$$T_2(Vf) = VT_1(f)V^*$$

for $f \in C(K_1\backslash G)$. As the T_i are isometric, one concludes that V is a *-isomorphism of $C(K_1\backslash G)$ onto $C(K_2\backslash G)$. The computation

$$\{V(\rho(h)\varphi_1^{(A)})\}(g) = \varphi_2(\gamma_{gh}(A)) = \{\rho(h)V\varphi_1^{(A)}\}(g)$$

shows that V commutes with the right regular representation ρ, and Observation 2 yields a $g \in G$ such that $\varphi_2^{(A)} = \lambda(g)\varphi_1^{(A)}$ for all $A \in \mathfrak{A}$, i.e.,

$$\varphi_2(A) = \varphi_1(\gamma_{g^{-1}}(A))$$

for all $A \in \mathfrak{A}$. This ends the proof of Theorem 5.4.24.

The main result on the existence of the chemical potential is the following.

Theorem 5.4.25. *Let $(\mathfrak{F}, \mathfrak{A}, G, \tau, \gamma, \sigma)$ be a field system, and ω an extremal τ-KMS state over $\mathfrak{A}$ at value $\beta \in \mathbb{R}\backslash\{0\}$ such that the corresponding representation of $\mathfrak{A}$ is faithful. Then each extremal τ-invariant extension φ of ω to $\mathfrak{F}$ is a KMS state at value β for a one-parameter group of *-automorphisms of $\mathfrak{F}$ of the form $t \mapsto \tau_t\gamma_{\xi_t}$, where $t \mapsto \xi_t$ is a continuous one-parameter subgroup of the center of the stabilizer $G_\varphi = \{g \in G;\ \varphi \circ \gamma_g = \varphi\}$ of φ. The group $t \mapsto \xi_t$ is uniquely determined by φ.*

Proof. The proof of this theorem requires at several points the spectral theory of the group G, i.e., the theory of the unitary representations of G. Since we have not developed this theory for general compact groups, we will content ourselves with proving the theorem for the slightly more transparent case of abelian groups G. The extension to general G is accomplished by replacing characters with irreducible representations (which are automatically finite dimensional), and products of characters with tensor products of representations. As a final remark on non-abelian G, note that if φ satisfies the $\tau\gamma_\xi$-KMS condition at value $\beta \in \mathbb{R}\backslash\{0\}$ for some one-parameter group $t \mapsto \xi_t$ in G, then φ is $\tau\gamma_\xi$-invariant by Proposition 5.3.3 and as φ is τ-invariant it follows that $\xi_t \in G_\varphi$ for all t. But if $g \in G_\varphi$, then $\varphi = \varphi \circ \gamma_g$ and hence $\gamma_{g^{-1}}\tau_t\gamma_{\xi_t}\gamma_g = \tau_t\gamma_{\xi_t}$ by Proposition 5.3.33, thus $g^{-1}\xi_t g = \xi_t$, i.e., $t \mapsto \xi_t$ is contained in the center of G. Throughout the sequel of the proof G is assumed to be abelian.

Let $\{\mathfrak{H}_\varphi, \pi_\varphi, U_\varphi, \Omega_\varphi\}$ be the covariant representation of the C^*-dynamical system $\{\mathfrak{F}, \mathbb{R} \times G_\varphi, \tau \times \gamma\}$, and let $\{\mathfrak{M}, \mathbb{R} \times G_\varphi, \tau \times \gamma\}$ denote the corresponding W^*-system, i.e., $\mathfrak{M} = \pi_\varphi(\mathfrak{F})''$, etc., and let $\mathfrak{F}^{G_\varphi}$ and $\mathfrak{M}^{G_\varphi}$ be the fixed-point algebras of the action of G_φ on $\mathfrak{F}$ and $\mathfrak{M}$, respectively. By integrating over the compact group G_φ one easily shows that $\mathfrak{M}^{G_\varphi}$ is the weak operator closure of $\mathfrak{F}^{G_\varphi}$, but in fact we can show more.

OBSERVATION 1

$$\mathfrak{M}^{G_\varphi} = \pi_\varphi(\mathfrak{A})'' \ .$$

Proof. Let $\hat{G}$ be the dual group of G, and if $\chi \in \hat{G}$, let

$$\mathfrak{F}^\gamma(\{\chi\}) = \{A \in \mathfrak{F}; \gamma_g(A) = \overline{\chi(g)}A\}$$

be the corresponding spectral subspace of $\mathfrak{F}$ (see Definition 3.2.37). Define the subset $\Sigma_\varphi \subseteq \hat{G}$ by

$$\Sigma_\varphi = \{\chi \in \hat{G};\ \text{there is an } A \in \mathfrak{F}^\gamma(\{\chi\}) \text{ with } \varphi(A) \neq 0\} \ .$$

OBSERVATION 2. Σ_φ is a closed subgroup of $\hat{G}$ with annihilator G_φ,

$$\Sigma_\varphi = G_\varphi^\perp = \{\chi \in \hat{G};\ \chi(g) = 1 \text{ for all } g \in G_\varphi\} \ ,$$
$$G_\varphi = \Sigma_\varphi^\perp = \{g \in G;\ \chi(g) = 1 \text{ for all } \chi \in \Sigma_\varphi\} \ .$$

PROOF. If $\chi,\ \chi' \in \Sigma_\varphi$ there are $A \in \mathfrak{F}^\gamma(\chi)$, $A' \in \mathfrak{F}^\gamma(\chi')$, with $\varphi(A) \neq 0$, $\varphi(A') \neq 0$. But then $A\tau_t(A') \in \mathfrak{F}^\gamma(\chi\chi')$ and as

$$\lim_{T-S\to\infty} \frac{1}{T-S}\int_S^T dt\, \varphi(A\tau_t(A')) = \varphi(A)\varphi(A') \neq 0 \ ,$$

by Proposition 5.4.23, it follows that $\varphi(A\tau_t(A')) \neq 0$ for some t. Hence $\chi\chi' \in \Sigma_\varphi$ and Σ_φ is additive. On the other hand, if $A \in \mathfrak{F}^\gamma(\chi)$ then $A^* \in \mathfrak{F}^\gamma(\overline{\chi})$ and as $\varphi(A^*) = \overline{\varphi(A)}$ it follows that Σ_φ is symmetric. Σ_φ is then a closed subgroup of $\hat{G}$ since $\hat{G}$ is discrete.

In general we have

$$\varphi(\gamma_g(A)) = \overline{\chi(g)}\varphi(A)$$

if $A \in \mathfrak{F}^\gamma(\chi)$. Thus if $\chi \in \Sigma_\varphi$ and $g \in G_\varphi$ we must have $\chi(g) = 1$, i.e.,

$$G_\varphi \subseteq \Sigma_\varphi^\perp \ .$$

Conversely, if $g \in \Sigma_\varphi^\perp$, and $A \in \mathfrak{F}^\gamma(\chi)$ then

$$\begin{aligned} \varphi(\gamma_g(A)) &= \varphi(A) && \text{if } \chi \in \Sigma_\varphi \\ &= 0 = \varphi(A) && \text{if } \chi \notin \Sigma_\varphi \ . \end{aligned}$$

Hence $g \in G_\varphi$ and the reverse inclusion

$$\Sigma_\varphi^\perp \subseteq G_\varphi$$

holds.

OBSERVATION 3. $\mathfrak{M}^{G_\varphi}$ is the von Neumann algebra generated by the $A \in \mathfrak{F}^\gamma(\chi), \chi \in \Sigma_\varphi$, i.e.,

$$\mathfrak{M}^{G_\varphi} = \left\{ \bigcup_{\chi \in \Sigma_\varphi} \mathfrak{F}^\gamma(\chi) \right\}'' \ .$$

PROOF. If $A \in \mathfrak{F}^\gamma(\chi), \chi \in \Sigma_\varphi$, Observation 2 implies that $A \in \mathfrak{M}^{G_\varphi}$, and hence the inclusion $\supseteq$ is valid. To show the converse, note that any $A \in \mathfrak{M}$ has the weak-operator convergent Fourier expansion

$$A = \sum_{\chi \in \hat{G}} A(\chi), \quad A(\chi) = \int_G dg\, \chi(g)\gamma_g(A) \ .$$

Thus if $A \in \mathfrak{M}^{G_\varphi}$, it follows from the uniqueness of this expansion that

$$(\overline{\chi(g)} - 1)A(\chi) = 0$$

for all $g \in G_\varphi$ and all $\chi \in \hat{G}$. Hence $\chi \in G_\varphi^\perp$ if $A(\chi) \neq 0$ and as $G_\varphi^\perp = \Sigma_\varphi$ by Observation 2, the reverse inclusion follows since

$$A = \sum_{\chi \in \Sigma_\varphi} A(\chi) \ .$$

We now finish the proof of Observation 1. The inclusion

$$\mathfrak{M}^{G_\varphi} \supseteq \pi_\varphi(\mathfrak{A})''$$

is evident since $\mathfrak{A} = \mathfrak{F}^G$. To show the converse, it suffices, by Observation 3, to show that if $A \in \mathfrak{F}^\gamma(\chi), \chi \in \Sigma_\varphi$, then $A \in \pi_\varphi(\mathfrak{A})''$. But since $\overline{\chi} \in \Sigma_\varphi$, by Observation 2, there exists a $B \in \mathfrak{F}^\gamma(\overline{\chi})$ with $\varphi(B) = 1$. But by Proposition 5.4.23 the limit

$$\lim_{T-S\to\infty} \frac{1}{T-S} \int dt\, \pi_\varphi(\tau_t(B)A) = \varphi(B)A = A$$

exists in the strong-operator topology. As $\tau_t(B)A \in \mathfrak{F}^G = \mathfrak{A}$ for all t, Observation 1 follows.

Since $\pi_\varphi(\mathfrak{A})'' \subseteq \pi_\varphi(\mathfrak{F}^{G_\varphi})'' \subseteq \mathfrak{M}^{G_\varphi}$ it follows from Observation 1 that

$$\pi_\varphi(\mathfrak{A})'' = \pi_\varphi(\mathfrak{F}^{G_\varphi})''$$

and hence Corollary 5.3.4 implies that the restriction of φ to $\mathfrak{F}^{G_\varphi}$ is still a τ-KMS state at value β. Hence, replacing $\mathfrak{A}$ by $\mathfrak{F}^{G_\varphi}$ and G by G_φ, it suffices to prove Theorem 5.4.25 in the case that $G_\varphi = G$, i.e., we may assume that φ is gauge invariant from now on. (Note that $\sigma \in G_\varphi$ by Proposition 5.4.23.) With this assumption we prove:

OBSERVATION 4. The set $C^2_\varphi(G)$ of functions of the form

$$g \in G \mapsto \varphi(A\gamma_g(B)) \ ,$$

where $A, B \in \mathfrak{F}$, linearly spans a norm-dense subspace of $C(G)$.

PROOF. $\overline{[C^2_\varphi(G)]}$ is closed under multiplication, because Proposition 5.4.23 implies that

$$\lim_{T-S\to\infty} \frac{1}{T-S} \int_S^T dt\, \varphi(A\tau_t(A')\gamma_g(B\tau_t(B'))) = \varepsilon_{A',B}\varphi(A\gamma_g(B))\varphi(A'\gamma_g(B')) \ ,$$

when $A,\ A',\ B,\ B' \in \mathfrak{F}_\pm$, uniformly in g. Thus

$$g \mapsto \varphi(A\gamma_g(B))\varphi(A'\gamma_g(B'))$$

is contained in $\overline{[C^2_\varphi(G)]}$, when $A,\ A',\ B,\ B' \in \mathfrak{F}_\pm$, and by linearity this is still true for general $A, A', B, B' \in \mathfrak{F}$.

We next show that $\overline{[C^2_\varphi(G)]}$ is closed under complex conjugation. First, note that as $\pi_\omega(\mathfrak{F})$ is strongly dense in $\mathfrak{M}$, $\overline{[C^2_\varphi(G)]}$ is also the norm closed linear span of the functions

$$\varphi^{(A,B)};\ g \mapsto (\Omega_\varphi,\ A\gamma_g(B)\Omega_\varphi) \ ,$$

where $A, B \in \mathfrak{M}$. But B has a weak-operator convergent Fourier expansion

$$B = \sum_{\chi \in \hat{G}} B(\chi) \ , \qquad B(\chi) = \int_G dg\, \chi(g)\gamma_g(B) \ ,$$

and hence it is enough to consider elements B which are eigenvectors for γ, i.e., $\gamma_g(B) = \overline{\chi(g)}B$. If $B\Omega_\varphi = 0$, then $\varphi^{(A,B)} = 0$ and there is nothing more to prove. If

$B\Omega_\varphi \neq 0$, then $BB^* \neq 0$. But since $BB^* \in \mathfrak{M}^G$ and $\varphi|_{\mathfrak{M}^G}$ is a KMS state at value β, it follows from Corollary 5.3.9 that $\varphi|_{\mathfrak{M}^G}$ is faithful and hence $\varphi(BB^*) \neq 0$, i.e., $B^*\Omega_\varphi \neq 0$. But $\gamma_g(B^*) = \chi(g)B^*$, and hence

$$\varphi^{(A,B)}(g) = \overline{\varphi^{(C,B^*)}(g)}$$

for a suitable $C \in \mathfrak{M}$. Now, $C^2_\varphi(G)$ is globally left and right invariant under translations by G by the relations

$$\lambda(g)\varphi^{(A,B)} = \varphi^{(\gamma_g(A),B)} \quad , \quad \rho(g)\varphi^{(A,B)} = \varphi^{(A,\gamma_g(B))} \ .$$

Hence, it follows from the Stone-Weierstrass theorem, as in the proof of Observation 1 in Theorem 5.4.24, that

$$N_\varphi = \{g \in G\,;\varphi(A\gamma_g(B)) = \varphi(AB) \text{ for all } A, B \in \mathfrak{F}\}$$

is a normal subgroup of G and

$$\overline{[C^2_\varphi(G)]} = C(G/N_\varphi) \ .$$

But N_φ is trivial because if $h \in N_\varphi$ and $B \in \mathfrak{M}^\gamma(\{\chi\})$ for some $\chi \in \hat{G}$, then $B - \overline{\chi(h)}B \in \mathfrak{M}^\gamma(\{\chi\})$. But

$$\varphi((B - \overline{\chi(h)}B)^*(B - \overline{\chi(h)}B)) = \varphi((B - \overline{\chi(h)}B)^*(B - \gamma_h(B))) = 0$$

by the definition of N_φ and as

$$(B - \overline{\chi(h)}B)^*(B - \overline{\chi(h)}B) \in \mathfrak{M}^G$$

and $\varphi|_{\mathfrak{M}^G}$ is faithful it follows that

$$B = \overline{\chi(h)}B = \gamma_h(B) \ .$$

By Fourier expansion we find that $B = \gamma_h(B)$ for all $B \in \mathfrak{M}$. But γ is a faithful representation of G on $\mathfrak{F}$, and π_φ is a faithful representation of $\mathfrak{F}$ as we shall subsequently show. It then follows from the last relation $h = e$. Hence $N_\varphi = \{e\}$ and one concludes that Observation 4 is valid.

To establish faithfulness of π_φ we assume that $A \in \mathfrak{F}$ and $\pi_\varphi(A) = 0$. But then the Fourier expansion of $\pi_\varphi(A)$ takes the form

$$\pi_\varphi(A) = \sum_{\chi \in \hat{G}} \pi_\varphi(A(\chi)) \ ,$$

where

$$A(\chi) = \int_G dg\, \chi(g)\gamma_g(A) \in \mathfrak{F} \ .$$

However $\pi_\varphi(A(\chi)) = 0$ by the uniqueness of this expansion, and hence $\pi_\varphi(A(\chi)^*A(\chi)) = 0$. Since $A(\chi)^*A(\chi) \in \mathfrak{A}$, it follows from the faithfulness of $\pi_\varphi|_{\mathfrak{A}}$ that $A(\chi)^*A(\chi) = 0$. Thus $A(\chi) = 0$ and $A = 0$.

We now complete the proof of Theorem 5.4.25. Since $\varphi|_{\mathfrak{A}}$ is a τ-KMS state at value β, we have

$$\int dg\, \varphi(A^*\tau_t(A')\tau_{i\beta}(\gamma_g(B^*\tau_t(B')))) = \int dg\, \varphi(\gamma_g(B^*\tau_t(B'))A^*\tau_t(A'))$$

when A, A', B, and B' are entire analytic for τ. If A, A', B, $B' \in \mathfrak{F}_\pm$ it follows from this relation and Proposition 5.4.23 that

$$\varepsilon_{A',B}\int dg\,\varphi(A^*\gamma_g(\tau_{i\beta}(B^*)))\varphi(A'\gamma_g((\tau_{i\beta}(B'))) = \varepsilon_{B',A}\int dg\,\varphi(\gamma_g(B^*)A^*)\varphi(\gamma_g(B')A') \ .$$

Now, using $\mathfrak{F}_+^2 \subseteq \mathfrak{F}_+$, $\mathfrak{F}_-^2 \subseteq \mathfrak{F}_+$, $\mathfrak{F}_+\mathfrak{F}_- \subseteq \mathfrak{F}_-$, $\mathfrak{F}_-\mathfrak{F}_+ \subseteq \mathfrak{F}_-$, and the fact that $\varphi|_{\mathfrak{F}_-} = 0$, it follows that both sides of this equation are zero if $\varepsilon_{A',B} \neq \varepsilon_{B',A}$, and as a consequence

$$\int dg\,\varphi(A^*\gamma_g(\tau_{i\beta}(B^*)))\varphi(A'\gamma_g(\tau_{i\beta}(B'))) = \int dg\,\varphi(\gamma_g(B^*)A^*)\varphi(\gamma_g(B')A') \ .$$

This relation extends by linearity to all entire τ-analytic A, A', B, $B' \in \mathfrak{F}$. Using $\tau_{i\beta}(B^*) = \tau_{-i\beta}(B)^*$ this may be written as

$$(s\varphi^{(\tau_{-i\beta}(B),\,A)}, \varphi^{(A',\,\tau_{i\beta}(B'))}) = (\varphi^{(A,\,B)}, s\varphi^{(B',\,A')}) \ ,$$

where (,) denotes the scalar product in $L^2(G)$, and $(sf)(g) = f(g^{-1})$ for all $g \in G$. Replacing B' by $\tau_{-i\beta}(B')$ in this relation we obtain

$$(s\varphi^{(\tau_{-i\beta}(B),\,A)}, \varphi^{(A',\,B')}) = (\varphi^{(A,\,B)}, s\varphi^{(\tau_{-i\beta}(B'),\,A')}) \ .$$

If A_i and B_i are entire analytic for τ and $\alpha_i \in \mathbb{C}, i = 1, ..., n$, we obtain from this relation

$$\left(\sum_{i=1}^n \alpha_i\, s\varphi^{(\tau_{-i\beta}(B_i),\,A_i)}, \varphi^{(A',\,B')}\right) = \left(\sum_{i=1}^n \alpha_i\, \varphi^{(A_i,\,B_i)}, s\varphi^{(\tau_{-i\beta}(B'),\,A')}\right) \ .$$

As $\overline{[C_\varphi^2(G)]} = C(G)$ by Observation 4 it follows that we may consistently define a linear operator S on $L^2(G)$ by

$$D(S) = \left\{\sum_{i=1}^n \alpha_i\, \varphi^{(A_i,\,B_i)};\ A_i, B_i \text{ entire analytic for } \tau\right\}$$

and

$$S\left(\sum_{i=1}^n \alpha_i\, \varphi^{(A_i,\,B_i)}\right) = \sum_{i=1}^n \alpha_i\, s\varphi^{(\tau_{-i\beta}(B_i),\,A_i)} \ .$$

One then obtains the relation

$$(S\psi, \varphi) = (\psi, S\varphi)$$

for $\psi, \varphi \in D(S)$. Hence S is a densely defined symmetric operator.

Using the relations

$$\lambda(g)\varphi^{(A,\,B)} = \varphi^{(\gamma_g(A),\,B)} \ , \quad \rho(g)\varphi^{(A,\,B)} = \varphi^{(A,\,\gamma_g(B))} \ ,$$

one then deduces that S commutes with the left and right regular representations of G on $L^2(G)$. Since $S\lambda(g) = \lambda(g)S$ for all g, it follows that S commutes with the projection

$$E_\chi = \int_G dg\,\overline{\chi(g)}\lambda(g) = \int_G dg\,\chi(g)\rho(g)$$

onto the one-dimensional subspace of $L^2(G)$ spanned by the element $g \mapsto \overline{\chi(g)}$. Hence S is essentially selfadjoint with spectral decomposition of the form

$$S = \sum_{\chi \in \hat{G}} S(\chi)E_\chi \ ,$$

where $S(\chi) \in \mathbb{R}$. Now, as the set of $\varphi^{(A,B)}$ spans $C(G)$ by Observation 4, there exists for all $\chi \in \hat{G}$ a pair A, B of τ-analytic elements such that

$$E_{\bar{\chi}}\varphi^{(A,B)} \neq 0 \ .$$

If one defines

$$B_{\bar{\chi}} = \int_G dg\, \overline{\chi(g)}\gamma_g(B) \ ,$$

then $B_{\bar{\chi}}$ is still τ-analytic since $\gamma\tau = \tau\gamma$. Moreover,

$$\varphi^{(A,B_{\bar{\chi}})} = E_\chi \varphi^{(A,B)} \neq 0$$

and in particular

$$\varphi(B_{\bar{\chi}}^* B_{\bar{\chi}}) \neq 0 \ .$$

Furthermore, $B = \tau_{i\beta/2}(B_\chi^*)$ satisfies

$$\varphi^{(B^*,B)} \in E_\chi C(G)$$

since

$$\varphi^{(B^*,B)}(g) = \varphi(\tau_{-i\beta/2}(B_{\bar{\chi}})\tau_{i\beta/2}(\gamma_g B_{\bar{\chi}}^*)) = \overline{\chi(g)}\varphi^{(B^*,B)}(e) \ .$$

We then compute

$$\begin{aligned} 0 < \varphi(B_{\bar{\chi}}^* B_{\bar{\chi}}) &= \varphi((\tau_{-i\beta/2}(B))(\tau_{-i\beta/2}(B))^*) \\ &= \varphi(\tau_{-i\beta}(B)B^*) \\ &= S\varphi^{(B^*,B)}(e) = S(\chi)\varphi(B^*B) \end{aligned}$$

and this implies

$$S(\chi) > 0 \ .$$

It follows that $\bar{S}$ is a strictly positive selfadjoint operator and hence $\bar{S}^{it}$ exists for all $t \in \mathbb{R}$.

The weak clustering of φ implies, by an argument which is by now standard, that

$$S(\varphi^{(A,B)}\varphi^{(A',B')}) = S(\varphi^{(A,B)})S(\varphi^{(A',B')}) \ .$$

In particular using $B = B_{\bar{\chi}}$, etc.,

$$S(\chi\chi') = S(\chi)S(\chi')$$

for all elements $\chi, \chi' \in \hat{G}$. But this implies

$$\bar{S}^{it}(\varphi^{(A,B)}\varphi^{(A',B')}) = \bar{S}^{it}(\varphi^{(A,B)})\bar{S}^{it}(\varphi^{(A',B')})$$

and hence

$$t \mapsto \bar{S}^{it} \cdot \bar{S}^{-it} = \mathrm{Ad}\ \bar{S}^{it}$$

defines a one-parameter group of *-isomorphisms of $C(G)$ acting by multiplication on $L^2(G)$. Since this action for each t commutes with left and right translations, it follows from Observation 2 in the proof of Theorem 5.4.24 that for each t there exists a $\xi_t \in G$ such that

$$\mathrm{Ad}\ \bar{S}^{it} = \lambda(\xi_{\beta t}) \ .$$

But as the automorphism Ad $\bar{S}^{it}$ of $C(G)$ is uniquely determined by the underlying homeomorphism of G, ξ_t is unique, and hence $t \mapsto \xi_t$ is a continuous one-parameter group in G. Thus,

$$\sigma_t = \tau_t \gamma_{\xi_t}$$

is a continuous one-parameter group of *-automorphisms of $\mathfrak{F}$.

Now, if $A, B \in \mathfrak{F}$ are entire analytic for the two commuting groups σ and τ, then the one-parameter curve

$$t \mapsto \varphi^{(A,\, \sigma_t(B))}$$

in $L^2(G)$ has an analytic extension to $t = i\beta$. But

$$\varphi^{(A,\sigma_t(B))}(g) = \varphi(A\gamma_{\xi_t}\gamma_g\tau_t(B)) = \bar{S}^{-it/\beta}\varphi(A\gamma_g\tau_t(B))$$

and so this extension is given by

$$S\varphi(A\gamma_g\tau_{i\beta}(B)) = \varphi(B\gamma_{-g}(A)) = \varphi(\gamma_g(B)A) \ .$$

In particular

$$\varphi(A\sigma_{i\beta}(B)) = \varphi(BA)$$

which is just the KMS condition at value β.

In the course of this proof we showed that π_φ is a faithful representation of $\mathfrak{F}$; hence the uniqueness of the group $t \mapsto \xi_t$ follows from Theorem 5.3.10.

We end this section with several remarks concerning Theorem 5.4.25. If G is a compact Lie group, the one-parameter group $t \mapsto \xi_t$ is defined by an element in the Lie algebra of G which may be called the *chemical potential* of φ. Since any two extremal τ-invariant extensions φ_1 and φ_2 of ω are related by a gauge transformation, Theorem 5.4.24, it follows from Proposition 5.3.33 that $t \mapsto \xi_t$ is uniquely determined by ω up to the transformation

$$(t \mapsto \xi_t) \mapsto (t \mapsto g^{-1}\xi_t g)$$

for $g \in G$. Hence, if $G_\varphi = G$ for some φ, or G is abelian, then the chemical potential is uniquely determined by ω alone. Note also that $t \mapsto \xi_t$ is trivial, i.e., the chemical potential vanishes, whenever G_φ is trivial, i.e., φ has no gauge symmetry whatsoever. In the usual case $G = \mathbb{T} = \mathbb{R}/\mathbb{Z}$, the chemical potential is a real number, and if it is nonzero φ is gauge invariant, i.e., $G_\varphi = \mathbb{T}$ for all φ.

In the situation covered by Theorem 5.4.25 assume that $\xi_{\mathbb{R}}$ is a closed subgroup of G_φ, i.e., $t \mapsto \xi_t$ is periodic, and define subgroups G_0 and H_0 of $\mathbb{R} \times G$ by

$$G_0 = \mathbb{R} \times G_\varphi, \quad H_0 = \{(t, \xi_t); t \in \mathbb{R}\} \ .$$

Then H_0 is a closed, normal subgroup of G_0 and G_0/H_0 is compact. Now $\tau_0 = \tau \times \gamma$ defines an action of G_0 on $\mathfrak{F}$, and since φ is extremal τ-invariant, φ is extremal τ_0-invariant. Assuming for simplicity that $\sigma = \iota$, i.e., $\mathfrak{F}$ is asymptotically abelian with respect to τ, it follows easily from the compactness of $\xi_{\mathbb{R}}$ that $\mathfrak{F}$ is asymptotically abelian with respect to $t \mapsto \tau_t\gamma_{\xi_t}$, and hence it follows

from Theorem 5.3.32 that the decomposition of φ into extremal KMS states for $t \mapsto \tau_t \gamma_{\xi_t}$, at value β, coincides with the decomposition into extremal H_0-invariant states. (This decomposition also coincides with the central decomposition by Theorem 5.3.30.) But then it follows from Theorem 4.3.37 that there exists a state $\tilde{\varphi} \in \mathscr{E}(E_{\mathfrak{F}}^{H_0})$ such that this decomposition is given by

$$\varphi(A) = \int_{G_0/H_0} dg\, \tilde{\varphi}(\tau_{0,g}(A)) \ ,$$

where dg is normalized Haar measure on G_0/H_0, and one may choose $\tilde{\varphi}$ to be $t \mapsto \tau_t \gamma_{\xi_t}$-KMS. Thus, all the translates $\tilde{\varphi} \circ \tau_{0,g}$ are $\tau\gamma_\xi$-KMS, and they are extensions of ω to $\mathfrak{F}$, but they are not necessarily time-invariant states, they are only periodic in time.

In our treatment of the chemical potential we assumed some form of asymptotic abelianess of the system $(\mathfrak{F}, \mathbb{R}, \tau)$. This assumption is usually not satisfied in quantum spin systems, and for the treatment of such systems it is more appropriate to consider ω which are invariant under space translations in some direction in addition to being time invariant. If α is the space-translation automorphism, then it is natural to assume that

$$\lim_{|n| \to \infty} \|A\alpha_n(B) - \varepsilon_{A,B}\alpha_n(B)A\| = 0$$

for $A, B \in \mathfrak{F}_\pm$, and then one can build up a theory of the chemical potential by considering extremal α-invariant extensions φ of ω to $\mathfrak{F}$. Theorem 5.4.25 remains valid in this setting by virtually the same proof.

Finally we note that a modified version of Theorem 5.4.25 remains valid when $\beta = 0$, i.e., when ω is a faithful extremal τ-invariant trace-state of $\mathfrak{A}$. In this case an extremal τ-invariant extension φ of ω to $\mathfrak{F}$ is not necessarily a trace-state. Nevertheless, there exists a continuous one-parameter subgroup $t \mapsto \xi_t$ of G_φ such that φ is a KMS state (at value -1) for $t \mapsto \gamma_{\xi_t}$. This follows by essentially the same proof, normalizing such that $\mathrm{Ad}\, \bar{S}^{it} = \lambda(\xi_{-t})$.

5.4.4. Passive Systems

Passive states of a dynamical system $(\mathfrak{A}, \tau)$ were introduced in Definition 5.3.21 as states satisfying

$$-i\omega(U^*\delta(U)) \geq 0$$

for all $U \in \mathscr{U}_0(\mathfrak{A}) \cap D(\delta)$, where δ is the generator of τ and $\mathscr{U}_0(\mathfrak{A})$ is the connected component of the identity of the group $\mathscr{U}(\mathfrak{A})$ of all unitary elements of $\mathfrak{A}$. This notion reflects a property of stability of equilibrium states which is basically kinematic. For Gibbs states of finite systems it is a consequence of the principle of minimum free energy. This was discussed in Section 5.3.1 prior to Theorem 5.3.15 and it follows from this discussion that $i\omega(U^*\delta(U))$ is exactly the difference in energy of the state ω and the perturbed state ω_U where $\omega_U(A) = \omega(U^*AU)$. We next demonstrate that this energy

difference can be directly interpreted as the energy transferred from the system when it undergoes a series of external changes. But this transferred energy is the mechanical work performed by the system and thus one establishes that a state is passive if, and only if, it is unable to perform work in a cyclic process. This is the second law of thermodynamics. Combination of this result with the characterization of τ-KMS states at positive β given by Theorem 5.3.22 then provides a different justification for the τ-KMS condition as a characterization of equilibrium.

It is first necessary to have a "time-dependent perturbation" analogue of Proposition 5.4.1.

Proposition 5.4.26. *Let $(\mathfrak{A}, \tau)$ be a C^*- or W^*-dynamical system and let δ denote the infinitesimal generator of τ. Furthermore, assume that $t \in \mathbb{R} \mapsto P_t = P_t^* \in \mathfrak{A}$ is a norm-continuous one-parameter family of selfadjoint elements.*

It follows that there exists a unique one-parameter family of *-automorphisms τ^P of $\mathfrak{A}$ satisfying

$$\frac{d\tau_t^P}{dt}(A) = \tau_t^P(\delta(A) + i[P_t, A])$$

and $\tau_0^P(A) = A$, for all $A \in \mathfrak{A}$. This family is given by

$$\tau_t^P(A) = \tau_t(A) + \sum_{n \geq 1} i^n \int_0^t dt_1 \int_0^{t_1} dt_2 \cdots \int_0^{t_{n-1}} dt_n [\tau_{t_n}(P_{t_n}), [\cdots [\tau_{t_1}(P_{t_1}), \tau_t(A)]]] \ .$$

Moreover, one has

$$\tau_t^P(A) = \Gamma_t^P \tau_t(A) \Gamma_t^{P*} \ ,$$

where Γ^P is the unique iterative solution of $\Gamma_0^P = \mathbb{1}$ and

$$\frac{d\Gamma_t^P}{dt} = i\Gamma_t^P \tau_t(P_t) \ ,$$

i.e., one has

$$\Gamma_t^P = \mathbb{1} + \sum_{n \geq 1} i^n \int_0^t dt_1 \int_0^{t_1} dt_2 \cdots \int_0^{t_{n-1}} dt_n \, \tau_{t_n}(P_{t_n}) \cdots \tau_{t_1}(P_{t_1}) \ .$$

We will not give the proof of this proposition as it is essentially identical to that of Proposition 5.4.1. The principal difference introduced by the time dependence of the perturbation is that the group property of τ^P and the cocycle property of Γ^P are no longer valid. Nevertheless, one can interpret the time development of states and observables in the same manner as when the perturbation is time independent.

We next consider perturbations $t \mapsto P_t$ with the property $P_t = 0$ for $t \leq 0$ or $t \geq T$ and we also assume that $t \mapsto P_t$ is norm-differentiable. This type of

perturbation can be thought of as a smooth, and temporary, alteration of the external conditions. But changing the external conditions transmits energy to the system, i.e., mechanical work is performed by the external forces. If ω is the state of the system at $t \leq 0$, then at time t the state is given by $\omega_t = \tau_t^{P*}\omega$ and the work performed on the system can be calculated by summation of the incremental energy changes of ω_t for all $t \in [0, T]$. Explicitly one divides $[0, T]$ into N intervals (t_i, t_{i+1}) which are sufficiently small that ω_t is essentially constant on each interval and defines the work by

$$L^P(\omega) = \sum_{i=1}^{N} \omega_{t_i}(P_{t_i} - P_{t_{i-1}}) \ .$$

Thus in the limit $N \mapsto \infty$ this definition takes the integral form

$$L^P(\omega) = \int_0^T dt\, \omega_t\left(\frac{dP_t}{dt}\right) = \int_0^T dt\, \omega\left(\tau_t^P\left(\frac{dP_t}{dt}\right)\right) \ .$$

An alternative way of calculating the work performed on the system is to subtract the energy of the initial state $\omega = \omega_0$ from the energy of the final state ω_T. But

$$\omega_T(A) = \omega(\Gamma_T^P \tau_T(A)\Gamma_T^{P*})$$

and analogy with the finite system, discussed prior to Theorem 5.3.15, indicates that this energy difference should be given by $-i\omega(\Gamma_t^P\delta(\Gamma_T^{P*}))$. This explains the following result.

Lemma 5.4.27. *Let $(\mathfrak{A}, \tau)$ be a C^*- or W^*-dynamical system and ω a state over $\mathfrak{A}$. Furthermore, let τ^P denote the perturbation of τ arising from a norm-differentiable family $\{P_t\}_{t\in\mathbb{R}}$ of selfadjoint elements $P_t \in D(\delta)$ such that $P_t = 0$ for $t \leq 0$, $t \geq T$, and $d\delta(P_t)/dt = \delta(dP_t/dt)$. Where δ is the generator of τ.*

It follows that

$$L^P(\omega) = \int_0^T dt\, \omega\left(\tau_t^P\left(\frac{dP_t}{dt}\right)\right) = -i\omega(\Gamma_T^P\delta(\Gamma_T^{P*})) \ ,$$

where Γ_T^P is the unitary element relating τ_T^P and τ_T.

Proof. The derivation δ is closed and it follows from Proposition 5.4.26 and the analysis of Section 3.2.2 that $\Gamma_t^P \in D(\delta)$, $t \mapsto \delta(\Gamma_t^P)$ is differentiable, and

$$\frac{d}{dt}\delta(\Gamma_t^P) = \delta\left(\frac{d\Gamma_t^P}{dt}\right) \ .$$

Therefore

$$-i\omega(\Gamma_T^P\delta(\Gamma_T^{P*})) = -i\int_0^T dt\, \omega\left(\frac{d\Gamma_t^P}{dt}\delta(\Gamma_t^{P*}) + \Gamma_t^P\delta\left(\frac{d\Gamma_t^{P*}}{dt}\right)\right) \ .$$

But the differential equation for Γ^P immediately yields

$$-i\omega(\Gamma_T^P\delta(\Gamma_T^{P*})) = \int_0^T dt\,\omega(\Gamma_t^P\tau_t(P_t)\delta(\Gamma_t^{P*}) - \Gamma_t^P\delta(\tau_t(P_t)\Gamma_t^{P*}))$$
$$= -\int_0^T dt\,\omega(\Gamma_t^P\tau_t(\delta(P_t))\Gamma_t^{P*}) \ .$$

The second step uses the derivation property of δ and $\delta\tau = \tau\delta$. But remembering that Γ^P relates τ and τ^P one can reexpress this as

$$-i\omega(\Gamma_T^P\delta(\Gamma_T^{P*})) = -\int_0^T dt\,\omega(\tau_t^P(\delta(P_t))) \ .$$

On the other hand one may integrate by parts and use $P_0 = 0 = P_T$ to find

$$L^P(\omega) = -\int_0^T dt\,\omega\left(\left(\frac{d\tau_t^P}{dt}\right)(P_t)\right) = -\int_0^T dt\,\omega(\tau_t^P(\delta(P_t))) \ .$$

This establishes the desired equality.

Combination of Lemma 5.4.27, Theorem 5.3.22, and an approximation argument then gives the following characterization of τ-KMS states.

Theorem 5.4.28. *Let $(\mathfrak{A}, \tau)$ be a C^*- or W^*-dynamical system and ω a state over $\mathfrak{A}$. Consider the following conditions.*

(1) *ω is a (τ, β)-KMS state for some $\beta \in [0, \infty]$ and ω is τ-invariant.*

(2) *The work performed on the system is positive, i.e.,*

$$L^P(\omega) = \int_0^T dt\,\omega\left(\tau_t^P\left(\frac{dP_t}{dt}\right)\right) \geq 0 \ ,$$

for every norm-differentiable family $\{P_t\}_{t\in\mathbb{R}}$ of selfadjoint perturbations $P_t \in \mathfrak{A}$ such that $P_t = 0$ for $t \leq 0$ and $t \geq T$.

It follows that (1) $\Rightarrow$ (2) and if there exists a group G and an action α of G as *-automorphisms of $\mathfrak{A}$ such that ω is α-invariant, α commutes with τ, and ω is weakly α-clustering, then (1) $\Leftrightarrow$ (2).

Proof. (1) $\Rightarrow$ (2). First, assume that $\{P_t\}_{t\in\mathbb{R}}$ satisfies the condition of Lemma 5.4.27. It follows from the passivity property established in Theorem 5.3.22, and Lemma 5.4.27 that

$$L^P(\omega) = -i\omega(\Gamma_T^P\delta(\Gamma_T^{P*})) \geq 0 \ .$$

Second, if $P_t \notin D(\delta)$, then one replaces it by the regularization

$$P_t^n = \sqrt{\frac{n}{\pi}}\int ds\,e^{-ns^2}\tau_s(P_t) \ .$$

In the C^*-case one has $\|P_t^n - P_t\| \to 0$ and $\|dP_t^n/dt - dP_t/dt\| \to 0$ by Proposition 2.5.22 and it follows easily that $L^{P^n}(\omega) \to L^P(\omega)$. Hence

$$L^P(\omega) = \lim_{n\to\infty} L^{P^n}(\omega) \geq 0$$

by the argument of the previous paragraph. In the W^*-case the argument is a little more delicate. As ω is τ-invariant the group τ is implemented by a unitary group U_ω in the representation $(\mathfrak{H}_\omega, \pi_\omega, \Omega_\omega)$. But if P_t^n are the above regularizations of P_t, one then has

$$\begin{aligned}\lim_{n\to\infty} \|\pi_\omega(P_t^n - P_t)\psi\| &\leq \lim_{n\to\infty} \pi^{-1/2} \int ds\, e^{-s^2} \|\pi_\omega(\tau_{s/\sqrt{n}}(P_t) - P_t)\psi\| \\ &\leq \lim_{n\to\infty} \pi^{-1/2} \int ds\, e^{-s^2} \{\|P_t\| \; \|(U_\omega(-s/\sqrt{n}) - \mathbb{1})\psi\| \\ &\quad + \|(U_\omega(s/\sqrt{n}) - \mathbb{1})\pi_\omega(P_t)\psi\|\} = 0\end{aligned}$$

for all $\psi \in \mathfrak{H}_\omega$, and similarly for dP_t^n/dt. It follows immediately from the uniform boundedness of strongly convergent sequences, and the Lebesgue-dominated convergence theorem, that $\pi_\omega(\Gamma_t^{P^n} - \Gamma_t^P) \to 0$ in the strong-operator topology. Therefore,

$$\begin{aligned}\omega\left(\tau_t^{P^n}\left(\frac{dP_t^n}{dt}\right)\right) &= \left(\Omega_\omega, \pi_\omega(\Gamma_t^{P^n}) U_\omega(t) \pi_\omega\left(\frac{dP_t^n}{dt}\right) U_\omega(-t) \pi_\omega(\Gamma_t^{P^n})^* \Omega_\omega\right) \\ &\to \omega\left(\tau_t^P\left(\frac{dP_t}{dt}\right)\right)\end{aligned}$$

and another application of the Lebesgue theorem gives

$$L^P(\omega) = \lim_{n\to\infty} L^{P^n}(\omega) \geq 0$$

as before.

(2) $\Rightarrow$ (1) : We argue that condition (2) implies that ω is passive and then apply Theorem 5.3.22.

Let U belong to the connected component $\mathscr{U}_0(\mathfrak{A})$ of the unit element in the group of all unitary elements of $\mathfrak{A}$. It follows that there exists a finite sequence $\{A_j\}_{1 \leq j \leq N}$ of selfadjoint elements $A_j \in \mathfrak{A}$ such that $\|A_j\| < \pi$ and

$$U = \prod_{j=1}^{N} e^{iA_j} \ .$$

(This follows because $\|U_1 - U_2\| < 2$ implies $U_1 = U_2 e^{iA}$ by spectral analysis.) Next let δ denote the generator of τ and assume that $A_j \in D(\delta)$ for all $j = 1, 2, \ldots, N$. Therefore, $U \in D(\delta)$ by Lemma 3.2.31. Now if f is a twice-differentiable function on $\mathbb{R}$ such that $f(t) = 0$ for $t \leq 0$ and $f(t) = 1$ for $t \geq T$ we define U_t by $U_t = \mathbb{1}$ for $t \leq 0$, $U_t = U$ for $t \geq T$, and

$$U_t = e^{iA_1} \cdots e^{iA_j} e^{if(t - jT/N)A_{j+1}}$$

for $jT/N \leq t \leq (j+1)T/N$. Further define perturbations P_t by

$$P_t = -i\tau_{-t}\left(U_t^* \frac{dU_t}{dt}\right) \ ,$$

i.e., P_t and U_t are linked by the differential equation

$$\frac{dU_t}{dt} = iU_t \tau_t(P_t) \ .$$

Thus, $U_t = \Gamma_t^P$ and in particular $U = \Gamma_T^P$. But P_t satisfies the conditions of Lemma 5.4.27 and hence

$$-i\omega(U\delta(U^*)) = L^P(\omega) \geq 0 \ .$$

Finally, the case that $U \in D(\delta)$ but $A_j \notin D(\delta)$ is handled by approximation. We omit the details.

Remark. There is one simple but interesting application of the identity

$$L^P(\omega) = -i\omega(\Gamma_T^P \delta(\Gamma_T^{P*}))$$

of Lemma 5.4.27. Assume that $\mathfrak{A} = \mathfrak{A}_1 \otimes \mathfrak{A}_2$, $\tau = \tau_1 \otimes \tau_2$, and $\omega = \omega_1 \otimes \omega_2$, where ω_i is a (τ, β_i)-KMS state with $\beta_i \geq 0$, $i = 1, 2$. Thus $(\mathfrak{A}, \tau)$ can be envisaged as two independent systems. Next consider an external interaction $\{P_t\}_{t \in \mathbb{R}}$, of the type considered in Lemma 5.4.27 which temporarily links the systems. As τ is a product, $\delta = \delta_1 \otimes \imath + \imath \otimes \delta_2$, where δ_i is the generator of τ_i and hence

$$L^P(\omega) = L_1^P(\omega) + L_2^P(\omega) \ ,$$

where

$$L_1^P(\omega) = -i\omega(\Gamma_T^P(\delta_1 \otimes \imath)(\Gamma_T^{P*})) \ , \quad L_2^P(\omega) = -i\omega(\Gamma_t^P(\imath \otimes \delta_2)(\Gamma_T^{P*})) \ .$$

These latter quantities represent the mechanical work performed on the first and second subsystems, respectively. But ω is a $(\tilde{\tau}, 1)$-KMS state where $\tilde{\tau}_t = \tau_{1,\, \beta_1 t} \otimes \tau_{2,\, \beta_2 t}$ and hence

$$\beta_1 L_1^P(\omega) + \beta_2 L_2^P(\omega) = \omega(\Gamma_T^P(\beta_1 \delta_1 \otimes \imath + \beta_2 \imath \otimes \delta_2)(\Gamma_T^{P*})) \geq 0$$

by Theorem 5.4.28. Thus setting $\beta_i = 1/T_i$ one finds

$$(T_1 - T_2) L_1^P(\omega) \leq T_1 L^P(\omega) \ .$$

Now if $T_1 \neq T_2$, then ω cannot be a (τ, β)-KMS state for any $\beta \geq 0$. Thus, it could happen that $L^P(\omega) \leq 0$. If, however, $T_1 > T_2$ then one must also have $L_1^P(\omega) < 0$ and

$$\frac{-L^P(\omega)}{-L_1^P(\omega)} \leq \frac{T_1 - T_2}{T_1} \ .$$

This is *Carnot's formula* which states that the efficiency of a heat motor is limited by $(T_1 - T_2)/T_1$ where T_1 and T_2 are the temperatures of the heat source and heat sink, respectively.

Notes and Remarks

Sections 5.2.1, 5.2.2, and 5.2.3

The study of the CCRs and CARs over $\mathfrak{h} = L^2(\mathbb{R}^3)$ was a direct outcome of attempts to combine quantum mechanics and classical field theory.

The CCRs were introduced by Dirac [Dir 1] in 1927 in the context of radiation theory and are generalizations of Heisenberg's commutation relations in quantum mechanics. The CARs were introduced by Jordan and Wigner [Jor 1] in 1928 for the purpose of quantizing the electron field. These authors also proved that the CARs over an n-dimensional Hilbert space generate the full $2^n \times 2^n$ complex matrix algebra. Since the late 1920s the theory of creation and annihilation operators has been developed by many people in a multitude of specific contexts, e.g., many-body physics, quantum optics, statistical mechanics, relativistic field theory, etc. Much of the analysis is, however, of a heuristic nature. Rigorous mathematical analysis of the commutation relations, and the associated algebras, only began in the 1950s, e.g., essential selfadjointness of $\Phi(f)$ was first proved in 1953 by Cook [Coo 1] who established that the $\Phi(f) \pm i\mathbb{1}$ have dense ranges. Cook also gave a precise description of the Fock space, introduced by Fock in 1932 [Foc 1], and the corresponding representation of the CCRs. Consequently, this representation is often called the Fock-Cook representation.

The abstract structure of the creation and annihilation operators was also studied in the 1950s, notably by Friederichs [[Fri 1]] and Segal (see [[Seg 1]] for a description of the subject during this period). In particular Segal emphasized the C^*-algebraic structure and introduced several new features and results. For example, it was traditional to analyze the CARs over a real Hilbert space $\mathfrak{h}$ in terms of "fields"

$$\Phi(f) = 2^{-1/2}(a(f) + a^*(f))$$

and their "conjugate fields"

$$\Pi(f) = -i\,2^{-1/2}(a(f) - a^*(f))$$

but Segal emphasized the advantages of considering complex $\mathfrak{h}$ and a single field.

The algebraic uniqueness of the CCR algebra, Theorem 5.2.8, was established in 1971 by Slawny [Sla 1] by the method we have described.

The Stone-von Neumann uniqueness theorem, Corollary 5.2.15, was announced by Stone in 1930 but the first published proof was given by von Neumann [Neu 4] a year later. The lack of uniqueness for systems over infinite-dimensional spaces $\mathfrak{h}$ caused a lot of confusion which was not fully clarified until the late 1950s, and early 1960s. Until 1950 it appeared that most people tacitly believed that a Weyl system over a general Hilbert space $\mathfrak{h}$ had a unique regular irreducible representation. Counterexamples appeared in various disguises in the 1950s. Segal realized that various canonical transformations of the Bogoliubov type were not unitarily implementable (see [[Seg 1]]), van Hove subsequently showed [Hov 1] that the uniqueness hypothesis led to a paradoxical "orthogonality of two complete orthogonal sets of eigenfunctions in Fock space," and Haag [Haag 4] established a general result which implied the existence of inequivalent representations. The work of Haag also clearly demonstrated that representations which are inequivalent to the Fock representation are crucial from the physical point of view. Roughly stated, Haag showed that each dynamics has a distinct set of relevant representations and different dynamics lead to inequivalent representations. (A precise statement of this type is given in Corollary 5.3.41.) Another aspect of inequivalent representation was provided by the work, in 1954, of Gårding and Wightman [Går 1]. These authors proposed a classification of the (regular) representations of the CCR and CAR algebras based upon properties of a number operator and, in particular, a result of the type given by Theorem 5.2.14. Various versions of this theorem were subsequently proved by several authors, e.g., Dell'Antonio, Doplicher, and Ruelle [Ant 1], Dell'Antonio and Doplicher [Ant 2], Chaiken [Cha 1], [Cha 2], and Courbage, Miracle, and Robinson [Cou 1]. Our discussion is an extension of this last reference. It should be emphasized that the CCR version of Theorem 5.2.14 may be false if $n_\omega(\psi)$ is defined by summing $\| a_\omega(f)\psi \|^2$ over all f in a fixed orthonormal basis of $\mathfrak{h}$ (see [Cha 1] for counterexamples) but the CAR version remains valid.

In 1964 Haag and Kastler [Haag 9] proposed a C^*-algebraic reformulation of quantum field theory which emphasized the quasi-local structure of the field algebra. They also clarified the importance of the global C^*-structure and the existence of inequivalent representations for the discussion of topics such as physical equivalence and superselection rules.

Truncated functions were introduced in quantum field theory by Haag [Haag 5] who realized their convenience for describing cluster properties (see Example 5.2.19). Analogues of these functions occur in other disciplines, e.g., cumulants in probability theory, Ursell-Mayer correlation functions in classical statistical mechanics, etc.

Bogoliubov exploited automorphisms arising from transformations of the one-particle space $\mathfrak{h}$ in his 1947 investigation of the equilibrium states of the Bose gas [Bog 1] and subsequently these automorphisms have been called Bogoliubov transformations. The names one-particle automorphism, or quasi-free automorphism, also occur. Combination of the Fock state with a Bogoliubov transformation immediately yields a quasi-free state and this was one of

the origins of such states. They also naturally occur as equilibrium states of the ideal gases and other noninteracting systems. The general notion of a quasi-free state as a state whose higher-order truncated functions vanish was independently introduced by Robinson [Rob 3] and Shale and Stinespring [Sha 1]. Robinson concentrated, however, on translationally invariant states while Shale and Stinespring only examined gauge-invariant states. The general theory was subsequently developed by numerous authors, e.g., Araki, Balslev, Dell'Antonio, Manuceau, Powers, Størmer, Verbeure (for a review up to 1969 see the proceedings of the Cargèse Summer School [[Car 1]]). One of the most striking early results was due to Powers who constructed a one-parameter family of mutually nonisomorphic type III factors as the weak closures of representations of the CAR algebra from quasi-free states [Pow 1]. Explicitly, the weak closure of $\pi_{\omega_\lambda}(\mathfrak{A})$, where ω_λ is the gauge-invariant quasi-free state given by

$$\omega_\lambda(a(f)^* a(g)) = \lambda(g, f) \ ,$$

is a factor of type $\mathrm{III}_{\lambda/1-\lambda}$ in the sense of Definition 2.7.24, for $0 < \lambda < 1/2$. Subsequently, the quasi-free factor states have been completely typed by properties of their two-point functions and criteria for quasi-equivalence of such states have also been given. For example, every gauge-invariant quasi-free state of the CAR algebra is a factor state and if ω_{A_1} and ω_{A_2} are such states with two-point functions given by

$$\omega_{A_i}(a(f)^* a(g)) = (g, \ A_i f), \quad i = 1, \ 2,$$

then $\pi_{\omega_{A_1}}$ is quasi-equivalent to $\pi_{\omega_{A_2}}$ if, and only if, $A_1^{1/2} - A_2^{1/2}$ and

$$(\mathbb{1} - A_1)^{1/2} - (\mathbb{1} - A_2)^{1/2}$$

are both Hilbert-Schmidt operators. The sufficiency of these latter conditions was derived by Dell'Antonio [Ant 3] and Rideau [Rid 1] while the necessity was established by Powers and Størmer [Pow 5].

Note that in particular π_{ω_A} is quasi-equivalent to the Fock representation if, and only if, $A^{1/2}$ and $(\mathbb{1} - A)^{1/2} - \mathbb{1}$ are both Hilbert-Schmidt operators. But as $\lambda \geq ((1-\lambda)^{1/2} - 1)^2$ the latter condition is redundant, i.e., π_{ω_A} is quasi-equivalent to the Fock representation if, and only if, A is of trace-class. But the trace of A defines the number of particles in ω_A,

$$\mathrm{Tr}(A) = \sum_{i \geq 1} \omega_A(a^*(f_i) a(f_i)) = n(\omega_A) \ .$$

Hence, ω_A is normal with respect to the Fock representation if, and only if, it has finite particle number.

It is interesting to note that the equivalence between A being trace-class and π_{ω_A} being quasi-equivalent to the Fock representation π_{ω_o} is formally clear from the identity

$$\omega_A(B) = \mathrm{Tr}(\Gamma(A) B) \ ,$$

where B is represented in the Fock representation. One uses that $\Gamma(A)$ is of trace-class if, and only if, A is of trace-class.

The generalization of these results to the CCR algebra and nongauge-invariant states was obtained by Araki [Ara 10], [Ara 11], Araki and Shiraishi [Ara 12], and van Daele [Dae 3].

Sections 5.2.4 and 5.2.5

The ideal gases are discussed in most standard textbooks on statistical mechanics (see, for example, Huang [[Hua 1]] or Landau and Lifschitz [[Lan 1]]) and it is common to perform the thermodynamic limit implicitly. Rigorous proofs of the existence of these limits are in fact quite recent. The most difficult case, the Bose gas in the region of condensation, was treated by Cannon [Can 1], and Lewis and Pulé [Lew 1], in 1973–1974. But both these works were partially based upon unpublished lecture notes of M. Kac. Our discussion is somewhat different and is based upon unpublished lectures of D.W. Robinson. The algebraic structure of the Gibbs thermodynamic limit states had, however, already been analyzed by Araki and Woods [Ara 8] for the Bose gas and by Araki and Wyss [Ara 9] for the Fermi gas. The Araki-Woods paper showed for the first time that equilibrium states lead to type III factors.

The ideal Bose gas exhibits more complex condensation phenomena than we have described. Theorem 5.2.30 establishes that if Λ_L is a parallelepiped with edges whose lengths tend to infinity in a homogeneous manner then at high densities a finite proportion of the particles occupy the lowest energy state, i.e., the ground state. But it is also possible to have a finite proportion of the particles occupying the energy levels in an arbitrary small band above the ground state with no macroscopic occupation of the ground state itself. This latter phenomena is referred to as generalized condensation. In general there are two critical densities $\rho_{gc} \leq \rho_c$. If the density $\rho \leq \rho_{gc}$ there is no form of condensation, if $\rho \in \langle \rho_{gc}, \rho_c]$ generalized condensation occurs and for all $\rho > \rho_c$ the system condenses into the ground state. For example [Ber 2], if Λ_L is a parallelepiped with sides $L_1 \geq L_2 \geq \ldots \geq L_\nu$ with $L_i \to \infty$ and $(L_2 \ldots L_\nu) / L_1 \to \infty$ but $\log L_2/(L_3 \ldots L_\nu) \to B$ then $\rho_c = \rho_{gc} + B\pi^{-1}$. Thus properties of condensation are sensitive both to shape and to boundary effects. The general theory of both forms of condensation was developed by van den Berg, Lewis and Pulé [Ber 3] and a variety of examples given by van den Berg, Lewis and Lunn [Ber 4]. But these papers were the sequel to various earlier investigations, see, for example, Girardeau [Gir 1], Schultz [Sch 1] and van den Berg and Lewis [Ber 1]. Other references and background material are given in these references.

The allusion to negative temperatures made in the footnote following Lemma 5.2.25 can be understood by reference to the models of magnetic materials discussed in Chapter 6. The equilibrium states for these spin systems are defined for all values of β and a change of sign of β corresponds to a change

of sign of the interaction. Thus if the temperature could be lowered beyond absolute zero, an attractive interaction would immediately become repulsive, and vice versa. Consequently, ferromagnetic materials would become antiferromagnetic, and conversely. But these two phenomena are physically quite distinct and hence the passage to negative temperatures would be heralded by a sudden change of magnetic properties. Such transitions have been observed, for example by Abragam and Proctor [Abr 1] in experiments on lithium fluoride and the same authors give a more detailed theoretical discussion in [Abr 2].

Section 5.3.1

The KMS condition was first introduced in quantum statistical mechanics by Kubo [Kub 1] in 1957 and Martin and Schwinger [Mart 1] in 1959 as a condition satisfied by thermodynamic Green's functions. This condition was systematically exploited in the analysis of Green's functions by Kadanoff and Baym [[Kada 1]]. It was first formulated in C^*-algebra language by Haag, Hugenholtz, and Winnink [Haag 6]. The original formulation of this condition is the one used in Proposition 5.3.12.

During the same period, 1966–1967, that Haag, Hugenholtz, and Winnink, investigated the algebraic formulation of the KMS condition, Tomita developed the essential points of the theory of the modular automorphism group (see Chapter 2). Although it was apparent that some connection existed between these two formalisms no complete synthesis was provided until 1970 when Takesaki [Tak 3] published his investigation and elaboration of Tomita's theory. In particular, Takesaki proved that the modular automorphism group satisfies the τ-KMS condition with $\beta = -1$ and that this condition uniquely determines the group τ when the state is given (Theorem 5.3.10). In the intervening period, 1967–1970, various other authors working on the KMS structure established partial results in this direction. For example, Winnink [Win 1] obtained the uniqueness of τ from the KMS condition and also [Win 2] proved that this condition implies invariance of the state and pointwise invariance of the center of the corresponding representation. Both these invariance results were obtained independently by Hugenholtz and the state invariance was also obtained by F. Rocca and M. Sirugue.

The multidimensional version of the edge of the wedge theorem, alluded to prior to Proposition 5.3.6, is discussed in [[Stre 1]], while more general forms of the Paley-Wiener theorem, Proposition 5.3.11, can be found in [[Hør 1]], [[Ree 2]], [[Rud 1]]. The three-line theorem can be found in the books by Titchmarsh and Rudin [[Tit 1]], Proposition 5.3.5 or [[Rud 1]], Theorem 12.8.

The earliest correlation inequality of the type encountered in Theorems 5.3.15 and 5.3.17 was given by Bogoliubov [Bog 2] who proved in 1962 that the Gibbs state ω of a finite system at inverse temperature β satisfies

$$|\omega([A,B])|^2 \leq -i\beta\omega(AA^* + A^*A)\omega([B^*, \delta(B)])/2 \ .$$

This inequality was extended to general (τ, β)-KMS states in 1972 by Garrison and Wong [Gar 1]. Basically, it follows from the Cauchy-Schwarz inequality applied to the Duhamel two-point function, introduced before Theorem 5.3.17. A detailed derivation and an application is given in Chapter 6 (see Section 6.2.6, Lemma 6.2.51).

Alternative upper bounds for the Duhamel function which improve the Bogoliubov inequality were subsequently derived for Gibbs states by Berman, Bruch, and Fortune [Ber 1] and by Roepstorff [Roe 1]. Falk and Bruch [Fal 1] and Roepstorff [Roe 1] also derived lower bounds. Roepstorff's results were extended to general KMS states by Naudts and Verbeure [Nau 1]. This generalization relied partially on earlier work of Naudts, Verbeure, and Weder [Nau 2]. Subsequently, Fannes and Verbeure [Fan 1], [Fan 2] established a converse to these results by showing that the KMS condition could be derived from the Roepstorff inequality.

Independently Sewell, partially in collaboration with Araki, had been attempting to prove the equivalence of a maximum entropy principle and the KMS condition for spin systems (for details and references to this development see Chapter 6) and the Fannes-Verbeure result provided the strategy for passing from the entropy principle to the KMS condition. Sewell [Sew 1] deduced the correlation inequality of Theorem 5.3.15 from the argument outlined prior to this theorem and also showed that this inequality implied the KMS condition. The converse implication followed for spin systems by the earlier work of Araki and Sewell [Ara 22]. For general KMS states it was given in the lecture notes of Araki [Ara 13].

Generators of positivity-preserving semigroups on C^*-algebras have been extensively studied in connection with the theory of irreversible quantum processes, [[Dav 1]], [[Eva 1]]. If the semigroup is norm continuous, one can give several equivalent characterizations of such generators, and the most complete result in this direction was proved by Evans and Hanche-Olsen in 1977, [Eva 1].

Theorem. *Let γ be a bounded map on a C^*-algebra $\mathfrak{A}$ with identity such that $\gamma(A^*) = \gamma(A)$ for all $A \in \mathfrak{A}$.*

The following conditions are equivalent:

(1) *$e^{t\gamma}$ is a positive map for all $t \in \mathbb{R}_+$.*
(2) *$(\lambda\iota - \gamma)^{-1}$ is a positive map for all large positive reals λ.*
(3) *If $A \in \mathfrak{A}_+, B \in \mathfrak{A}$ satisfy $AB = 0$, then $B^*\gamma(A)B = 0$.*
(4) *If $A \in \mathfrak{A}_+$ and $\omega \in E_{\mathfrak{A}}$ satisfy $\omega(A) = 0$, then $\omega(\gamma(A)) \geq 0$.*
(5) *$\gamma(A^2) + A\gamma(\mathbb{1})A \geq \gamma(A)A + A\gamma(A)$ for all selfadjoint $A \in \mathfrak{A}$.*
(6) *$\gamma(\mathbb{1}) + U^*\gamma(\mathbb{1})U \geq \gamma(U^*)U + U^*\gamma(U)$ for all unitaries $U \in \mathfrak{A}$.*

Note that in the special case $\gamma(\mathbb{1}) = 0$ conditions (5) and (6) follow from the condition

$$\gamma(A^*A) \geq \gamma(A^*)A + A^*\gamma(A)$$

mentioned prior to Theorem 5.3.15 and in Proposition 3.2.22, but in fact the latter condition is strictly stronger than (5) and (6). An explicit example, [Eva 1], is given by $\mathfrak{A} = \mathscr{L}(\mathbb{C}^2)$, the complex 2×2 matrices, and $\gamma(A) = A^t - A$, where A^t is the transposed matrix of A,

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix}^t = \begin{pmatrix} a & c \\ b & d \end{pmatrix} .$$

In fact the groups generated by a generator γ satisfying the strong condition are characterized by the generalized Schwarz inequality, i.e.,

Corollary [Eva 1]. *Let γ be a linear map on a C^*-algebra $\mathfrak{A}$ such that $\gamma(A^*) = \gamma(A)^*$ for all $A \in \mathfrak{A}$.*
The following conditions are equivalent:

(1) $e^{t\gamma}(A^*A) \geq e^{t\gamma}(A^*)e^{t\gamma}(A)$ *for all* $A \in \mathfrak{A}, t \in \mathbb{R}_+$.
(2) $\gamma(A^*A) \geq \gamma(A^*)A + A^*\gamma(A)$ *for all* $A \in \mathfrak{A}$.

One has an even better understanding of norm-continuous semigroups of completely positive maps on von Neumann algebras. The notion of a *completely positive map* between two C^*-algebras $\mathfrak{A}$ and $\mathfrak{B}$ was introduced by Stinespring in 1955 [Sti 1]. Let $\mathfrak{A}_n = \mathfrak{A} \otimes \mathscr{L}(\mathbb{C}^n)$ be the C^*-algebra of all $n \times n$ matrices with entries in $\mathfrak{A}$. A linear map $\varphi : \mathfrak{A} \mapsto \mathfrak{B}$ is said to be *n-positive* if the induced map $\varphi_n : \mathfrak{A}_n \mapsto \mathfrak{B}_n$ defined by

$$\varphi((A_{ij})_{i,j=1}^n) = (\varphi(A_{ij}))_{i,j=1}^n$$

is positive. φ is said to be *completely positive* if it is n-positive for $n = 1, 2, 3, \ldots$. For example, an automorphism of a C^*-algebra is completely positive, while an anti-automorphism of a non-abelian C^*-algebra is positive, but not 2-positive. For all n there exist maps which are n-positive but not $n+1$-positive.

There does not seem to be any deep inherent reason for studying completely positive maps among all positive maps except that they are relatively easy to handle due to the following result, which is often referred to as Stinespring's theorem.

Proposition [Sti 1]. *If $\mathfrak{A}$ is a C^*-algebra with identity, and $\varphi : \mathfrak{A} \mapsto \mathscr{L}(\mathfrak{H})$ is a linear map, then φ is completely positive if and only if it has the form*

$$\varphi(A) = V^*\pi(A)V$$

for some representation π of $\mathfrak{A}$ on a Hilbert space $\mathfrak{K}$, and some bounded linear map $V : \mathfrak{H} \mapsto \mathfrak{K}$. If $\mathfrak{A}$ and $\mathfrak{H}$ are separable, then $\mathfrak{K}$ can be taken to be separable. If $\mathfrak{A}$ is a von Neumann algebra and φ is normal, then π can be taken to be normal.

The observant reader may have noticed that this proposition was actually established during the proof of the generalized Schwarz inequality, Proposition 3.2.4, where it was also established that a positive, identity-preserving map

from an abelian C^*-algebra into another C^*-algebra is completely positive. One can also show that a positive, identity-preserving map from an arbitrary C^*-algebra into an abelian C^*-algebra is completely positive, in particular states are completely positive [Stø 1].

During the course of the proof of Proposition 3.2.4 we established that the generalized Schwarz inequality

$$\varphi(\mathbb{1})\varphi(A^*A) \geq \varphi(A)^*\varphi(A)$$

is always valid for a completely positive map φ. Araki proved in 1973 that this inequality follows from 2-positivity alone [Ara 23]. In 1976 Evans [Eva 2] proved that if $\varphi\colon \mathfrak{A} \mapsto \mathscr{L}(\mathfrak{H})$ is a $n+1$-positive map, where $n \geq 1$, then the matrix inequality

$$(\varphi(A_i^*A_j))_{i,j=1}^n \geq (\varphi(A_i^*B)\varphi(B^*B)^{-1}\varphi(B^*A_j))_{i,j=1}^n$$

is valid for all B, A_1, $A_2, \ldots, A_n \in \mathfrak{A}$ (with the proper interpretation of $\varphi(B^*B)^{-1}$). In particular

$$\|\varphi(B^*B)\|(\varphi(A_i^*A_j))_{i,j=1}^n \geq (\varphi(A_i^*B)\varphi(B^*A_j))_{i,j=1}^n$$

and, setting $B = \mathbb{1}$,

$$\|\varphi\|(\varphi(A_i^*A_j))_{i,j=1}^n \geq (\varphi(A_i^*)\varphi(A_j))_{i,j=1}^n \ .$$

For $n = 1$ this is just the generalized Schwarz inequality. One can show conversely that if a bounded linear map $\varphi\colon \mathfrak{A} \mapsto \mathscr{L}(\mathfrak{H})$ satisfies these inequalities for all n, then φ is completely positive.

If $\mathfrak{A}$ is a von Neumann algebra on a Hilbert space $\mathfrak{H}$ (or $\mathfrak{A} = \mathscr{L}\mathscr{C}(\mathfrak{H})$) it follows from Stinespring's theorem and Theorem 2.4.26 that a normal map $\varphi\colon \mathfrak{A} \mapsto \mathfrak{A}$ is completely positive if and only if it has the form

$$\varphi(A) = \sum_\alpha V_\alpha^* A V_\alpha$$

for a suitable set $\{V_\alpha\} \subseteq \mathscr{L}(\mathfrak{H})$, where the convergence is in the weak-operator topology. The set can be taken to be countable if $\mathfrak{H}$ is separable, and finite if $\mathfrak{H}$ is finite dimensional.

The following theorem is a generalization of the derivation theorem, Corollary 3.2.47, to generators of norm-continuous semigroups of completely positive maps. It was proved in some special cases by Lindblad and independently by Gorini, Kossakowski, and Sudarshan in 1976, and was extended by various authors until the final version was proved by Christensen and Evans in 1978 [Chr 1]. The latter paper contains a complete history and bibliography of the subject, and the final result is

Theorem [Chr 1]. *Suppose that $t \in \mathbb{R}_+ \mapsto e^{t\gamma}$ is a norm-continuous semigroup of completely positive maps on a C^*-algebra $\mathfrak{A}$ acting on a Hilbert space $\mathfrak{H}$. Then there exists a completely positive map φ from $\mathfrak{A}$ into its weak closure $\overline{\mathfrak{A}}$ and a selfadjoint element $H = H^* \in \overline{\mathfrak{A}}$ such that the generator γ has the form*

$$\gamma(A) = [iH, A] - \{R, A\}/2 + \varphi(A) \ .$$

Here $R = \varphi(\mathbb{1}) - \gamma(\mathbb{1})$ *and* $\{\cdot,\cdot\}$ *denotes the anti-commutator.*

In particular, if the maps $e^{t\gamma}$ are normal the map φ can be taken to be normal and γ has the form

$$\gamma(A) = [iH, A] - \{R,\ A\}/2 + \sum_{\alpha} V_\alpha^* A V_\alpha$$

for suitable $V_\alpha \in \mathscr{L}(\mathfrak{H})$.

The theory for generators of norm-continuous, normal, completely positive semigroups on von Neumann algebras can thus be summed up as follows:

Corollary. *Suppose that* $t \in \mathbb{R}_+ \mapsto e^{t\gamma}$ *is a norm-continuous* C_0^**-semigroup on a von Neumann algebra* $\mathfrak{M}$ *on a Hilbert space* $\mathfrak{H}$*, such that* $e^{t\gamma}(\mathbb{1}) = \mathbb{1}$ *for all* $t \in \mathbb{R}_+$.

The following statements are equivalent:

(1) $e^{t\gamma}$ *is a completely positive map for each* $t \in \mathbb{R}_+$.

(2) $(\gamma \otimes \iota)(A^*A) \geq (\gamma \otimes \iota)(A^*)A + A^*(\gamma \otimes \iota)(A)$ *for each* $A \in \mathfrak{M} \otimes \mathscr{L}(\mathbb{C}^n)$ *and each* $n = 1, 2, 3, \ldots$ *(here* $\iota\colon \mathscr{L}(\mathbb{C}^n) \mapsto \mathscr{L}(\mathbb{C}^n)$ *is the identity map).*

(3) *There exists a set* $\{V_\alpha\}$ *of operators in* $\mathscr{L}(\mathfrak{H})$ *such that* $R = \sum_\alpha V_\alpha^* V_\alpha$ *is a bounded operator in* $\mathfrak{M}$*, and such that* $\sum_\alpha V_\alpha^* A V_\alpha \in \mathfrak{M}$ *whenever* $A \in \mathfrak{M}$*, and a selfadjoint operator* $H = H^* \in \mathfrak{M}$ *such that*

$$\gamma(A) = [iH, A] - \{R, A\}/2 + \sum_{\alpha} V_\alpha^* A V_\alpha$$

for all $A \in \mathfrak{M}$.

To prove that (3) $\Rightarrow$ (1) in this corollary, one uses that γ_1, γ_2, and γ_3 defined by

$$\gamma_1(A) = [iH, A], \quad \gamma_2(A) = -\{R, A\}/2, \quad \gamma_3(A) = \sum_{\alpha} V_\alpha^* A V_\alpha$$

are all generators of completely positive semigroups, i.e.,

$$e^{t\gamma_1}(A) = e^{itH} A e^{-itH}, \quad e^{t\gamma_2}(A) = e^{-(t/2)R} A e^{-(t/2)R} \ ,$$

$$e^{t\gamma_3}(A) = \sum_{n=0}^{\infty} \frac{t^n}{n!} \gamma_3^n(A) \ ,$$

and then the Trotter product formula, Corollary 3.1.31, implies that γ generates a completely positive semigroup.

The theory of non-norm-continuous semigroups of positivity-preserving maps has not been developed very much, but there exist some results on quasi-free evolutions on the CCR and CAR algebras (see Evans' review paper [Eva 3] for results up to 1980). For other results in this direction see [[Bra 1]], [[Rob 2]] and [Arv l].

The connection between the Duhamel two-point function of a KMS state and various quantities of linear response theory has been described by Naudts, Verbeure, and Weder [Nau 2].

Ground states, as described in Definition 5.3.18, are versions of the positive-energy vacuum states studied by innumerable authors since the early 1950s and Proposition 5.3.19 is an algebraic reformulation of standard results in this field. The set of ground states of a C^*-dynamical system was studied by Araki in 1964 [Ara 7], and Sirugue and Testard in 1971 [Sir 1] examined these states as $\beta \to \infty$ limits of (τ, β)-KMS states.

The notion of passive states and Theorem 5.3.22 is due to Pusz and Woronowicz in 1977 [Pus 1].

The results on convergence of KMS states are more or less folklore, but the proofs by means of the auto-correlation lower bound appear to be new.

The algebras $\mathcal{O}_n$ in Example 5.3.27 were introduced and studied by Cuntz in 1976 [Cun 2]. An alternative definition was suggested by Evans in 1979 [Eva 4]. Let $\mathfrak{H}$ be an n-dimensional Hilbert space, where $2 \leq n \leq \aleph_0$. Define $\mathcal{O}_n^F$ as the C^*-algebra generated by creation and annihilation operators on the full (unsymmetrized) Fock Space

$$\mathfrak{F}(\mathfrak{H}) = \bigoplus_{r=0}^{\infty} (\otimes^r \mathfrak{H}) \ .$$

Evans' definitions are then

$$\mathcal{O}_n = \mathcal{O}_n^F / \mathcal{LC}(\mathfrak{F}(\mathfrak{H})), \quad \mathcal{O}_\infty = \mathcal{O}_\infty^F \ .$$

Then the group τ_t on $\mathcal{O}_n$ is induced from the group $\Gamma(e^{it})(\cdot)\Gamma(e^{-it})$ on $\mathcal{O}_n^F$, where

$$\Gamma(e^{it}) = \bigoplus_{r=0}^{\infty} (\otimes^r e^{it}) = e^{iNt}$$

and N is the number operator. (In particular $N \geq 0$, so the ground state for $(\mathcal{O}_\infty, \tau)$ identifies with the Fock vacuum state.)

The algebras $\mathcal{O}_n$ have several interesting properties, e.g., although the weak closure of $\mathcal{O}_n$ is a hyperfinite von Neumann algebra in any representation ($\mathcal{O}_n$ is nuclear), $\mathcal{O}_n$ is not the inductive limit of an increasing sequence of type I C^*-algebras.

Example 5.3.27 is due to Olesen and Pedersen [Ole 5]. More refined examples will be described in the Notes and Remarks to Sections 5.3.2 and 5.3.3.

Sections 5.3.2 and 5.3.3

The simplex property of K_β and the coincidence of the central decomposition with the decomposition of KMS states emerged from studies of the set of KMS states by Araki, Hugenholtz, Lanford, Ruelle, and Takesaki in 1967–1970, [Ara 14], [Ara 15], [Lan 4], [Rue 5], [Tak 3]. The possible breakdown of Euclidean symmetry in the decomposition of KMS states has been discussed by

Emch, Knops, and Verboven [Emc 1]. Various invariance properties of the type given in Proposition 5.3.33 were initially derived by Sirugue and Winnink [Sir 2]. The absence of breakdown of symmetry in Theorem 5.3.33A was proved by Fannes, Vanheuverzwijn and Verbeure [Fan 4] and will be discussed further in the Notes and Remarks to Section 6.2.6.

Connes' cocycle theorem, Theorem 5.3.34, is a key result in the classification theory for von Neumann algebras and was proved in 1973 [Con 4]. The disjointness of KMS states at different temperatures, Theorem 5.3.35, was demonstrated by Takesaki in 1970 [Tak 5]. The type III property of the weak closure of a KMS representation of asymptotic abelian systems, Corollary 5.3.36, was shown by Araki and Størmer in 1972 [Ara 16], [Stø 5], and with a little more work they could show that the type III part occurring is actually type III_1.

Although Remark 2 after Theorem 5.3.32 has no later applications it is rather striking because it equates a physically natural algebraic-ergodic property, weak-asymptotic abelianness in mean for all $\omega \in K_\beta$, with a purely geometric property, the facial property of K_β. Equivalences of this type occurred in the decomposition theory described in Chapter 4, e.g., $E^G_{\mathfrak{A}}$ is a simplex if and only if $(\mathfrak{A}, \omega)$ is G-abelian for all $\omega \in E^G_{\mathfrak{A}}$, but these involved slightly more artificial ergodic assumptions, e.g., G-abelianness or G-centrality.

Parts of Theorem 5.3.37 and Corollary 5.3.40 can be recovered from Araki's 1964 paper [Ara 7]. The characterization (4) in Corollary 5.3.40 for separable C^*-algebras is due to Dang-Ngoc [Dan 2]. The idea of considering more general faces in $E^G_{\mathfrak{A}}$ than the set of ground states, as well as characterizations (5)–(7) in Theorem 5.3.38 are essentially due to Batty [Bat 1] [Bat 2] and he also proves the theorem without any topological restriction on the group G. If $\mathfrak{B}$ is a C^*-algebra, F is a closed face in $E_{\mathfrak{B}}$ and $\omega \in F$ he defines P^F_ω as the projection onto those vectors $\eta \in \mathfrak{H}_\omega$ such that

$$(\eta, \pi_\omega(\cdot)\eta) \in \mathbb{R}_+ F \ .$$

These vectors form a closed subspace in $\mathfrak{H}_\omega$ since F is a face. Using the facial property of F, it follows that $P^F_\omega \in \pi_\omega(\mathfrak{B})''$, and ω is said to be *F-abelian* if $P^F_\omega \pi_\omega(\mathfrak{B})'' P^F_\omega$ is abelian. The face F is said to be *abelian* if every state in F is F-abelian. The *F-multiplicity* of $\omega \in F$ is defined to be the dimension dim $(P^F_\omega \mathfrak{H}_\omega)$.

Batty [Bat 1], [Bat 2] proves that the following conditions are equivalent

1. F is abelian.
2. For each $\omega \in F, \pi_\omega(\mathfrak{B})'$ is abelian.
3. F is a simplex.
4. Every pure state in F has F-multiplicity 1.
5. Any factorial state in F is pure.
6. Any two distinct pure states in F are disjoint.
7. If ω_1, ω_2 are distinct pure states in F then the face generated by ω_1 and ω_2 in $E_{\mathfrak{B}}$ is equal to the convex set $\{\lambda\omega_1 + (1-\lambda)\omega_2;\ \lambda \in [0,1]\}$.

He proves this without any separability assumption whatsoever by invoking Pedersen's noncommutative integration theory [Ped 3] rather than the more pedestrian measure theory used in our proof of Theorem 5.3.38.

In order to prove Theorem 5.3.38 from the above theorem Batty relies upon a very useful observation due to Ed Effros and in more rudimentary form to Kastler and Robinson [Kas 1]. Let $\mathfrak{A}$ be a C^*-algebra with identity, G a discrete group and τ an action of G on $\mathfrak{A}$. Let $\mathfrak{A} \otimes_\tau G$ be the crossed product of $\mathfrak{A}$ by the action τ, Definition 2.7.2. Then $\mathfrak{A}$ and G are canonically embedded in $\mathfrak{A} \otimes_\tau G$. If $A \in \mathfrak{A}$ and $g \in G$ we use A, g also to denote the images of A, g in $\mathfrak{A} \otimes_\tau G$. Then there is a bijective correspondence between the state space of $\mathfrak{A} \otimes_\tau G$ and the set of all bounded functions $\Phi : G \mapsto \mathfrak{A}^*$ such that $\Phi(e)$ is a state and Φ is positive definite in the sense

$$\sum_{i,j=1}^{n} \Phi(g_i^{-1} g_j)(\tau_{g_i}^{-1}(A_i^* A_j)) \geq 0$$

for any $A_i \in \mathfrak{A}, g_i \in G$. The correspondence is given by $\rho \mapsto \Phi_\rho$, where

$$\Phi_\rho(g)(A) = \rho(Ag) \ .$$

The correspondence is a homeomorphism for the weak*-topology on $E_{\mathfrak{A} \otimes_\tau G}$ and the topology of pointwise weak*-convergence on the space of functions from G into $\mathfrak{A}^*$. In particular, if $\omega \in E_{\mathfrak{A}}^G$ the function $\Phi_\omega(g) = \omega$, for all $g \in G$, is positive definite. This establishes an affine homeomorphism between $E_{\mathfrak{A}}^G$ and the closed face $F_{\mathfrak{A}}^G$ of states ρ on $\mathfrak{A} \otimes_\tau G$ with the property

$$\rho(g_1 A g_2) = \rho(A)$$

for all g_1, $g_2 \in G, A \in \mathfrak{A}$. If ρ is such a state, and $\omega = \rho|_{\mathfrak{A}}$, then $\mathfrak{H}_\rho = \mathfrak{H}_\omega$, $\pi_\rho(A) = \pi_\omega(A)$ and $\pi_\rho(g) = U_\omega(g)$. Thus if F is a face in $E_{\mathfrak{A}}^G$ then its image F_0 in $F_{\mathfrak{A}}^G$ is a face in $F_{\mathfrak{A}}^G$, and hence in $E_{\mathfrak{A} \otimes_\tau G}$. One now shows for $\omega \in F$ that $P_\omega = P_\rho^{F_0}$ is exactly the projection onto the vectors $\eta \in E_\omega \mathfrak{H}_\omega$ such that $A \in \mathfrak{A} \mapsto (\eta, \pi_\omega(A)\eta)$ is contained in $\mathbb{R}_+ F$. If the statements of the previous theorem of Batty are translated into this new situation, we see that the following conditions are equivalent for each closed face $F \in E_{\mathfrak{A}}^G$:

1. $P_\omega \pi_\omega(\mathfrak{A})'' P_\omega$ is abelian for all $\omega \in F$.
2. $\{\pi_\omega(\mathfrak{A}) \cup U_\omega(G)\}'$ is abelian for all $\omega \in F$.
3. F is a simplex.
4. Each extremal state in F is weakly clustering in the sense that

$$\inf_{A' \in Co(\tau_G(A))} |\omega(A'B) - \omega(A)\omega(B)| = 0$$

   for all $A, B \in \mathfrak{A}$.
5. Any state $\omega \in F$ such that $\{\pi_\omega(\mathfrak{A}) \cup U_\omega(G)\}'$ is a factor is ergodic.
6. If ω_1 and ω_2 are distinct ergodic states in F then the covariant representations $(\mathfrak{H}_{\omega_1}, \pi_{\omega_1}, U_{\omega_1})$ and $(\mathfrak{H}_{\omega_2}, \pi_{\omega_2}, U_{\omega_2})$ are unitarily equivalent (as covariant representations).

7. If ω_1 and ω_2 are distinct ergodic states in F then the face generated by ω_1 and ω_2 in $E_{\mathfrak{A}}^G$ is equal to the convex set $\{\lambda\omega_1 + (1-\lambda)\omega_2;\ \lambda \in [0,1]\}$.

As $P_\omega \leq E_\omega$ Condition (1) of this theorem is weaker than Condition (1) of Theorem 5.3.38. The special condition on F in Theorem 5.3.38 immediately implies $P_\omega = E_\omega$. Since Condition (1) of the theorem is equivalent to $E_\omega \pi_\omega(\mathfrak{A})'' E_\omega$ being abelian, Proposition 4.3.7, this shows that Theorem 5.3.38 is also true for general groups G.

Batty also gives examples of C^*-dynamical systems based on simple C^*-algebras where the sets of ground states form n-dimensional simplices, $n = 1, 2....$

Let $(\mathfrak{A}, \tau)$ be a C^*-dynamical system and assume that $\mathfrak{A}$ has an identity. For each $\beta \in [-\infty, \infty]$, let K_β be the set of (τ, β)-KMS states of $(\mathfrak{A}, \tau)$. In particular $K_{+\infty}(K_{-\infty})$ is the set of ground (ceiling) states. Define $T(\mathfrak{A}, \tau) = \bigcup_{\beta \in [-\infty,\infty]} K_\beta$ with the topology inherited from the weak*-topology on $E_{\mathfrak{A}}$. Further endow this space with the fibre bundle structure as a bundle of compact convex sets defined by the map $\omega \mapsto \beta(\omega)$ where $\beta(\omega)$ is the β such that $\omega \in K_\beta$. In order for the latter map to be well defined we assume that $K_{\beta_1} \cap K_{\beta_2} = \emptyset$ for $\beta_1 \neq \beta_2$, i.e., that the one-parameter group defined by τ on $\mathfrak{A}/\mathfrak{J}$ for any τ-invariant closed two-sided ideal $\mathfrak{J} \subset \mathfrak{A}$ is nontrivial. The bundle $T(\mathfrak{A}, \tau)$ is called the *temperature state space* of $(\mathfrak{A}, \tau)$.

It follows from Proposition 5.3.25 that $T(\mathfrak{A}, \tau)$ is closed in $E_{\mathfrak{A}}$, and hence compact. By Theorem 5.3.30, each K_β is a simplex if $\beta \in \mathbb{R}$ and by Theorem 5.3.37 both $K_{+\infty}$ and $K_{-\infty}$ are faces in $E_{\mathfrak{A}}$. The explicit computation of the temperature state space of $(\mathfrak{A}, \tau)$ is in general a very hard task, as we will see in Chapter 6, but there are a few cases, apart from Example 5.3.37 where it can be achieved. In 1979, Bratteli, Elliott and Herman [Bra 14] proved that if F is an arbitrary closed subset of $[-\infty, \infty]$ then there exists a C^*-dynamical system $(\mathfrak{A}, \tau)$ such that $\mathfrak{A}$ is a simple C^*-algebra with identity and $(\mathfrak{A}, \tau)$ admits a (τ, β)-KMS state if and only if $\beta \in F$. The C^*-algebra $\mathfrak{A}$ was obtained as the crossed product of an AF-algebra by an automorphism with τ the dual action. (A C^*-algebra is said to be an *approximately finite dimensional C^*-algebra* or an AF-*algebra* if it contains an increasing sequence of finite-dimensional *-subalgebras with dense union. (Particular examples are the UHF-algebras of Example 2.6.12, [Bra 1]). The analysis in [Bra 14] was extended by Bratteli, Elliott and Kishimoto in 1980–83 [Bra 18], [Bra 19]. They proved that each metrizable simplex bundle $\mathbb{R} \in \beta \mapsto K_\beta$ can be realized as the finite β part of the temperature state space of a C^*-dynamical system $(\mathfrak{A}, \tau)$ where $\mathfrak{A}$ is simple, separable with identity and τ is periodic with period 2π. (The formal definition of a locally compact bundle of compact convex sets can be found in [Bra 19], page 210). This is even proved for the chemical potential-inverse temperature state space in [Bra 19]. The construction can be made such that $F_{\pm\infty}$ are isomorphic to the state spaces of two arbitrary simple AF-algebras $\mathfrak{A}^{\pm\infty}$ with identity. Furthermore, if $F_{\pm\infty}$ are arbitrary faces of the state spaces of $\mathfrak{A}^{\pm\infty}$ one can perturb the dynamics τ by an inner perturbation P, as in Proposition 5.4.1, to obtain a new C^*-dynamical system $(\mathfrak{A}, \tau^P)$ such that the finite β part of the

temperature state space is as before, but the set of $(\tau^P, \pm\infty)$-KMS states is affinely isomorphic to $F_{\pm\infty}$. The paper [Bra 18] concludes by showing that any metrizable simplex is affinely isomorphic to a face in the state space of a simple AF-algebra with identity. Hence $F_{\pm\infty}$ can be taken to be arbitrary metrizable simplices (but this certainly does not exhaust all possibilities for $F_{\pm\infty}$, see, for example, Corollary 5.3.40).

For quantum spin systems, as described in Chapter 6, there are a few specific systems where the temperature state space has been completely analyzed. In addition there are many partial results. These matters will be discussed in Sections 6.2.5–7 and the associated Notes and Remarks. In this case the simplices K_β are always nonempty, Proposition 6.2.15, and generically there is a critical inverse temperature β_c such that K_β consists of only one point for $|\beta| < \beta_c$, Proposition 6.2.45, and $\beta_c = +\infty$ for one-dimensional systems, Theorem 6.2.47. This feature is also shared by the only other non-trivial C^*-dynamical system $(\mathfrak{A}, \tau)$ for which $T(\mathfrak{A}, \tau)$ is known in detail. This example was analyzed by Bost and Connes in 1995, [Bos 1], [[Con 1]]. Their C^*-dynamical system is intimately connected with the statistical theory of the distribution of prime numbers. It is defined as follows: Let $\mathbb{Q}$ be the rational numbers and define

$$\Gamma = \left\{ \begin{pmatrix} 1 & b \\ 0 & a \end{pmatrix}; a, b \in \mathbb{Q},\ a > 0 \right\} .$$

Using the formulae

$$\begin{pmatrix} 1 & b \\ 0 & a \end{pmatrix}\begin{pmatrix} 1 & b' \\ 0 & a' \end{pmatrix} = \begin{pmatrix} 1 & ba' + b' \\ 0 & aa' \end{pmatrix} , \begin{pmatrix} 1 & b \\ 0 & a \end{pmatrix}^{-1} = \begin{pmatrix} 1 & -b/a \\ 0 & 1/a \end{pmatrix} ,$$

one checks that Γ is a group under matrix multiplication. Let $\Gamma_0 \simeq \mathbb{Z}$ be the subgroup

$$\Gamma_0 = \left\{ \begin{pmatrix} 1 & n \\ 0 & 1 \end{pmatrix}; n \in \mathbb{Z} \right\} .$$

It follows from the identity

$$\begin{pmatrix} 1 & n \\ 0 & 1 \end{pmatrix}\begin{pmatrix} 1 & b \\ 0 & a \end{pmatrix}\begin{pmatrix} 1 & \mathbb{Z} \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} 1 & na + b + \mathbb{Z} \\ 0 & a \end{pmatrix}$$

that the Γ_0-orbit through $\gamma\Gamma_0$, when Γ_0 acts on the left on Γ/Γ_0, contains exactly q points when $\gamma = \left(\begin{smallmatrix} 1 & b \\ 0 & a \end{smallmatrix}\right)$and $a = p/q$ with p, q mutually prime. Since all these orbits are finite, one may define the Hecke algebra $\mathfrak{H}(\Gamma, \Gamma_0)$ as the algebra of functions f on $\Gamma_0\backslash\Gamma/\Gamma_0$, with finite support, with product

$$(f * f')(\gamma) = \sum_{\gamma_1 \in \Gamma_0\backslash\Gamma} f(\gamma\gamma_1^{-1}) f'(\gamma_1) .$$

where $f, f' \in \mathfrak{H}(\Gamma, \Gamma_0)$ are viewed as Γ_0-biinvariant functions on Γ. The C^*-algebra $\mathfrak{A}$ is defined as the norm closure of $\mathfrak{H}(\Gamma, \Gamma_0)$ in the regular representation λ on $L^2(\Gamma_0\backslash\Gamma)$, defined by

$$(\lambda(f)\xi)(\gamma) = \sum_{\gamma_1 \in \Gamma_0 \backslash \Gamma} f(\gamma\gamma_1^{-1})\xi(\gamma_1) \ .$$

The algebra is closed under involution, since $\lambda(f)^* = \lambda(f^*)$ where $f^*(\gamma) = \overline{f(\gamma^{-1})}$. The automorphism group τ_t on $\mathfrak{A}$ is defined through its action on $\mathfrak{H}(\Gamma, \Gamma_0)$ by

$$\tau_t(f)(\gamma) = a^{it} f(\gamma)$$

if

$$\gamma = \begin{pmatrix} 1 & b \\ 0 & a \end{pmatrix} \ .$$

In fact τ is the modular automorphism group for the state on $\mathfrak{M} = \lambda(\mathfrak{H}(\Gamma, \Gamma_0))''$ given by the unit vector corresponding to the coset $\Gamma_0 \in \Gamma_0 \backslash \Gamma$, i.e., this state is a $(\tau, -1)$-KMS state.

There is a natural action σ of the group $W = \times_p(\mathbb{Z}/p\mathbb{Z})$ on $\mathfrak{A}$ commuting with τ, where p ranges over all prime numbers. For $0 < \beta \leq 1$ there is a unique (τ, β)-KMS state φ_β on $(\mathfrak{A}, \tau)$ which is a type III_1 factor state. Moreover, for $1 < \beta < \infty$ each extremal (τ, β)-KMS state is a type I factor state and if φ is any such extremal state then the map $W \ni g \mapsto \varphi \circ \sigma_g$ is a homeomorphism between W and the set of extremal (τ, β)-KMS states. All of these are computed explicitly in [Bos 1].

Corollary 5.3.41 is related to a famous theorem of Haag proved in 1955 [Haag 4] which gave an important impetus to the C^*-algebraic approach to quantum field theory. Let $\mathfrak{A}$ be the C^*-algebra generated by the time zero fields in a free, relativistic, irreducible quantum field theory (we refer to the monograph by Streater and Wightman [[Stre 1]] for definitions and a complete account of the theorem), and let τ_t^{free} be the free time evolution,

$$\tau_t^{\text{free}}(A) = e^{itH_0} A e^{-itH_0} \ ,$$

where H_0 is the free Hamiltonian and $A \in \mathfrak{A}$. Now, assume that there exists another relativistic field theory on the same Hilbert space with the same time-zero fields and time evolution τ_t^{int}. Moreover, assume that for each $t \in \mathbb{R}$ there exists a unitary operator $V(t)$ such that

$$\tau_t^{\text{int}}(A) = V(t)\tau_t^{\text{free}}(A)V(t)^*$$

for all $A \in \mathfrak{A}$. Haag's theorem then states that the new theory is unitary equivalent with the free theory. The operators $V(t)$ played a large role in the early attempts of constructing interacting quantum fields in the so-called interaction picture, but Haag's theorem implied that the interaction picture only exists when there is no interaction. A program of circumventing these difficulties by using automorphisms of C^*-algebras instead of unitary operators on Hilbert space was proposed by Guenin in 1966 [Gue 1] and this program was followed in the early days of constructive quantum field theory. Around 1972 these methods were replaced by the more powerful probabilistic methods of Euclidean quantum field theory (see Notes and Remarks to Chapter 6).

Modular theory and the theory of KMS states have entered into quantum field theory for various reasons some of which are discussed in Chapter 5 of the book by Haag [[Haa 1]]. First, the relativistic vacuum is separating for the W*-algebras of observables corresponding to space-time regions whose causal complement contains a non-empty open set. Hence the field theory has a modular structure. Bisognano and Wichmann [Bis 1]. [Bis 2] established an unexpected identification between the modular automorphisms for wedge-shaped regions and the Lorentz boosts in the relativistic symmetry group. The wedge-shaped regions provide the simplest examples of horizons (see Rindler [Rin 1]) and the Bisognano-Wichmann result has an interesting interpretation in terms of the Hawking temperature of the corresponding black hole (see [[Haa 1]] page 248). In general wedge-shaped regions are the only ones for which the modular automorphisms correspond to point transformations in Minkowski space. Hislop and Longo [His 1] have, however, extended this identification to other regions for theories with a conformal invariance. Secondly, Jaffe, Lesniewski, Osterwalder and Wisniowski [Jaf 1] [Jaf 2] have introduced a super-KMS condition in the context of Connes' theory of entire cyclic cohomology of quantum algebras [[Con 1]]. This concept allows one to deal with situations such as supersymmetric field theory on noncompact manifolds for which the Hamiltonian has continuous spectrum. It relies on the existence of a super-derivation whose square is the generator of a one-parameter semigroup on the quantum algebra. The analytic properties of this super-derivation were discussed further by Kishimoto and Nakamura [Kis 6]. This super-KMS condition was partially inspired by work of Kastler [Kas 4]. Thirdly, Bros and Buchholz [Bro 1] [Bro 2] have suggested a relativistic formulation of the KMS condition for thermal equilibrium in which the group of time translations is replaced by the group of space-time symmetries. This suggestion is based on the observation that the relativistic correlation functions have stronger analyticity properties than those characteristic of the usual KMS condition.

Theorem 5.3.43 was proved by Kishimoto [Kis 4] and he also generalized the Borchers-Arveson theorem, Theorem 3.2.46.

For classical systems the KMS condition is not an appropriate condition of equilibrium because it forces the dynamics to be trivial. An alternative characterization was proposed by Katz [Kat 1] and has the form

$$\omega(\{f,g\}) = \beta\omega(g\{f,H\}) \ .$$

Here β is the inverse temperature, H is the Hamiltonian, and $\{,\}$ is the Poisson bracket:

$$\{f,g\} = \sum_i \left(\frac{\partial f}{\partial q_i}\frac{\partial g}{\partial p_i} - \frac{\partial f}{\partial p_i}\frac{\partial g}{\partial q_i} \right) \ .$$

This condition has been studied by several authors and the equivalence between states satisfying this condition and canonical Gibbs states has, for example, been established in [Aiz 1].

Section 5.4.1

The perturbation expansion for $\Gamma_t^P = U_t^P U_{-t}$ in Proposition 5.4.1 and Corollary 5.4.2 goes back at least to work in the late forties by Tomonaga [Tomo 1], Schwinger [Schw 1], Feynman [Fey 1], and Dyson [Dys 1], (see also [Ara 19]), while the direct expansion of τ_t^P was defined by Robinson in 1973 [Rob 8]. The existence of a normal τ^P-KMS state ω^P for the perturbed dynamics τ^P, and the expansion for the corresponding vector Ω^P in Theorem 5.4.4 is due to Araki in 1973 [Ara 20] (see also [Ara 21]), while the expansion of ω^P in terms of the truncated functions of ω in the same theorem was derived by Bratteli, Kishimoto, and Robinson in 1978 [Bra 13]. Note that Theorem 5.4.4 is a partial converse of Connes' cocycle theorem, Theorem 5.3.34, and the investigation of ω^P was partially inspired by Connes 1973 paper [Con 4].The notions of perturbed state and perturbed dynamics were extended to some unbounded relative Hamiltonians by Donald [Don 1] [Don 2] using completely different methods from those of Araki.

The time-dependent approach to stability was initiated by Robinson in 1973, [Rob 8], and Definition 5.4.8, Example 5.4.9, and Proposition 5.4.10 come from this paper.

The morphisms $\gamma_\pm$ are not always automorphisms under the assumptions of Proposition 5.4.10. This problem has been discussed by Golodets [Gol 1] and Maassen [Maa1]. Proposition 5.4.13 and most of the remaining results in this section were proved in [Bra 13].

Example 5.4.11 is basically the second quantization of quantum-mechanical scattering theory with a rank-one projection as perturbation, i.e., interaction. The abstract theory of this problem is described fully in Kato's book on perturbation theory [[Kat 1]] and in particular the Møller matrices are proved to be unitary. This latter result was crucial in the Birman-Kato proofs of unitarity of the S-matrix for physically more relevant scattering problems.The explicit form of the kernels of the Møller matrices can be found in a variety of places, for example, in Newton's book on scattering theory [New 1].

The equivalence of normality and finite density for quasi-free states which is used in Example 5.4.15 has already been discussed in the Notes and Remarks to Sections 5.2.1–5.2.3. It is a special case of the criterion for quasi-equivalence of representations generated by two quasi-free states.

Section 5.4.2

The original idea of deriving the KMS condition from conditions of stability and purity of a state appeared in a paper by Haag, Kastler, and Trych-Pohlmeyer in 1974 [Haag 7]. This paper assumed L^1-clustering of the truncated n-point functions for $n = 2, 3, \cdots, 6$. By exploiting the additivity of the joint spectrum of the Hamiltonian and the modular operator, Bratteli and Kastler were subsequently able to replace 6 by 4 [Bra 12]. However, both these papers

had a gap in the proof (Observation 3 of Theorem 5.4.19 was not explicitly proved). This gap was finally filled by Hoekman [Hoe 1]. The proof of Theorem 5.4.19 is based on these three papers.

In 1977, Haag and Trych-Pohlmeyer [Haag 8] suggested that one could replace the L^1-clustering assumption of the truncated n-point functions up to $n = 4$ by simple three-point clustering.

$$\lim_{\inf_{i \neq j} |t_i - t_j| \to \infty} \omega(\tau_{t_1}(A_1)\tau_{t_2}(A_2)\tau_{t_3}(A_3)) = \omega(A_1)\omega(A_2)\omega(A_3)$$

or alternatively by the assumption that ω is a factor state, in the presence of an $L^1(\mathfrak{A}_0)$-asymptotic abelianness, and they proved Observation 1 of Theorem 5.4.20 under these assumptions. The proof of the theorem itself was however incomplete. The final version of Theorem 5.4.20 was proved by Bratteli, Kishimoto, and Robinson [Bra 13]. The stability condition (2b) of Corollary 5.4.21 was also suggested by these latter authors, while the stability condition.

$$\lim_{\lambda \to 0} \|\omega_{\pm}^{\lambda P} - \omega\| = 0$$

in the subsequent remarks was proposed by Haag and Trych-Pohlmeyer [Haag 8]. The final remark of this section is due to Kastler [Kas 2].

Section 5.4.3

The theory of the chemical potential presented in this section was developed in 1975–1976 by Araki and Kishimoto [Ara 17], and Araki, Haag, Kastler, and Takesaki [Ara 18]. We benefited greatly from the lecture notes by Kastler in preparing this section [Kas 3].

Section 5.4.4

This section is based entirely on material from the 1977 paper by Pusz and Woronowicz [Pus 1].

Models of Quantum Statistical Mechanics

6.1. Introduction

In the previous chapter we examined various applications of the formalism of *-algebras to quantum statistical mechanics. These applications principally concerned equilibrium properties of macroscopic systems and fell into one of two categories. First, we analyzed thermodynamic limit phenomena of specific particle models by use of the Gibbs ansatz for the equilibrium states. Second, we examined the structure of a set of states, the KMS states, which appeared appropriate for the description of equilibrium. The first of these approaches was developed for the ideal quantum gases in Sections 5.1 and 5.2, while the second was contained in Sections 5.3 and 5.4. It should be reemphasized that the thermodynamic limits of the Gibbs equilibrium states of the ideal Fermi gas are exactly the KMS states of the C^*-system formed by the CAR algebra and the corresponding free evolution. For the Bose gas, however, the situation is more complex because the free evolution τ is not a strongly continuous group of *-automorphisms of the CCR algebra $\mathfrak{A}$ and hence $(\mathfrak{A}, \tau)$ does not form a C^*-system. Thus, it is not evident that one can use a global C^*-structure to characterize the set of equilibrium states. Nevertheless, the Gibbs equilibrium states ω are faithful states of the CCR algebra $\mathfrak{A}$, the free evolution τ has extensions $\hat{\tau}$ to the corresponding von Neumann algebras $\pi_\omega(\mathfrak{A})''$, and the $(\pi_\omega(\mathfrak{A})'', \hat{\tau})$ form W^*-dynamical systems for which ω is $\hat{\tau}$-KMS. Thus, the modular or KMS structure is still a characteristic of the equilibrium states but it is manifested state by state without the synthesizing C^*-dynamical system.

The aim of this chapter is to extend these investigations by examination of a larger class of models. In the latter half of the chapter we analyze point particles interacting at a distance but before this we describe a simpler, but more artificial, type of model, quantum spin systems. Spin systems were first introduced in the discussion of magnetic properties of crystalline substances but have subsequently been reinterpreted as models of liquids and gases with restraints on the movements of the constituent particles. There are two advantages in examining spin systems. First, there is a certain understanding of the collective effects occurring in these models which lead to phase transitions and, second there is a fairly well-developed analysis of the KMS structure, at the C^*-level, of these models. The results for continuous systems are much more modest, however, and even the collective phenomena are barely understood.

Basically there are two directions for analysis, the existence and properties of the dynamical evolution, and the properties and structure of the equilibrium

states. For most quantum spin systems the evolution can be handled independently of the equilibrium structure but for more general models, including continuous systems, this is not the case. There is virtually nothing known about the evolutions of continuous systems of interacting particles except in, or close to, equilibrium and even in the equilibrium situation knowledge is scant.

6.2. Quantum Spin Systems

6.2.1. Kinematical and Dynamical Descriptions

Basically a quantum spin system consists of a set of particles confined to a lattice and interacting at a distance. There are, however, two possible physical interpretations of these models, either as a *lattice gas* or as a *spin system*. The first views each point of the lattice as a possible site for a finite number N of particles, i.e., each point of the configuration space can be either empty or occupied by $1, 2, \ldots, N$ particles. These particles then interact with one another and this leads to an evolution in which one envisages the particles jumping from lattice site to lattice site. The second interpretation assumes that every lattice site is permanently occupied by a particle but the particles have various internal degrees of freedom, e.g., the particles could have an intrinsic spin with several possible orientations. The interaction between the particles then follows from a coupling of the internal degrees of freedom and this yields, for example, an evolution in which the spin orientations are constantly changing.

In some applications of these models it is important that the lattice L has a symmetry. For example one commonly examines the case $L = \mathbb{Z}^\nu$, i.e., the lattice is a ν-dimensional cubic array, and then the configuration space of the model is invariant under the group of lattice translations. More complex symmetries are also possible.

Invariance properties of this type reflect the traditional view of crystals as objects with a regular spatial order. There are, however, other crystalline structures, quasicrystals, which appear to lack a precise spatial symmetry. Experimentally quasicrystals are characterized by a discrete diffraction spectrum which is incompatible with any translation symmetry. The determination of the quasicrystal structure from the diffraction data is, however, extremely difficult if not impossible. One possible model of quasicrystals is by a lattice associated with an aperiodic tiling of the configuration space $\mathbb{R}^\nu$ but there appears to be no compelling evidence for any particular aperiodicity. Lattices constructed from aperiodic tilings have a homogeneous structure, but no complete spatial symmetry, and homogeneity rather than symmetry should be the essential feature for any model of a crystal. In the sequel we will see that for some properties such as the construction of dynamics it suffices to assume that the lattice L is a countable set of points. We assume throughout that L is both countable and infinite. For many results some homogeneity is required

and we usually assume symmetry and specialize to the simplest case, $L = \mathbb{Z}^\nu$ although other symmetries or weaker homogeneity properties would often suffice.

The kinematic structure associated with a quantum spin system has already been described in Chapters 2 and 3. It consists of a quasi-local UHF algebra constructed over the finite subsets of L. (See Examples 2.6.12 and 3.2.25.) Explicitly, one first orders the set of finite subsets of L by inclusion. Next, one associates with each point $x \in L$ an $(N+1)$-dimensional Hilbert space $\mathfrak{H}_{\{x\}}$ and with each finite subset $\Lambda \subset L$ the tensor product space

$$\mathfrak{H}_\Lambda = \bigotimes_{x \in \Lambda} \mathfrak{H}_{\{x\}} \ .$$

The local C^*-algebra $\mathfrak{A}_\Lambda$ is then defined by $\mathfrak{A}_\Lambda = \mathscr{L}(\mathfrak{H}_\Lambda)$. If $\Lambda_1 \cap \Lambda_2 = \varnothing$, then $\mathfrak{H}_{\Lambda_1 \cup \Lambda_2} = \mathfrak{H}_{\Lambda_1} \otimes \mathfrak{H}_{\Lambda_2}$ and $\mathfrak{A}_{\Lambda_1}$ is isomorphic to the C^*-subalgebra $\mathfrak{A}_{\Lambda_1} \otimes \mathbb{1}_{\Lambda_2}$ of $\mathfrak{A}_{\Lambda_1 \cup \Lambda_2}$, where $\mathbb{1}_{\Lambda_2}$ denotes the identity operator on $\mathfrak{H}_{\Lambda_2}$. Identifying $\mathfrak{A}_{\Lambda_1}$ and $\mathfrak{A}_{\Lambda_1} \otimes \mathbb{1}_{\Lambda_2}$ one concludes that the algebras $\{\mathfrak{A}_\Lambda\}_{\Lambda \subset L}$ form an increasing family of matrix algebras whose union is a normed *-algebra, which is incomplete because L is infinite. The norm completion $\mathfrak{A}$ of this union is a quasi-local C^*-algebra when equipped with the net of C^*-subalgebras $\mathfrak{A}_\Lambda$ (the orthogonality relation $\perp$ between the Λ is defined by $\Lambda_1 \perp \Lambda_2$ if $\Lambda_1 \cap \Lambda_2 = \varnothing$).

The local algebras $\mathfrak{A}_\Lambda$ represent the physical observables associated with the particles at the points of Λ and the algebra $\mathfrak{A}$ corresponds to the observables of the complete spin system. The quasi-local structure of $\mathfrak{A}$, $\bigcup_\Lambda \mathfrak{A}_\Lambda$, is summarized by the following;

(1) $$\mathfrak{A}_{\Lambda_1} \subseteq \mathfrak{A}_{\Lambda_2} \quad \text{if } \Lambda_1 \subseteq \Lambda_2 \ ,$$

(2) $$\mathfrak{A} = \overline{\bigcup_{\Lambda \subset L} \mathfrak{A}_\Lambda} \ ,$$

where the bar denotes uniform closure,

(3) $\mathfrak{A}$ and each $\mathfrak{A}_\Lambda$ have a common identity $\mathbb{1}$,

(4) $$[\mathfrak{A}_{\Lambda_1}, \mathfrak{A}_{\Lambda_2}] = 0$$

whenever $\Lambda_1 \cap \Lambda_2 = \varnothing$,

(5) $\mathfrak{A}$ is simple.

The first four properties follow by construction and the fifth follows from Corollary 2.6.19. The first property reflects the isotony of observables and the fourth the quantum-mechanical independence of observables associated with disjoint subsystems.

If $L = \mathbb{Z}^\nu$, then the group $\mathbb{Z}^\nu$ has an action τ as *-automorphisms of $\mathfrak{A}$. This action was constructed in Example 4.3.26. Referring to this construction one finds that the translations τ have the properties

(6) (a) if $A \in \mathfrak{A}_\Lambda$, then $\tau_x(A) \in \mathfrak{A}_{\Lambda+x}$,

(b) $$\lim_{|x| \to \infty} \|[A, \tau_x(B)]\| = 0$$

for all $A, B \in \mathfrak{A}$.

The asymptotic abelianness follows from conditions (2), (4), and (6a), and ensures that the theory of ergodic states described in Chapter 4 is applicable to the group $\mathbb{Z}^\nu$ of lattice translations. Physically the group τ corresponds to translations in the configuration space and the asymptotic abelianness demonstrates that any pair of observations becomes independent when performed sufficiently far apart.

Classical-mechanical spin systems can be described in a similar algebraic fashion. One associates with each $x \in L$ a maximal abelian C^*-subalgebra $\mathfrak{C}_{\{x\}} \subset \mathscr{L}(\mathfrak{H}_{\{x\}})$ and defines the local algebra $\mathfrak{C}_\Lambda$ by

$$\mathfrak{C}_\Lambda = \bigotimes_{x \in \Lambda} \mathfrak{C}_{\{x\}}$$

for each $\Lambda \subset L$. The global C^*-algebra $\mathfrak{C}$ is introduced by

$$\mathfrak{C} = \overline{\bigcup_{\Lambda \subset L} \mathfrak{C}_\Lambda} \ .$$

If $L = \mathbb{Z}^\nu$, the $\mathfrak{C}_{\{x\}}$ are chosen such that the group τ of space translations leaves $\mathfrak{C}$ invariant, i.e., one takes

$$\mathfrak{C}_{\{x+y\}} = \tau_y \mathfrak{C}_{\{x\}}$$

for all $x, y \in \mathbb{Z}^\nu$.

EXAMPLE 6.2.1. Assume $N = 1$, then each $\mathfrak{H}_{\{x\}}$ is two dimensional, $\mathfrak{A}_{\{x\}}$ is an algebra of 2×2 matrices and each such matrix can be decomposed as a sum of multiples of the Pauli matrices $\sigma_0^x (= \mathbb{1}), \sigma_1^x, \sigma_2^x, \sigma_3^x$ defined in Example 4.2.7. Thus if $|\Lambda|$ denotes the number of points in Λ, then $\mathfrak{A}_\Lambda$ is a full algebra of $2^{|\Lambda|} \times 2^{|\Lambda|}$-matrices corresponding to polynomials in the Pauli matrices $\{\sigma_i^x; i = 0, 1, 2, 3, x \in \Lambda\}$. A general element of the quasi-local algebra $\mathfrak{A}$ is a function of the σ_i^x which can be constructed as the uniform limits of polynomials. If $L = \mathbb{Z}^\nu$, one has $\tau_x(\sigma_i^y) = \sigma_i^{x+y}$, etc. In this latter case the classical algebra is *-isomorphic to the C^*-subalgebra $\mathfrak{C} \subset \mathfrak{A}$ generated by the third-component Pauli matrices $\{\sigma_3^x; x \in L\}$.

This model is often referred to as a spin-$\frac{1}{2}$ system because a quantum-mechanical spin-$\frac{1}{2}$ particle has exactly two degrees of freedom. The general case corresponds to spin-$N/2$ because spin-$N/2$ particles have $2(N/2) + 1 = N + 1$ degrees of freedom.

The foregoing structure defines the kinematics of the quantum spin systems, i.e., the instantaneous observables. We next consider the dynamics and for this purpose it is necessary to introduce interactions. An *interaction* Φ is defined as a function from the finite subsets $X \subset L$ into the hermitian elements of $\mathfrak{A}$ such that $\Phi(X) \in \mathfrak{A}_X$. Each $\Phi(X)$ represents the energy of interaction of the set of all particles in the finite subset X. Now in the spin system the particles are considered to be fixed at the lattice sites and hence the total energy of interaction in a subset Λ consists of the interaction energy of all subsystems. This total energy is defined to be the *Hamiltonian* $H_\Phi(\Lambda)$ *associated with* Λ. Explicitly

$$H_\Phi(\Lambda) = \sum_{X \subseteq \Lambda} \Phi(X) \ .$$

Clearly, $H_\Phi(\Lambda)$ is a hermitian element of $\mathfrak{A}_\Lambda$.

An interaction Φ is said to be of finite range if the only non-zero contribution to the energy arises from finite clusters of neighboring particles. In order to make this precise one must assume that the lattice has some rudimentary form of homogeneity or symmetry. If, for example, L is equipped with a metric $d(\cdot;\cdot)$ then we define L to be homogeneous if the metric has the following two properties. First, $d(x;y) \geq 1$ for all $x, y \in L$. Second, for each $r \geq 1$ there are at most a finite number N_r of points y with $d(x;y) \leq r$ uniformly for $x \in L$. The interaction Φ is then defined to have finite range if there exists a $d_\Phi \geq 1$ such that $\Phi(X) = 0$ whenever $D(X) = \sup_{x,y \in X} d(x;y) > d_\Phi$. The minimum possible value of d_Φ is called the *range* of Φ and there is no mutual interaction between particles whose separation is greater than this range. Lattices that are homogeneous include $\mathbb{Z}^\nu$, equipped with the usual metric, or more complicated periodic sublattices of $\mathbb{R}^\nu$, and the lattices associated with aperiodic tilings of $\mathbb{R}^\nu$.

If $L = \mathbb{Z}^\nu$, or some other subgroup of $\mathbb{R}^\nu$, one can also consider *translationally invariant interactions*. These are the Φ satisfying the additional requirements

$$\Phi(X + x) = \tau_x \Phi(X)$$

for all $X \subset \mathbb{Z}^\nu$ and $x \in \mathbb{Z}^\nu$.

If $\mathfrak{C} \subset \mathfrak{A}$ is the abelian algebra describing a classical spin system and $\Phi(X) \in \mathfrak{C}_X \subset \mathfrak{A}_X$ for all $X \subset L$, then Φ is called a *classical interaction*.

The set of interactions of a quantum spin system forms a real vector space when equipped with the obvious linear structure $(\Phi_1 + \Phi_2)(X) = \Phi_1(X) + \Phi_2(X)$ and $(\lambda\Phi)(X) = \lambda\Phi(X)$. Moreover, the finite-range interactions form a real vector subspace. Subsequently, it will be convenient to consider certain real Banach subspaces of interactions. For example, if $X \subset L \mapsto \xi(X) \geq 0$ is a family of positive functions, one can specify a norm by

$$\|\Phi\|_\xi = \sup_{x \in L} \sum_{X \ni x} \|\Phi(X)\| \xi(X)$$

and then introduce a Banach space B_ξ of interactions by

$$B_\xi = \{\Phi; \|\Phi\|_\xi < +\infty\} \ .$$

This method, and variations of it, will often be used in the sequel. The $\xi(X)$ will always be taken as a simple functions of the number of points $|X|$ in X and the diameter $D(X)$ of X if $L = \mathbb{Z}^\nu$. The conditions $\|\Phi\|_\xi < +\infty$ often have a physical interpretation. For example, if $\xi(X) = 1$ and one defines

$$E_\Phi(x) = \sum_{X \ni x} \Phi(X) \ .$$

it follows that $E_\Phi(x) \in \mathfrak{A}$ and $\|E_\Phi(x)\| \leq \|\Phi\|_\xi$. But $E_\Phi(x)$ corresponds to the energy of interaction of particles at the point $x \in L$ with their surroundings. Thus this choice of ξ corresponds to a restriction of finite energy per particle.

Note that if one considers only translationally invariant interactions, then each of the Banach spaces B_ξ contains the subspace of finite-range interactions. This follows because.

$$\sup_{x \in \mathbb{Z}^\nu} \sum_{X \ni x} \|\Phi(X)\| \xi(X) = \sum_{X \ni 0} \|\Phi(X)\| \xi(X)$$

and the right-hand side is a finite sum, and hence bounded.

EXAMPLE 6.2.2. Let $L = \mathbb{Z}^\nu$ and consider the spin-$\frac{1}{2}$ system described in Example 6.2.1. The simplest interesting interaction is a one-body and two-body translationally invariant interaction, i.e., $\Phi(\{x\}) = \tau_x \Phi(\{0\})$, $\Phi(\{x, y\}) = \tau_x \Phi(\{0, y - x\})$ and $\Phi(X) = 0$ if $|X| > 2$. One such choice is determined by

$$\Phi(\{0\}) = h\sigma_3^0 \ ,$$

$$\Phi(\{0,x\}) = \sum_{i=1}^{3} j_i(x) \sigma_i^0 \sigma_i^x \ ,$$

where $h \in \mathbb{R}$ and the j_i are real functions over $\mathbb{Z}^\nu$. This model is usually referred to as the *anisotropic Heisenberg model* if the $j_i \neq 0$ and $j_i \neq j_j$ for some pair i, j; the *isotropic Heisenberg model* if $j_1 = j_2 = j_3 \neq 0$; the *X–Y model* if $j_i \neq 0, i = 1, 2$ but $j_3 = 0$; the *Ising model* if $j_1 = j_2 = 0$. In each case the energy of the system confined to Λ consists of two parts

$$\sum_{x \in \Lambda} h\sigma_3^x, \qquad \sum_{x, y \in \Lambda} \sum_{i=1}^{3} j_i(x - y) \sigma_i^x \sigma_i^y \ .$$

The first contribution corresponds to the interaction of the spin-$\frac{1}{2}$ particles with an external electromagnetic field of strength h at x and the second corresponds to an interaction, at a distance, of particles x and y.

The dynamical evolution of any system can be defined in terms of the evolution of the associated observables. For a finite spin system confined to $\Lambda \subset L$, with interaction Φ and Hamiltonian $H_\Phi(\Lambda)$, this evolution is given by the Heisenberg relations $A \in \mathfrak{A}_\Lambda \mapsto \tau_t^\Lambda(A) \in \mathfrak{A}_\Lambda$, where

$$\tau_t^\Lambda(A) = e^{itH_\Phi(\Lambda)} A e^{-itH_\Phi(\Lambda)} \ ,$$

i.e., $t \in \mathbb{R} \mapsto \tau_t^\Lambda$ is a one-parameter group of *-automorphisms of the matrix algebra $\mathfrak{A}_\Lambda$. We now want to analyze this evolution for various classes of interactions and for systems which consist of a large number of particles. The standard method of approach to this type of problem is by asymptotic expansion in terms of inverse powers of the total number of particles. The first term of such an expansion corresponds to the approximation that the system has an infinite number of particles and this approximation then coincides with the thermodynamic limit discussed in Chapter 1 and applied to the ideal gases in Chapter 5. Thus, computation of the time evolution of a fixed observable $A \in \mathfrak{A}_{\Lambda_0}$ consists of calculating limits

$$\tau_t(A) = \lim_{\Lambda \to \infty} \tau_t^\Lambda(A)$$

of the evolutes $\tau_t^\Lambda(A)$ as the system grows indefinitely in size. We adopt for simplicity the convention that $\Lambda \to \infty$ indicates Λ eventually contains any finite subset of L.

There are various possible senses in which the limits $\tau_t(A)$ might exist and these govern some of the basic properties of the evolutions τ, e.g., the continuity of the map $t \mapsto \tau_t(A)$. For many classes of interactions the limits actually exist in the norm sense for all $A \in \mathfrak{A}_{\Lambda_0}$ and all $\Lambda_0 \subset L$. Therefore, the evolution τ extends by continuity to a strongly continuous one-parameter group of *-automorphisms of the quasi-local algebra

$$\mathfrak{A} = \overline{\bigcup_{\Lambda \subset L} \mathfrak{A}_\Lambda}$$

and $(\mathfrak{A}, \tau)$ forms a C^*-dynamical system. For more general interactions the limits only exist in certain representations and the evolution determines a W^*-system. Our immediate purpose is to describe the C^*-results.

There are several methods of proving the existence of the norm limits of the evolutes $\tau_t^\Lambda(A)$. Each method applies to a slightly different class of interactions and emphasizes a different physical feature of the interaction. All known methods are either implicitly, or explicitly, dependent upon the equations of motion

$$\frac{d\tau_t^\Lambda}{dt}(A) = \delta_\Lambda(\tau_t^\Lambda(A))$$

of $\tau_t^\Lambda(A)$. Here δ_Λ denotes the bounded derivation defined by

$$\delta_\Lambda(A) = i[H_\Phi(\Lambda), A], \quad A \in \mathfrak{A} \ .$$

First we examine convergence of the τ^Λ via convergence of the infinitesimal generators δ_Λ. For this one needs the following version of Proposition 3.2.52.

Proposition 6.2.3. *Let Φ be an interaction of a quantum spin system satisfying*

$$p_\Phi(x) = \sum_{X \ni x} \|\Phi(X)\| < +\infty$$

for all $x \in L$.

It follows that there exists a derivation δ of the quantum spin algebra $\mathfrak{A}$ such that

$$D(\delta) = \bigcup_{\Lambda \subset L} \mathfrak{A}_\Lambda$$

and for $A \in \mathfrak{A}_\Lambda$

$$\delta(A) = i \sum_{X \cap \Lambda \neq \varnothing} [\Phi(X), A].$$

The derivation δ is norm-closable and its closure $\bar{\delta}$ is the infinitesimal generator of a strongly continuous one-parameter group of *-automorphisms τ of $\mathfrak{A}$ if, and only if, one of the following conditions is satisfied:

either

$$\bar{\delta} \text{ possesses a dense set of analytic elements}$$

or

$$(\imath + \alpha\bar{\delta})(D(\bar{\delta})) = \mathfrak{A}, \quad \alpha \in \mathbb{R}\backslash\{0\} \ .$$

Finally if $\bar{\delta}$ generates the group τ and if

$$\tau_t^\Lambda(A) = e^{it H_\Phi(\Lambda)} A e^{-it H_\Phi(\Lambda)} \ ,$$

$$\lim_{\Lambda \to \infty} \|\tau_t(A) - \tau_t^\Lambda(A)\| = 0$$

for all $A \in \mathfrak{A}$, uniformly for t in compacts.

PROOF. First for $A \in \mathfrak{A}_\Lambda$

$$\left\| i \sum_{X \cap \Lambda \neq \varnothing} [\Phi(X), A] \right\| \leq \sum_{x \in \Lambda} \sum_{X \ni x} \|[\Phi(X), A]\| \leq 2\,|\Lambda| \|A\| \sup_{x \in \Lambda} p_\Phi(x) < +\infty$$

and hence δ is a norm densely defined derivation. But δ satisfies the hypothesis of Proposition 3.2.22 and thus $\pm\delta$ are dissipative. Consequently, δ is norm-closable by Lemma 3.1.14 and

$$\|(\imath + \alpha\bar{\delta})(A)\| \geq \|A\|$$

for all $\alpha \in \mathbb{R}$, and $A \in D(\delta)$, by Lemma 3.1.15. The criteria for $\bar{\delta}$ to be a generator follow directly from Theorem 3.2.50.

Finally, if δ_Λ is the bounded derivation defined by

$$\delta_\Lambda(A) = i[H_\Phi(\Lambda), A]$$

for all $A \in \mathfrak{A}$, then

$$\lim_{\Lambda \to \infty} \|\delta_\Lambda(A) - \bar{\delta}(A)\| = 0$$

for all $A \in D(\delta)$. Thus

$$\lim_{\Lambda \to \infty} \|\tau_t(A) - e^{t\delta_\Lambda}(A)\| = 0$$

for all $A \in \mathfrak{A}$, uniformly for t in compacts, by Theorem 3.1.28.

Remark. Proposition 6.2.3 has a converse, i.e., any derivation δ of the quantum spin algebra $\mathfrak{A}$ with $D(\delta) = \bigcup_{\Lambda \subset L} \mathfrak{A}_\Lambda$ can be obtained from an interaction Φ. To see this first note that the last remark in Example 3.2.25 implies that for all finite sets $\Lambda \subset L$, there exists an $\tilde{H}(\Lambda) = \tilde{H}(\Lambda)^* \in \mathfrak{A}$ such that

$$\delta(A) = i\,[\tilde{H}(\Lambda), A] \qquad (*)$$

for all $A \in \mathfrak{A}_\Lambda$. Moreover, $\tilde{H}(\Lambda)$ is determined by δ up to addition by elements in $\mathfrak{A}'_\Lambda \cap \mathfrak{A} = \mathfrak{A}_{\Lambda^c}$. Here Λ^c denotes the complement of Λ and

$$\mathfrak{A}_{\Lambda^c} = \overline{\bigcup_{\Lambda' \subset \Lambda^c} \mathfrak{A}_{\Lambda'}} \ .$$

To normalize $\tilde{H}(\Lambda)$ we define a projection E_Λ of norm one from $\mathfrak{A}$ onto $\mathfrak{A}_\Lambda$ for any (finite or infinite) region Λ as follows. Write $\mathfrak{A} = \mathfrak{A}_\Lambda \otimes \mathfrak{A}_{\Lambda^c}$, and let τ be the unique normalized trace on the UHF algebra $\mathfrak{A}_{\Lambda^c}$. Then E_Λ is defined by

$$E_\Lambda\Big(\sum_i A_i \otimes B_i\Big) = \sum_i \tau(B_i)A_i$$

for $A_i \in \mathfrak{A}_\Lambda$ and $B_i \in \mathfrak{A}_{\Lambda^c}$.

By replacing $\tilde{H}(\Lambda)$ by $\tilde{H}(\Lambda) - E_{\Lambda^c}(\tilde{H}(\Lambda))$ we may choose an $\tilde{H}(\Lambda)$ satisfying $(*)$ and

$$E_{\Lambda^c}(\tilde{H}(\Lambda)) = 0 \ , \tag{$**$}$$

and conditions $(*)$ and $(**)$ determine $\tilde{H}(\Lambda)$ uniquely.

Now, define

$$H(\Lambda) = E_\Lambda(\tilde{H}(\Lambda)), \quad W(\Lambda) = \tilde{H}(\Lambda) - H(\Lambda)$$

and define inductively

$$\Phi(\varnothing) = 0, \quad \Phi(\Lambda) = H(\Lambda) - \sum_{X \subsetneq \Lambda} \Phi(X) \ .$$

Then one has

$$H(\Lambda) = \sum_{X \subseteq \Lambda} \Phi(X), \quad \tilde{H}(\Lambda) = H(\Lambda) + W(\Lambda) \ .$$

Using the normalization condition one can now show that

$$W(\Lambda) = \lim_{\Lambda' \to \infty} W(\Lambda; \Lambda')$$

where the limit converges in norm, and

$$W(\Lambda; \Lambda') = \sum \{\Phi(X);\ X \cap \Lambda \neq \varnothing,\ X \cap \Lambda^c \neq \varnothing,\ X \subset \Lambda'\} \ .$$

To prove this note that if $\Lambda_1 \subset \Lambda$, the following computation is valid

$$\begin{aligned} E_{\Lambda_1}(\tilde{H}(\Lambda)) - H(\Lambda_1) &= E_{\Lambda_1}(\tilde{H}(\Lambda) - \tilde{H}(\Lambda_1)) \\ &= \tau(\tilde{H}(\Lambda) - \tilde{H}(\Lambda_1)) \\ &= \tau(E_{\Lambda^c}(\tilde{H}(\Lambda))) - \tau(E_{\Lambda_1^c}(\tilde{H}(\Lambda_1))) = 0 \ . \end{aligned} \tag{$\binom{*}{**}$}$$

Here the second equality follows from

$$\tilde{H}(\Lambda) - \tilde{H}(\Lambda_1) \in \mathfrak{A}_{\Lambda_1'} \cap \mathfrak{A} = \mathfrak{A}_{\Lambda_1^c}$$

which is a consequence of $(*)$, while the last equality follows from $(**)$.

Next one computes that if $\Lambda \subseteq \Lambda'$, then

$$\begin{aligned} H(\Lambda'\backslash\Lambda) &= E_{\Lambda'\backslash\Lambda}(\tilde{H}(\Lambda')) \\ &= E_{\Lambda'\backslash\Lambda}(\tilde{H}(\Lambda') - \tilde{H}(\Lambda)) \\ &= E_{\Lambda'}E_{\Lambda^c}(\tilde{H}(\Lambda') - \tilde{H}(\Lambda)) = E_{\Lambda'}(\tilde{H}(\Lambda') - \tilde{H}(\Lambda)) \ , \qquad \binom{**}{**} \end{aligned}$$

where the first two equalities follow from $\binom{*}{**}$ and $(**)$, respectively, and the last from

$$\tilde{H}(\Lambda') - \tilde{H}(\Lambda) \in \mathfrak{A}_{\Lambda^c} \ .$$

We can now derive a manageable expression for the surface term $W(\Lambda;\Lambda')$,

$$\begin{aligned} W(\Lambda;\Lambda') &= H(\Lambda') - H(\Lambda'\backslash\Lambda) - H(\Lambda) \\ &= E_{\Lambda'}(\tilde{H}(\Lambda')) - E_{\Lambda'}(\tilde{H}(\Lambda') - \tilde{H}(\Lambda)) - H(\Lambda) \\ &= E_{\Lambda'}(\tilde{H}(\Lambda)) - H(\Lambda) \end{aligned}$$

for all $\Lambda' \supseteq \Lambda$, where $\binom{**}{**}$ was used in the second step. But $E_{\Lambda'}(A) \to A$ in norm when $\Lambda' \to \infty$, for all $A \in \mathfrak{A}$, and hence

$$\lim_{\Lambda' \to \infty} W(\Lambda;\Lambda') = \tilde{H}(\Lambda) - H(\Lambda) = W(\Lambda) \ .$$

The first specific result on existence of a time evolution is based upon the first criterion of the above proposition and is applicable to interactions for which the many-body forces are negligible in a suitable sense.

Theorem 6.2.4. *Let Φ be an interaction of a quantum spin system satisfying the requirement*

$$\|\Phi\|_\lambda = \sum_{n \geq 0} e^{\lambda n} \left(\sup_{x \in L} \sum_{\substack{X \ni x \\ |X| = n+1}} \|\Phi(X)\| \right) < +\infty$$

for some $\lambda > 0$, and define a derivation δ by

$$D(\delta) = \bigcup_{\Lambda \subset L} \mathfrak{A}_\Lambda$$

and

$$\delta(A) = i \sum_{X \cap \Lambda \neq \emptyset} [\Phi(X), A], \quad A \in \mathfrak{A}_\Lambda \ .$$

It follows that $D(\delta)$ is a norm-dense *-subalgebra of analytic elements of the closure $\bar{\delta}$ of δ. Therefore, $\bar{\delta}$ generates a strongly continuous one-parameter group of *-automorphisms τ of $\mathfrak{A}$ and

$$\lim_{\Lambda \to \infty} \|\tau_t(A) - \tau_t^\Lambda(A)\| = 0$$

for all $A \in \mathfrak{A}$, uniformly for t in compacts, where

$$\tau_t^\Lambda(A) = e^{itH_\Phi(\Lambda)} A e^{-itH_\Phi(\Lambda)} \ .$$

Remark. Less severe restrictions on the growth of $\|\Phi(X)\|$ with $|X|$ may be imposed at the cost of making the elements of $D(\delta)$ non-analytic, but nevertheless $\bar{\delta}$ remains a generator. (See Notes and Remarks.)

PROOF. Once we have established that each element of $D(\delta)$ is analytic for δ then the remaining statements follow directly from Proposition 6.2.3 because $p_\Phi(x) \leq \|\Phi\|_\lambda$ for all $x \in L$.

Now take $A \in \mathfrak{A}_\Lambda$. One has $\Phi(X) \in \mathfrak{A}_X$, and $\mathfrak{A}_\Lambda$ and $\mathfrak{A}_X$ commute whenever $X \cap \Lambda = \varnothing$. Therefore,

$$\delta^n(A) = i^n \sum_{X_1 \cap S_0 \neq \varnothing, \ldots, X_n \cap S_{n-1} \neq \varnothing} [\Phi(X_n), [\cdots [\Phi(X_1), A]]] \ ,$$

where $S_0 = \Lambda$ and

$$S_j = X_j \cup X_{j-1} \cup \cdots \cup X_1 \cup \Lambda$$

for $j \geq 1$. But

$$\sum_{X_i} \cdot = \sum_{n_i \geq 0} \sum_{\substack{X_i \\ |X_i| = n_i + 1}} \cdot$$

and

$$|S_j| \leq |X_j| + |X_{j-1}| + \cdots + |X_1| + |\Lambda| - j \ .$$

Thus

$$\|\delta^n(A)\| \leq 2^n \sum_{n_1, \ldots, n_n \geq 0} \prod_{i=1}^{n} (n_1 + \cdots + n_{i-1} + |\Lambda|) \|\Phi\|_{n_i} \|A\| \ ,$$

where

$$\|\Phi\|_{n_i} = \sup_{x \in L} \sum_{\substack{X \ni x \\ |X| = n_i + 1}} \|\Phi(X)\| \ .$$

But $a^n \leq n! \lambda^{-n} e^{a\lambda}$ for $\lambda, a > 0$ and hence

$$\|\delta^n(A)\| \leq (2/\lambda)^n \|\Phi\|_\lambda^n \|A\| n! \exp(\lambda |\Lambda|) \ .$$

This establishes that A is an analytic element for δ with radius of analyticity $t_A \geq (\lambda / 2\|\Phi\|_\lambda)$, i.e.,

$$\sum_{n \geq 0} \frac{|t|^n}{n!} \|\delta^n(A)\| < +\infty$$

for $|t| < (\lambda / 2\|\Phi\|_\lambda)$, and the proof is complete.

EXAMPLE 6.2.5. Assume Φ contains only one- and two-body interactions, i.e., $\Phi(X) = 0$ for $|X| > 2$. The conclusions of Theorem 6.2.4 are then valid whenever

$$\sup_{x \in L} \|\Phi(\{x\})\| < +\infty, \qquad \sup_{x \in L} \sum_{y \in L} \|\Phi(\{x, y\})\| < +\infty \ .$$

If $L = \mathbb{Z}^\nu$ and Φ is translationally invariant, these conditions reduce to the single restraint

$$\sum_{0 \neq y \in \mathbb{Z}^\nu} \|\Phi(\{0, y\})\| < +\infty \ .$$

This is obviously satisfied if Φ is of finite range and in general it can be understood as a restriction on the range of the two-body interactions.

The evolution τ constructed in Theorem 6.2.4 can be considered as a function of the interaction Φ and the perturbation estimates used in the proof establish that τ is continuous in Φ. For example if Φ_1 and Φ_2 both satisfy the requirements of the theorem, and if δ_{Φ_1} and δ_{Φ_2} denote the generators of the corresponding groups τ^{Φ_1} and τ^{Φ_2}, then

$$\tau_t^{\Phi_1}(A) - \tau_t^{\Phi_2}(A) = \sum_{n \geq 1} \frac{t^n}{n!} \sum_{m=0}^{n-1} \delta_{\Phi_1}^m (\delta_{\Phi_1} - \delta_{\Phi_2}) \delta_{\Phi_2}^{n-m-1}(A) \ .$$

Hence for $A \in \mathfrak{A}_\Lambda$ the above estimation procedure gives

$$\begin{aligned} \|\tau_t^{\Phi_1}(A) - \tau_t^{\Phi_2}(A)\| &\leq \sum_{n \geq 1} |t|^n \left(\frac{2}{\lambda}\right)^n \sum_{m=0}^{n-1} \|\Phi_1\|_\lambda^m \|\Phi_2\|_\lambda^{n-m-1} \\ &\quad \times \|\Phi_1 - \Phi_2\|_\lambda \|A\| e^{\lambda|\Lambda|} \\ &\leq \frac{2|t|}{\lambda} \|\Phi_1 - \Phi_2\|_\lambda \|A\| e^{\lambda|\Lambda|} \left(1 - \frac{2|t|}{\lambda} \|\Phi_1\|_\lambda\right)^{-1} \\ &\quad \times \left(1 - \frac{2|t|}{\lambda} \|\Phi_2\|_\lambda\right)^{-1} , \end{aligned}$$

whenever $(2|t|/\lambda)\|\Phi_i\|_\lambda < 1, i = 1, 2$. Continuity for general A and small t then follows by approximation of A by strictly local elements. Finally, continuity for all A and t results from the group property of $t \mapsto \tau_t^\Phi$.

The second result concerning the existence of dynamics emphasizes properties of the *energy interaction across the surface* of each finite subset $\Lambda \subset L$. This energy is defined by

$$W_\Phi(\Lambda) = \sum_{\substack{X \cap \Lambda \neq \varnothing \\ X \cap \Lambda^c \neq \varnothing}} \Phi(X)$$

where Λ^c again denotes the complement of Λ. The following theorem, which is a consequence of the result of Section 3.1.4, covers two cases which are typically applicable to one- and two-dimensional systems respectively.

Theorem 6.2.6. *Let Φ be an interaction of a quantum spin system satisfying the requirement*

$$p_\Phi(x) = \sum_{X \ni x} \|\Phi(X)\| < +\infty$$

for all $x \in L$, and define a derivation δ by

$$D(\delta) = \bigcup_{\Lambda \subset L} \mathfrak{A}_\Lambda$$

and

$$\delta(A) = i \sum_{X \cap \Lambda \neq \varnothing} [\Phi(X), A], \quad A \in \mathfrak{A}_\Lambda \ .$$

Assume that there exists an increasing sequence $\Lambda_n \subset L$ such that $\Lambda_n \to \infty$ and

$$\textit{either} \qquad \left\| \sum_{\substack{X \cap \Lambda_n \neq \varnothing \\ X \cap \Lambda_n^c \neq \varnothing}} \Phi(X) \right\| \leq M$$

for some $M > 0$

$$\textit{or} \qquad \left\| \sum_{\substack{X \cap \Lambda_n \neq \varnothing \\ X \cap \Lambda_{n+m}^c \neq \varnothing}} \Phi(X) \right\| \leq O(n) e^{-\alpha m}$$

for some $\alpha > 0$.

It follows that the closure $\bar{\delta}$ of δ generates a strongly continuous one-parameter group of *-automorphism of $\mathfrak{A}$ and, furthermore,

$$\lim_{n \to \infty} \|\tau_t(A) - \tau_t^{\Lambda_n}(A)\| = 0$$

for all $A \in \mathfrak{A}$, uniformly for t in compacts.

Proof. This result follows from Theorem 3.1.34, and the discussion subsequent to the theorem, when one makes the identifications $X = \mathfrak{A}$, $X_n = \mathfrak{A}_{\Lambda_n}$, $S = \delta$, and $S_{n,m} = S_{n+m,0} = \delta_{n+m}$, where

$$\delta_n(A) = i[H_\Phi(\Lambda_n), A]$$

for all $A \in \mathfrak{A}$.

Thus under the first assumption of the theorem the result follows from the discussion at the end of Section 3.1.4 because

$$\|S|_{X_n} - S_{n,0}\| = \|(\delta - \delta_n)|_{\mathfrak{A}_{\Lambda_n}}\| \leq 2 \left\| \sum_{\substack{X \cap \Lambda_n \neq \varnothing \\ X \cap \Lambda_n^c \neq \varnothing}} \Phi(X) \right\| \leq 2M \ .$$

Similarly, the second assumption of theorem implies that

$$\|S|_{X_n} - S_{n,m}\| = \|(\delta - \delta_{n+m})|_{\mathfrak{A}_{\Lambda_n}}\| \leq 2 \left\| \sum_{\substack{X \cap \Lambda_n \neq \varnothing \\ X \cap \Lambda_{n+m}^c \neq \varnothing}} \Phi(X) \right\| = O(n) e^{-\alpha m}$$

and the result follows from Theorem 3.1.34.

Theorems 6.2.4 and 6.2.6 both give conditions on the interaction which are sufficient for the construction of dynamics. The conditions of Theorem 6.2.4 imply that

$$\sup_{x \in L} \|\Phi(\{x\})\| < +\infty \ ,$$

i.e., the interaction energy is uniformly bounded on the lattice. Theorem 6.2.6 does not impose this type of boundedness and $\|\Phi(X)\|$ could grow indefinitely provided that the surface energies are appropriately bounded. Thus, Theorem 6.2.6 appears more general than Theorem 6.2.4. Unfortunately, the bounds of Theorem 6.2.6 are rather restrictive and essentially limit the result to one- and two-dimensional models. These applications are illustrated by the following examples.

EXAMPLE 6.2.7. Let $L = \mathbb{Z}, \Lambda_n = [-n, n]$, and assume that Φ is a translation invariant interaction. It follows that

$$\left\| \sum_{\substack{X \cap \Lambda_n \neq \emptyset \\ X \cap \Lambda_n^c \neq \emptyset}} \Phi(X) \right\| \leq 2 \sum_{X \ni 0} D(X) \|\Phi(X)\| \ .$$

Thus if the right-hand side is finite the first case of Theorem 6.2.6 is applicable. This requirement differs from that of Theorem 6.2.4 insofar the possible growth of

$$\|\Phi\|_n = \sum_{\substack{X \ni 0 \\ |X| = n+1}} \|\Phi(X)\|$$

with n is less restricted. On the other hand, the range of Φ is more restricted. For example, if Φ is a two-body interaction, i.e., if $\Phi(X) = 0$ for $|X| > 2$, then the condition becomes

$$\sum_{x \neq 0} |x| \, \|\Phi(\{0, x\})\| < +\infty \ .$$

Thus, the two-body interactions should decrease roughly as $|x|^{-2-\varepsilon}$.

EXAMPLE 6.2.8. Let $L = \mathbb{Z}^2$,

$$\Lambda_n = \{x; x = (x_1, x_2) \in \mathbb{Z}^2, |x_i| \leq n, i = 1, 2\} \ ,$$

and assume that Φ is an interaction with finite range d_Φ. It follows that

$$\left\| \sum_{\substack{X \cap \Lambda_n \neq \emptyset \\ X \cap \Lambda_{n+m}^c \neq \emptyset}} \Phi(X) \right\| \leq \sum_{x \in \Lambda_n \setminus \Lambda_{n-d_\Phi}} \left\| \sum_{\substack{X \ni x \\ D(X) \geq m}} \Phi(X) \right\| \leq 4 n d_\Phi \sup_{x \in \Lambda_n \setminus \Lambda_{n-d_\Phi}} \left\| \sum_{\substack{X \ni x \\ D(X) \geq m}} \Phi(X) \right\| \ .$$

But the right-hand side vanishes identically if $m > d_\Phi$ and hence the second case of Theorem 6.2.6 is applicable.

The third and final method of discussing the dynamics of quantum spin systems applies only to a subclass of the interactions covered by Theorem 6.2.4 but it establishes more detailed propagation properties. This method only applies to regular lattices, e.g., $L = \mathbb{Z}^\nu$, and differs from the previous methods insofar it establishes the Cauchy convergence property of $\Lambda \mapsto \tau_t^\Lambda(A)$ directly. The starting point of the method is the estimate

$$\begin{aligned}\|\tau_t^{\Lambda_1}(A) - \tau_t^{\Lambda_2}(A)\| &= \left\| \int_0^t ds \frac{d}{ds}(\tau_s^{\Lambda_1}\tau_{t-s}^{\Lambda_2}(A)) \right\| \\ &= \left\| \int_0^t ds\, \tau_s^{\Lambda_1}([H_\Phi(\Lambda_1) - H_\Phi(\Lambda_2),\ \tau_{t-s}^{\Lambda_2}(A)]) \right\| \\ &\leq \sum_{x \in \Lambda_1 \setminus \Lambda_2} \sum_{X \ni x} \int_0^{|t|} ds \|[\Phi(X), \tau_s^{\Lambda_2}(A)]\|\end{aligned}$$

which is valid for $\Lambda_2 \subseteq \Lambda_1$, and $A \in \mathfrak{A}_{\Lambda_2}$. Thus to prove the Cauchy property one must estimate the commutators occurring in the last summand. These estimates can be understood as bounds on propagation velocities. We discuss this interpretation subsequently.

Proposition 6.2.9. *Let Φ be an interaction of a quantum spin system on the lattice $L = \mathbb{Z}^\nu$ and assume that*

$$\|\Phi\|_\lambda = \sup_{x \in \mathbb{Z}^\nu} \sum_{X \ni x} |X|(N+1)^{2|X|} e^{\lambda D(X)} \|\Phi(X)\| < +\infty$$

for some $\lambda > 0$. Let τ^Λ denote the evolution associated with Φ and $\Lambda \subset \mathbb{Z}^\nu$ and $x \in \mathbb{Z}^\nu \mapsto \tau_x$ the action of space translations.

It follows that

$$\|[\tau_t^\Lambda(A), B]\| \leq \|A\| \sum_{x \in \mathbb{Z}^\nu} \sup_{C \in \mathfrak{A}_{\{0\}}} \left(\frac{\|[\tau_x(C), B]\|}{\|C\|} \right) e^{-|x|\lambda + 2|t|\,\|\Phi\|_\lambda}$$

for all $A \in \mathfrak{A}_{\{0\}}$ and $B \in \mathfrak{A}$.

Proof. First define

$$C_{A,B}^\Lambda(x,t) = [\tau_x \tau_t^\Lambda(A),\ B]$$

and remark that

$$\begin{aligned}C_{A,B}^\Lambda(x,t) &= C_{A,B}^\Lambda(x,0) + \int_0^t ds \frac{\partial}{\partial s} C_{A,B}^\Lambda(x,s) \\ &= C_{A,B}^\Lambda(x,0) + i \sum_{X \ni 0} \int_0^t ds\, [\tau_x \tau_s^\Lambda([\Phi(X),\ A]), B]\ .\end{aligned}$$

Next define

$$C_B(x,\ t) = \sup_{\Lambda \subset \mathbb{Z}^\nu} \sup_{A \in \mathfrak{A}_{\{0\}}} \frac{\|C_{A,B}^\Lambda(x,t)\|}{\|A\|}\ .$$

The integral relation for $C_{A,B}^\Lambda$, and several applications of the triangle inequality, yields the integral inequality

$$C_B(x,t) \leq C_B(x,0) + \sum_{X \ni 0} \int_0^{|t|} ds \sup_{\Lambda \subset \mathbb{Z}^\nu} \sup_{A \in \mathfrak{A}_{\{0\}}} \frac{\|[\tau_x \tau_s^\Lambda([\Phi(X), A]), B]\|}{\|A\|}\ .$$

Next we seek a majorization of the integrand in terms of C_B.

Let $e(i_x, j_x), i_x, j_x = 0, 1, \ldots, N$, be a set of matrix units for $\mathfrak{A}_{\{x\}}$. Each $[\Phi(X), A]$ has a unique decomposition of the form

$$[\Phi(X), A] = \sum_{\{i_x\}\{j_x\}} C_\Phi(\{i_x\}, \{j_x\}) \prod_{x \in X} e(i_x, j_x)$$

with coefficients $C_\Phi \in \mathbb{C}$ satisfying

$$|C_\Phi(\{i_x\}, \{j_x\})| \leq \|[\Phi(X), A]\| \leq 2\|\Phi(X)\| \, \|A\| \ .$$

Substitution of this decomposition into the integrand of the above inequality, use of the linearity properties of commutators and the triangle inequality then gives the new integral inequality

$$C_B(x,t) \leq C_B(x,0) + \sum_{X \ni 0} \sum_{y \in X} 2(N+1)^{2|X|} \|\Phi(X)\| \int_0^{|t|} ds \, C_B(x+y, s) \ .$$

But this takes the simple form

$$C_B(x,t) \leq C_B(x,0) + 2 \sum_{y \in \mathbb{Z}^\nu} \varepsilon(y) \int_0^{|t|} ds \, C_B(x+y, s) \ ,$$

where

$$\varepsilon(y) = \sum_{\substack{X \ni 0 \\ X \ni y}} (N+1)^{2|X|} \|\Phi(X)\| \ .$$

Iterating this last inequality yields

$$C_B(x,t) \leq \sum_{y \in \mathbb{Z}^\nu} C_B(y,0) \frac{1}{(2\pi)^\nu} \int_{0 < \theta_i \leq 2\pi} d^\nu\theta \, e^{i\theta(x-y)} e^{2|t|\hat{\varepsilon}(\theta)} \ ,$$

where $\hat{\varepsilon}$ is the $\mathbb{Z}^\nu$-Fourier transform of ε. (This use of Fourier transformation is where the regularity assumption $L = \mathbb{Z}^\nu$ is important.) As $\hat{\varepsilon}$ is analytic and periodic one may change the integration to an integration along $\operatorname{Im} \theta = \gamma$ to estimate

$$\left| \frac{1}{(2\pi)^\nu} \int d^\nu\theta \, e^{i\theta(x-y)} e^{2|t|\hat{\varepsilon}(\theta)} \right| \leq e^{-(x-y)\gamma} \frac{1}{(2\pi)^\nu} \int d^\nu\theta \, |e^{2|t|\hat{\varepsilon}(\theta+i\gamma)}| \ .$$

But

$$\hat{\varepsilon}(\theta + i\gamma) = \sum_{y \in \mathbb{Z}^\nu} e^{-i(\theta+i\gamma)y} \varepsilon(y) \ .$$

Hence, using $\varepsilon(y) \geq 0$, one concludes that

$$|\hat{\varepsilon}(\theta + i\gamma)| \leq \sum_{y \in \mathbb{Z}^\nu} e^{\gamma y} \varepsilon(y) = \hat{\varepsilon}(i\gamma) \ .$$

Consequently

$$|e^{2|t|\hat{\varepsilon}(\theta+i\gamma)}| \leq e^{2|t|\hat{\varepsilon}(i\gamma)} \ .$$

Combination of these estimates immediately yields the bound

$$C_B(x,t) \leq \sum_{y \in \mathbb{Z}^\nu} C_B(y,0) e^{-(x-y)\gamma} e^{2|t|\hat{\varepsilon}(i\gamma)} \ .$$

But choosing $\gamma = ((x-y)/|x-y|)\lambda$ with $\lambda > 0$ gives

$$\begin{aligned}\hat{\varepsilon}(i\gamma) &= \sum_{X \ni 0} \sum_{y \in X} (N+1)^{2|X|} \|\Phi(X)\| e^{\lambda(x-y)y/|x-y|} \\ &\leq \sum_{X \ni 0} |X|(N+1)^{2|X|} \|\Phi(X)\| e^{\lambda D(X)} \leq \|\Phi\|_\lambda \ .\end{aligned}$$

Consequently

$$C_B(x,t) \leq \sum_{y \in \mathbb{Z}^\nu} C_B(y,0) e^{-\lambda|x-y|} e^{2|t|\|\Phi\|_\lambda} \ .$$

The statement of the proposition now follows from the definition of C_B.

Corollary 6.2.10. *If*

$$C(x,t) = \sup_{\Lambda \subset \mathbb{Z}^\nu} \sup_{A,B \in \mathfrak{A}_{\{0\}}} \frac{\|[\tau_x \tau_t^\Lambda(A), B]\|}{\|A\| \|B\|} \ ,$$

then $C(x,0) \leq 2\delta_{x,0}$ *and hence*

$$C(x,t) \leq 2\exp\{-|t|(\lambda|x|/|t| - 2\|\Phi\|_\lambda)\} \ .$$

These estimates now allow a new discussion of dynamical evolution for a suitable class of interactions.

Theorem 6.2.11. *Let* Φ *be an interaction of a quantum spin system on the lattice* $L = \mathbb{Z}^\nu$ and *assume*

$$\|\Phi\|_\lambda = \sup_{x \in \mathbb{Z}^\nu} \sum_{X \ni x} |X|(N+1)^{2|X|} e^{\lambda D(X)} \|\Phi(X)\| < +\infty$$

for some $\lambda > 0$. *Further let* τ^Λ *denote the evolution associated with* Φ *and* Λ.

It follows that τ^Λ *converges strongly to a one-parameter group of* **-automorphisms* τ *of* $\mathfrak{A}$, *i.e.,*

$$\lim_{\Lambda \to \infty} \|\tau_t(A) - \tau_t^\Lambda(A)\| = 0$$

for all $A \in \mathfrak{A}$, *and the convergence is uniform for* t *in compacts.*

Moreover, for $A, B \in \mathfrak{A}_{\{0\}}$ *one has*

$$\left.\begin{aligned}&\|[\tau_x \tau_t(A), B]\| \\ &\|[\tau_t \tau_x(A), B]\|\end{aligned}\right\} \leq 2\|A\| \ \|B\| e^{-|t|\{\lambda|x|/|t| - 2\|\Phi\|_\lambda\}} \ ,$$

where $x \in \mathbb{Z}^\nu \mapsto \tau_x$ *denotes space translations.*

Finally if Φ_1 *and* Φ_2 *are two interactions of the above class and* τ^{Φ_1} *and* τ^{Φ_2} *the appropriate automorphism groups, then*

$$\|\tau_t^{\Phi_1}(A) - \tau_t^{\Phi_2}(A)\| \leq \|A\| \ |\Lambda_0| \ \|\Phi_1 - \Phi_2\|_\lambda \left[\frac{e^{2|t| \ \|\Phi\|_\lambda} - 1}{\|\Phi\|_\lambda}\right] \left[\sum_{x \in \mathbb{Z}^\nu} e^{-\lambda|x|_0}\right]$$

for all $A \in \mathfrak{A}_{\Lambda_0}$ *where* $\|\Phi\|_\lambda = \min(\|\Phi_1\|_\lambda, \|\Phi_2\|_\lambda)$ *and*

$$|x|_0 = \min_{y \in \Lambda_0} |x - y| \ .$$

PROOF. Prior to Proposition 6.2.9 we established the estimate

$$\|\tau_t^{\Lambda_1}(A) - \tau_t^{\Lambda_2}(A)\| \leq \sum_{x \in \Lambda_1 \setminus \Lambda_2} \sum_{X \ni x} \int_0^{|t|} ds \|[\Phi(X), \tau_s^{\Lambda_2}(A)]\|$$

whenever $A \in \mathfrak{A}_{\Lambda_0}$ with $\Lambda_0 \subset \Lambda_2 \subset \Lambda_1$. But then decomposition of $\Phi(X)$ in terms of matrix units, as in the proof of Proposition 6.2.9, yields the estimate

$$\begin{aligned}\|\tau_t^{\Lambda_1}(A) - \tau_t^{\Lambda_2}(A)\| \leq & \sum_{x \in \Lambda_1 \setminus \Lambda_2} \sum_{X \ni x} \|\Phi(X)\|(N+1)^{2|X|} \\ & \times \sum_{y \in X} \int_0^{|t|} ds \sup_{B \in \mathfrak{A}_{\{0\}}} \frac{\|[\tau_y(B), \tau_s^{\Lambda_2}(A)]\|}{\|B\|} \ .\end{aligned}$$

Therefore, an application of the bound of Proposition 6.2.9 gives

$$\begin{aligned}\|\tau_t^{\Lambda_1}(A) - \tau_t^{\Lambda_2}(A)\| \leq & \sum_{x \in \Lambda_1 \setminus \Lambda_2} \sum_{X \ni x} (N+1)^{2|X|} \|\Phi(X)\| \, 2 \, \|A\| \\ & \times \sum_{y \in X} \sum_{z \in \Lambda_0} e^{-\lambda|y-z|} \int_0^{|t|} ds \, e^{2s\|\Phi\|_\lambda} \ .\end{aligned}$$

But $-|y-z| \leq -|z-x| + |x-y|$ and $|x-y| \leq D(X)$ for $x, y \in X$. Thus one obtains

$$\begin{aligned}\|\tau_t^{\Lambda_1}(A) - \tau_t^{\Lambda_2}(A)\| \leq & \, 2\|A\| \sum_{x \in \Lambda_1 \setminus \Lambda_2} \sum_{X \ni x} |X|(N+1)^{2|X|} \|\Phi(X)\| e^{\lambda D(X)} \\ & \times \sum_{z \in \Lambda_0} e^{-\lambda|x-z|} \int_0^{|t|} ds \, e^{2s\|\Phi\|_\lambda} \\ \leq & \, \|A\| |\Lambda_0| (e^{2|t|\|\Phi\|_\lambda} - 1) \sum_{x \in \Lambda_1 \setminus \Lambda_2} e^{-\lambda|x|_0} \ .\end{aligned}$$

Hence $\tau_t^\Lambda(A)$ converges in norm for all strictly local A and the convergence is uniform on compacts. Convergence for general A follows by continuity.

The second statement of the theorem follows directly from Corollary 6.2.10.

The final statement follows from the estimate

$$\|\tau_t^{\Phi_1}(A) - \tau_t^{\Phi_2}(A)\| \leq \int_0^{|t|} ds \sum_{X \subset \mathbb{Z}^\nu} \|[\Phi_1(X) - \Phi_2(X), \tau_s^{\Phi_2}(A)]\|$$

and an argument similar to the above.

EXAMPLE 6.2.12. Assume Φ is translationally invariant and contains only two-body interactions. The condition of Theorem 6.2.11 then reduces to the condition

$$\sum_{x \in \mathbb{Z}^\nu} \|\Phi(\{0, x\})\| e^{\lambda|x|} < \infty$$

for some $\lambda > 0$, i.e., the interaction must decrease exponentially with distance.

Let us now consider in a little more detail the significance of the foregoing commutator estimates. If $A \in \mathfrak{A}_{\{0\}}$, then A corresponds to an observation at the origin and $\tau_x\tau_t(A)$ can be thought of as an observation at the point x at time t. The commutator $[\tau_x\tau_t(A), B]$ with $B \in \mathfrak{A}_{\{0\}}$ then gives a measure of dependence of this observation on the observation B at the origin at time $t = 0$, i.e., the commutator measures the effect of the observation $\tau_x\tau_t(A)$ at the origin. Thus, the estimate

$$\frac{\|[\tau_x\tau_t(A), B]\|}{2\|A\|\ \|B\|} < \exp\left\{-|t|\left[\frac{\lambda|x|}{|t|} - 2\|\Phi\|_\lambda\right]\right\}$$

shows that this effect is exponentially decreasing with time outside of the cone

$$|x| < |t|\left(\frac{2\|\Phi\|_\lambda}{\lambda}\right) .$$

Thus physical disturbances propagate with velocities less than

$$V_\Phi = \inf_\lambda \frac{2\|\Phi\|_\lambda}{\lambda} .$$

Another way of arriving at this same qualitative conclusion is to reexamine the essential localization of $\tau_t(A)$. The estimate used in the proof of Theorem 6.2.11 shows that

$$\begin{aligned}\|\tau_t(A) - \tau_t^\Lambda(A)\| &\le \|A\|(e^{2|t|\|\Phi\|_\lambda} - 1)\sum_{x\in\Lambda^c} e^{-\lambda|x|} \\ &\le 2\|A\|\ \|\Phi\|_\lambda|t|\sum_{x\in\Lambda^c} e^{-\lambda|x|}e^{2|t|\|\Phi\|_\lambda}\end{aligned}$$

for $A \in \mathfrak{A}_{\{0\}}$. But if $\Lambda = \{x; |x| < V|t| + D\}$, then

$$\sum_{x\in\Lambda^c} e^{-\lambda|x|} \le S_\nu \int_{r > V|t|+D-1} dr\ r^{\nu-1}e^{-\lambda r} ,$$

where S_ν is the surface area of the ν-dimensional unit sphere. Therefore,

$$\|\tau_t(A) - \tau_t^\Lambda(A)\| \le 2\|A\|\ \|\Phi\|_\lambda F(|t|)e^{-\lambda|t|(V-V_\lambda)}$$

where $V_\lambda = 2\|\Phi\|_\lambda/\lambda$ and $F(|t|)$ has the form

$$F(|t|) = |t|P_{\nu-1}(V|t| + D)e^{-\lambda D|t|} ,$$

where $P_{\nu-1}$ is a polynomial of order $\nu - 1$. Thus, if $V > V_\Phi$ and $\varepsilon > 0$, one may choose D such that

$$\|\tau_t(A) - \tau_t^\Lambda(A)\| < \varepsilon\|A\|$$

for all $t \in \mathbb{R}$, i.e., $\tau_t(A)$ is essentially localized in a cone

$$|x| < V_\Phi|t| + D .$$

This conclusion that the propagation of physical effects is exponentially damped outside of a causal cone determined by a group velocity V_Φ is essen-

tially restricted to interactions which are exponentially decreasing in configuration space (see Example 6.2.12). If the interaction decreases more slowly, then one would expect the damping to be less important but no quantitative results in this direction have been obtained.

Although these results show that propagation takes place only in a causal cone with asymptote determined by V_Φ the method provides no information concerning the distribution of effects within the cone. The characteristics of this distribution depend much more intimately on the details of the interaction. For certain interactions the maximum velocity of propagation is sensibly smaller than the estimate V_Φ and it is typically zero for classical interactions such as the Ising interaction.

EXAMPLE 6.2.13. Consider the spin-$\frac{1}{2}$ Ising model introduced in Example 6.2.2. If $A \in \mathfrak{A}_{\{x\}}$ is of the form

$$A = a_0 \sigma_0^x + a_3 \sigma_3^x$$

with $a_0, a_3 \in \mathbb{C}$, then the commutation relations $[\sigma_3^x, \sigma_3^y] = 0$ and the identification $\sigma_0^x = \mathbb{1}$ show that A is a fixed point for the Ising evolution, i.e.,

$$\tau_t(A) = A \ .$$

Alternatively if

$$A' = a_+ \sigma_+^x + a_- \sigma_-^x \ ,$$

where $a_\pm \in \mathbb{C}$ and $\sigma_\pm^x$ are the spin raising and lowering operators defined by

$$\sigma_\pm^x = (\sigma_1^x \pm i\sigma_2^x)/2 \ .$$

then one finds

$$\tau_t(A') = a_+ e^{itH_\Phi^x} \sigma_+^x + a_- e^{-itH_\Phi^x} a_-^x \ ,$$

where

$$H_\Phi^x = \sum_{y \in \mathbb{Z}^\nu} j_3(x-y) \sigma_3^y \ .$$

Thus the time development $t \mapsto \tau_t(A')$ has a multiperiodic nature which is periodic if Φ has finite range. In this latter case $\tau_t(A)$ remains localized within a distance d_Φ (the range of Φ) of the point x. Finally a general element of $\mathfrak{A}_{\{x\}}$ has the form $A + A'$ and combination of the above cases gives the generic behavior.

The Ising model illustrates a behavior typical of classical interactions. If $\mathfrak{C} \subset \mathfrak{A}$ is a classical spin algebra and Φ takes values in $\mathfrak{C}$, then all elements of $\mathfrak{C}$ are fixed points of the corresponding evolution. This follows because $\mathfrak{C}$ is abelian.

More interesting types of propagation are expected for models such as the Heisenberg model and the X–Y model. To analyze the dynamics of the latter we first describe a connection between the kinematics of the one-dimensional spin-$\frac{1}{2}$ system of Example 6.2.1 and the corresponding CAR algebra of Theorem 5.2.5.

EXAMPLE 6.2.14A Consider the spin-$\frac{1}{2}$ model with $L = \mathbb{Z}$. The C*-algebra of local observables $\mathfrak{A}_\Lambda$ is generated by polynomials in the Pauli operators $\{\sigma_i^x; i = 0, 1, 2, 3, x \in \Lambda\}$ and the corresponding quasi-local algebra $\mathfrak{A}^P$ is isomorphic to the UHF-algebra $\otimes_{x=-\infty}^{\infty} M_2$. An explicit matrix representation of the Pauli operators was given in Example 4.2.7. They satisfy the Pauli relations

$$(\sigma_j^x)^2 = \mathbb{1}, \quad \sigma_j^{x*} = \sigma_j^x, \quad \sigma_j^x \sigma_{j+1}^x = -\sigma_{j+1}^x \sigma_j^x = i\sigma_{j+2}^x$$

where addition of the indices is modulo 3. Moreover, $[\sigma_i^x, \sigma_j^y] = 0$ if $x \neq y$.

Now define the Fermi algebra $\mathfrak{A}^F$ as the C*-algebra generated by elements $\{a_x, a_x^*; x \in Z\}$ satisfying the anticommutation relations

$$\{a_x, a_y^*\} = \delta_{x,y}\ , \quad \{a_x, a_y\} = 0$$

for all $x, y \in Z$. In Theorem 5.2.5 it was established that $\mathfrak{A}^F$ is also isomorphic to the UHF-algebra $\otimes_{x=-\infty}^{\infty} M_2$ but due to the anticommutation at large distances there cannot be an isomorphism between $\mathfrak{A}^F$ and $\mathfrak{A}^P$ which respects the spin structure. Nevertheless one can embed $\mathfrak{A}^F$ and $\mathfrak{A}^P$ in a larger UHF-algebra $\widehat{\mathfrak{A}}$ in such a way that $\mathfrak{A}^F \cap \mathfrak{A}^P$ is the C*-subalgebra of even elements, i.e., the C*-subalgebra generated by even polynomials in the a and a^*, or in the σ. The embedding is defined as follows.

Let Θ_- be the automorphism, of order 2, of $\mathfrak{A}^F$ defined by

$$\Theta_-(a_x) = \begin{cases} a_x & \text{if } x \geq 1\ , \\ -a_x & \text{if } x \leq 0\ . \end{cases}$$

The crossed product $\widehat{\mathfrak{A}} = \mathfrak{A} \otimes_{\Theta_-} \mathbb{Z}_2$, of $\mathfrak{A}$ and this action of $\mathbb{Z}_2 = \mathbb{Z}/2\mathbb{Z}$, is then the C*-algebra generated by $\mathfrak{A}^F$ and an operator $T \in \widehat{\mathfrak{A}}$ satisfying $T^2 = \mathbb{1}, T = T^*$ and $TA = \Theta_-(A)T$ for $A \in \mathfrak{A}^F$. One can check that $\widehat{\mathfrak{A}}$ is also isomorphic to $\otimes_{x=-\infty}^{\infty} M_2$.

Now realize the Pauli algebra $\mathfrak{A}^P$ as the C*-subalgebra of $\widehat{\mathfrak{A}}$ generated by

$$\sigma_1^x = TS_x(a_x + a_x^*)\ , \quad \sigma_2^x = iTS_x(a_x - a_x^*), \quad \sigma_3^x = 2a_x^* a_x - \mathbb{1}$$

where

$$S_x = \begin{cases} \prod_{y=1}^{x-1} \sigma_3^y & \text{if } x \geq 1\ , \\ \mathbb{1} & \text{if } x = 1\ , \\ \prod_{y=x}^{0} \sigma_3^y & \text{if } x < 1\ . \end{cases}$$

The operators then satisfy the Pauli spin relations and this defines an embedding of $\mathfrak{A}^P$ into $\widehat{\mathfrak{A}}$. (The significance of the operators $TS_x = S_x T$ is explained by noting that one has the formal relation

$$TS_x = \prod_{y=-\infty}^{x-1} \sigma_3^y.)$$

Next define an action Θ of the group $\mathbb{Z}_2 \times \mathbb{Z}_2$ on $\widehat{\mathfrak{A}}$ by

$$\Theta(i,j)(a_x) = (-1)^i a_x,\ \Theta(i,j)(a_x^*) = (-1)^i a_x^*,\ \Theta(i,j)(T) = (-1)^j T$$

for all $i, j = 0, 1$, and let $\widehat{\mathfrak{A}}_{\pm\pm}$ denote the four spectral subspaces of $\widehat{\mathfrak{A}}$ defined by this action (see Section 3.2.3). Then one checks that $\widehat{\mathfrak{A}}_{++}$ is the even subalgebra of $\mathfrak{A}^F$ alluded to in the previous paragraph and

$$\mathfrak{A}^F = \widehat{\mathfrak{A}}_{++} + \widehat{\mathfrak{A}}_{-+} \ ,$$

$$\mathfrak{A}^P = \widehat{\mathfrak{A}}_{++} + \widehat{\mathfrak{A}}_{--} \ .$$

The even subalgebra $\widehat{\mathfrak{A}}_{++} = \mathfrak{A}^P \cap \mathfrak{A}^F$ is itself isomorphic to $\otimes_{x=-\infty}^{\infty} M_2$.

An interesting automorphism σ of $\widehat{\mathfrak{A}}$ is defined by

$$\sigma(a_x) = a_{x+1}, \quad \sigma(T) = \sigma_3^1 T = T\sigma_3^1 \ .$$

One checks that σ restricted to $\mathfrak{A}^F$ is the twosided quasi-free shift and its restriction to $\mathfrak{A}^P$ is the twosided shift. Thus these shifts coincide on the even subalgebra.

Finally note that $\mathfrak{A}^P$ is also generated by the spin raising and lowering operators

$$\sigma_\pm^x = (\sigma_1^x \pm i\sigma_2^x)/2$$

which satisfy the relations

$$\{\sigma_+^x, \sigma_-^x\} = \mathbb{1}, \quad [\sigma_+^x, \sigma_-^x] = \sigma_3^x \ .$$

The $\sigma_\pm^x, \sigma_\pm^y$ commute if $x \neq y$. The a_x, a_x^* can be recovered from the $\sigma_\pm^x$ by

$$a_x = TS_x\sigma_-^x, \quad a_x^* = TS_x\sigma_+^x \ .$$

We now use this description of the kinematical structure of the spin-$\frac{1}{2}$ system to analyze the time development of the X–Y model.

EXAMPLE 6.2.14B Consider the X–Y-model of Example 6.2.2 for $\nu = 1$ but assume, for simplicity, that $j_i(x) = 0$ for $|x| \neq 1$. On the algebra $\widehat{\mathfrak{A}}$ the local Hamiltonian then has the form

$$\begin{aligned} H_n = H_\Phi([-n,n]) &= -J \sum_{x=-n}^{n-1} ((1+\gamma)\sigma_1^x\sigma_1^{x+1} + (1-\gamma)\sigma_2^x\sigma_2^{x+1}) + h \sum_{x=-n}^{n} \sigma_3^x \\ &= 2J \sum_{x=-n}^{n-1} (a_x^* a_{x+1} + a_{x+1}^* a_x + \gamma a_x^* a_{x+1}^* + \gamma a_{x+1} a_x) \\ &\quad + h \sum_{x=-n}^{n} (2a_x^* a_x - \mathbb{1}) \ . \end{aligned}$$

Therefore the Hamiltonian H_Φ defines a time development of $\widehat{\mathfrak{A}}$ which leaves the two subalgebras $\mathfrak{A}^F$ and $\mathfrak{A}^P$ invariant. Assume, for simplicity, that $h = 0$. The infinitesimal time change of the a is then given by

$$\delta_\Phi(a_x) = \lim_{n\to\infty} i[H_n, a_x] = -2iJ(a_{x+1} + a_{x-1} + \gamma(a_{x+1}^* + a_{x-1}^*)) \ .$$

For $h = (f, g)$ with $f, g \in l_2(\mathbb{Z})$ it is now convenient to introduce

$$B(h) = a^*(f) + a(g) = \sum_j f_j a_j^* + \sum_j g_j a_j \ .$$

One then computes that the derivation δ_Φ generates the one-parameter group

$$\tau_t(B(h)) = B(e^{i2JKt}h)$$

where

$$K = \begin{pmatrix} (U+U^*) & \gamma(U-U^*) \\ -\gamma(U-U^*) & -(U+U^*) \end{pmatrix}$$

and

$$(Uf)_j = f_{j+1}, \quad (U^* f)_j = f_{j-1} \ .$$

The time evolution of $T \in \widehat{\mathfrak{A}}$ is given by $\tau_t(T) = TV_t$ where

$$\begin{aligned} V_t &= \lim_{n\to\infty} Te^{itH_n}Te^{-itH_n} \\ &= \lim_{n\to\infty} e^{it\Theta_-(H_n)}e^{-itH_n} = \sum_{j=0}^{\infty} i^n \int_0^t dt_1 \int_0^{t_1} dt_2 \ldots \int_0^{t_{n-1}} dt_n\, \tau_{t_n}(A)\ldots\tau_{t_1}(A) \ , \end{aligned}$$

by Theorem 3.1.33, with

$$A = \lim_{n\to\infty}(\Theta_-(H_n) - H_n) = -4J(a_0^*a_1 + a_1^*a_0 + \gamma(a_0^*a_1^* + a_1a_0)) \ .$$

These formulae give the time-development on $\widehat{\mathfrak{A}}$. Next, using Fourier transformation, one deduces that K has a Lebesgue spectrum on $[-2,-2\gamma] \cup [2\gamma, 2]$ with uniform multiplicity 4. Therefore $e^{it2JK}h \to 0$ weakly as $t \to \pm\infty$ for all $h \in l_2(\mathbb{Z}) \oplus l_2(\mathbb{Z})$. Hence the limits

$$\tilde{\Theta}_\pm(A) = \lim_{t\to\pm\infty} V_tAV_t^*$$

exist for all $A \in \mathfrak{A}^F$ and define automorphisms of $\mathfrak{A}^F$. In fact

$$\tilde{\Theta}_\pm(B(h)) = B(U_\pm h)$$

where $U_\pm$ are unitary operators which can be computed explicitly. Using these observations, and a method similar to that of Example 5.4.9, one now establishes the following twisted asymptotic abelianness for $A, B \in \mathfrak{A}^P$: if $A, B \in \widehat{\mathfrak{A}}_{++}$ then

$$\lim_{t\to\pm\infty} \|[A, \tau_t(B)]\| = 0 \ ,$$

if $A \in \widehat{\mathfrak{A}}_{--}$ and $B \in \widehat{\mathfrak{A}}_{++}$ then

$$\lim_{t\to\pm\infty} \|A\tau_t(B) - \widetilde{\Theta}_+(\tau_t(B))A\| = 0 \ ,$$

and if $A \in \widehat{\mathfrak{A}}_{++}$ and $B \in \widehat{\mathfrak{A}}_{--}$ then

$$\lim_{t\to\pm\infty} \|A\tau_t(B) - \tau_t(B)\widetilde{\Theta}_+(A)\| = 0 \ .$$

These general conclusions remain valid if $h \neq 0$. Note that it is also possible to show that the automorphisms $\widetilde{\Theta}_\pm$ do not extend to $\widehat{\mathfrak{A}}$ (see Notes and Remarks).

A special case which is illuminating is the case $\gamma = 0$, i.e., the isotropic X–Y model. Then the infinitesimal time change is given by

$$\delta_\Phi(a_x^*) = \lim_{n\to\infty} i[H_n, a_x^*] = 2iJ(a_{x-1}^* + a_{x+1}^*) + 2iha_x^*$$

and this can be integrated by Fourier transformation to give

$$\tau_t(a_x^*) = \sum_{y\in\mathbb{Z}} G_t(x-y)a_y^*$$

where

$$G_t(x) = (2\pi)^{-1}\int_0^{2\pi} d\theta\, e^{ix\theta}e^{it(4J\cos\theta+2h)} \ .$$

Thus if $A = a_0^*a_0 = \sigma_+^0\sigma_-^0 = (\sigma_3^0 + \mathbb{1})/2$ then $\|[\tau_x\tau_t(A), A]\|$ is proportional to $|G_t(x)|$. But one finds that $|G_t(Vt)|$ decreases exponentially with t if $|V| > 4|J|$ and decreases

like $|t|^{-1/2}$ if $|V| < 4|J|$. Within the cone $|x|/|t| < 4|J|$ there is propagation which is essentially homogeneous and decreasing proportionally to $|t|^{-1/2}$ and outside the cone the propagation effects are exponentially small.

Throughout this subsection we have analyzed the time development of quantum spin systems as a norm limit of the local dynamics. For many interactions, e.g., long-range interactions, it is possible that the appropriate limits only exist in certain representations. (See Notes and Remarks.)

The periodic time behavior exhibited by the Ising interaction in Example 6.2.13 is easily seen to be typical of classical interactions and of course all elements of the classical subalgebra $\mathfrak{C}$ are left invariant. On the other hand it is not at all evident that the propagation exhibited by the X–Y model in Example 6.2.14 is typical of quantum interactions although this is believed to be the case.

6.2.2. The Gibbs Condition for Equilibrium

Throughout the rest of this section we analyze the equilibrium states of quantum spin systems and we often assume that the dynamics is given by a strongly continuous one-parameter group τ of *-automorphisms of the quantum spin algebra $\mathfrak{A}$. In this paragraph we compare the traditional Gibbs definition of equilibrium and the definition through the τ-KMS condition. Subsequently we discuss other characterizations of equilibrium.

First define the *local Gibbs state* associated with the interaction Φ by

$$\omega_\Lambda(A) = \frac{\mathrm{Tr}_{\mathfrak{H}_\Lambda}(e^{-H_\Phi(\Lambda)}A)}{\mathrm{Tr}_{\mathfrak{H}_\Lambda}(e^{-H_\Phi(\Lambda)})}$$

for all $A \in \mathfrak{A}_\Lambda$. Occasionally it is useful to indicate the dependence of ω_Λ on Φ and then we use the notation ω_Λ^Φ. It is also natural to insert a factor $\beta \in \mathbb{R}$, corresponding to the inverse temperature, in front of $H_\Phi(\Lambda)$ but for simplicity we often omit β.

Although ω_Λ is defined as a state on $\mathfrak{A}_\Lambda$, it has an extension to a state on $\mathfrak{A}$ by Proposition 2.3.24. Let ω_Λ^G denote an arbitrary such extension. The thermodynamic limit of ω_Λ as $\Lambda \to \infty$ can now be analyzed with the aid of the ω_Λ^G.

The spin algebra $\mathfrak{A}$ contains an identity and hence the state space $E_{\mathfrak{A}}$ is compact in the weak* topology. Therefore, there exist nets of extensions $\omega_{\Lambda_\alpha}^G$ of ω_{Λ_α} such that $\Lambda_\alpha \to \infty$ and $\omega_{\Lambda_\alpha}^G$ converges in the weak* topology to a state ω over $\mathfrak{A}$, i.e.,

$$\lim_\alpha \omega_{\Lambda_\alpha}^G(A) = \omega(A)$$

for all $A \in \mathfrak{A}$. Hence, ω is a thermodynamic limit point of the local Gibbs states in the sense that

$$\omega(A) = \lim_\alpha \omega_{\Lambda_\alpha}(A)$$

for all $A \in \mathfrak{A}_\Lambda$ and all Λ. Henceforth we define a state ω^Φ over $\mathfrak{A}$ to be a *thermodynamic limit point* of the local Gibbs states ω_Λ^Φ if it is the weak* limit of a net of extensions of ω_Λ^Φ to $\mathfrak{A}$.

It is a consequence of the general analysis of Chapter 5 that the thermodynamic limit points ω are KMS states.

Proposition 6.2.15. *Let Φ be an interaction of a quantum spin system, $\omega_\Lambda^{\beta\Phi}$ the local Gibbs states*

$$\omega_\Lambda^{\beta\Phi}(A) = \frac{\mathrm{Tr}_{\mathfrak{H}_\Lambda}(e^{-\beta H_\Phi(\Lambda)}A)}{\mathrm{Tr}_{\mathfrak{H}_\Lambda}(e^{-\beta H_\Phi(\Lambda)})}, \qquad A \in \mathfrak{A}_\Lambda \ ,$$

and τ^Λ the local automorphism groups

$$\tau_t^\Lambda(A) = e^{itH_\Phi(\Lambda)}Ae^{-itH_\Phi(\Lambda)}, \quad A \in \mathfrak{A} \ .$$

Assume that τ^Λ converges strongly to an automorphism group τ, i.e.,

$$\lim_{\Lambda\to\infty} \|\tau_t^\Lambda(A) - \tau_t(A)\| = 0$$

for all $A \in \mathfrak{A}$ and $t \in \mathbb{R}$.

It follows that every thermodynamic limit point $\omega^{\beta\Phi}$ of $\omega_\Lambda^{\beta\Phi}$ is a (τ, β)-KMS state over $\mathfrak{A}$.

Proof. As $\mathfrak{A}$ is separable $\omega^{\beta\Phi}$ is the weak* limit of a sequence of extensions of the local Gibbs states. Therefore the result follows from Proposition 5.3.25.

This proposition shows that the thermodynamic limits of the usual Gibbs states are KMS states and our aim is to derive a converse of this statement and thus deduce that the Gibbs equilibrium states are completely characterized by the KMS condition. It is, however, overly optimistic to expect a strict converse to the proposition. The difficulty is that the foregoing notion of Gibbs state is too restricted. The state ω_Λ^Φ describes a closed system, i.e., a system completely isolated in Λ and lacking interaction with the exterior. But external interactions, or interactions across the boundary of Λ, are of relevance whenever multiple phases, i.e., multiple thermodynamic equilibrium states are possible because these interactions influence the relative proportion and disposition of the phases. Thus, variation of the external interactions is necessary if one wishes to describe all equilibrium distributions. Hence, it is necessary to broaden the notion of Gibbs states to allow these external effects. There are two approaches. Either one may modify the interaction near the boundary of Λ in order to reproduce the boundary effects or one may consider the system as a subsystem of a larger system. Although these methods are conceptually different they are technically similar. We adopt the second point of view and refer to the subsystem as an *open system*, i.e., open to external interaction. We next introduce a set of states which describes equilibrium for open systems.

For orientation let us first examine the Gibbs state $\omega_{\Lambda'}$ of a finite spin system with interaction $\beta\Phi$. If $\Lambda \subset \Lambda'$ is a subsystem then the restriction of the Gibbs

state $\omega_{\Lambda'}$ to $\mathfrak{A}_\Lambda$ is not the Gibbs state ω_Λ of $\mathfrak{A}_\Lambda$. The restricted state describes particles in Λ interacting with particles in the external region $\Lambda'\backslash\Lambda$. If, however, the state $\omega_{\Lambda'}$ is modified by removal of the interaction across the boundary of Λ and $\Lambda'\backslash\Lambda$, then the restriction of the modification is equal to ω_Λ. In order to express this quantitatively reintroduce

$$W_\Phi(\Lambda\,;\Lambda') = \sum\{\Phi(X);\, X\cap\Lambda\neq\varnothing,\, X\cap\Lambda^c\neq\varnothing, X\subseteq\Lambda'\}\ ,$$

the energy of interaction across the border of Λ and $\Lambda'\backslash\Lambda$. Now subtraction of this external interaction corresponds to a perturbation of the state ω_Λ in the sense of Section 5.4.1 with the perturbation $P = \beta W_\Phi(\Lambda\,;\Lambda')$. Explicitly

$$\omega^P_{\Lambda'}(A) = \frac{\mathrm{Tr}_{\mathfrak{H}_{\Lambda'}}(e^{-\beta H_\Phi(\Lambda')+P}A)}{\mathrm{Tr}_{\mathfrak{H}_{\Lambda'}}(e^{-\beta H_\Phi(\Lambda')+P})} = \frac{\mathrm{Tr}_{\mathfrak{H}_{\Lambda'}}(e^{-\beta H_\Phi(\Lambda)}e^{-\beta H_\Phi(\Lambda'\backslash\Lambda)}A)}{\mathrm{Tr}_{\mathfrak{H}_{\Lambda'}}(e^{-\beta H_\Phi(\Lambda)}e^{-\beta H_\Phi(\Lambda'\backslash\Lambda)})}$$

and therefore

$$\omega^P_{\Lambda'} = \omega_\Lambda\otimes\omega_{\Lambda'\backslash\Lambda}\ .$$

In particular $\omega^P_{\Lambda'}\,|_{\mathfrak{A}_\Lambda} = \omega_\Lambda$.

Next consider the infinite system and assume that the interaction energy

$$W_\Phi(\Lambda) = \sum_{\substack{X\cup\Lambda\neq\varnothing\\ X\cup\Lambda^c\neq\varnothing}}\Phi(X) = \lim_{\Lambda'\to\infty} W_\Phi(\Lambda\,;\Lambda')$$

is well defined, i.e., the limit exists in norm. This energy represents the interaction of the subsystem Λ with the remainder of the system in the complement Λ^c of Λ. The above observations then motivate the following definition.

Definition 6.2.16. Let Φ be an interaction of a quantum spin system such that the surface energy $W_\Phi(\Lambda)$ is a well-defined element of $\mathfrak{A}$ for all $\Lambda\subset L$.

A state ω over $\mathfrak{A}$ is defined to satisfy the *Gibbs condition* with respect to $\beta\Phi$ if the following conditions are fulfilled.

(1) ω is faithful, i.e., Ω_ω is separating for $\pi_\omega(\mathfrak{A})''$

(2) $$\omega^{P_\Lambda} = \omega_\Lambda\otimes\tilde{\omega}$$

for all $\Lambda\subset L$, where ω_Λ is the local Gibbs state corresponding to Φ, $\tilde{\omega}$ is a state over $\mathfrak{A}_{\Lambda^c}$, ω^{P_Λ} is the perturbation of ω constructed in Theorem 5.4.4, and $P_\Lambda = \beta W_\Phi(\Lambda)$.

All limit points of the local Gibbs states satisfy the Gibbs condition. This follows from combining Proposition 6.2.15 and the following result.

Proposition 6.2.17. *Let Φ be an interaction of a quantum spin system and τ^Λ the corresponding local automorphism group. Assume that*

(1) *τ^Λ converges strongly to an automorphism group τ, i.e.,*

$$\lim_{\Lambda\to\infty}\|\tau^\Lambda_t(A) - \tau_t(A)\| = 0$$

for all $A\in\mathfrak{A}$ and $t\in\mathbb{R}$.

(2) *The surface energies* $W_\Phi(\Lambda)$ *are well-defined elements of* $\mathfrak{A}$ *for all* $\Lambda \subset L$.

It follows that every (τ, β)*-KMS state satisfies the Gibbs condition with respect to* $\beta\Phi$*, for all* $\beta \in \mathbb{R}$.

PROOF. If $\beta = 0$, the implication is trivial. If $\beta \neq 0$, it suffices, by rescaling, to consider the case $\beta = -1$. First let $Q = -(W_\Phi(\Lambda) + H_\Phi(\Lambda))$ and consider the perturbation $\tau^{\Lambda',Q}$ of the local groups $\tau^{\Lambda'}$ for all $\Lambda' \supset \Lambda$. It follows from assumption (1) and the definition of τ^Q that $\tau^{\Lambda',Q}$ converges strongly to an automorphism group τ^{Λ^c} which acts trivially on $\mathfrak{A}_\Lambda$ and which leaves $\mathfrak{A}_{\Lambda^c}$ invariant. Similarly if $P = -W_\Phi(\Lambda)$, one finds

$$\tau^P = \tau^\Lambda \otimes \tau^{\Lambda^c} \quad ,$$

where we identify τ^{Λ^c} with its restriction to $\mathfrak{A}_{\Lambda^c}$. But the corresponding perturbation ω^P of ω is a τ^P-KMS state by Theorem 5.4.4.

Next for $0 < B \in \mathfrak{A}_{\Lambda^c}$ define the state ω_B^P over $\mathfrak{A}_\Lambda$ by

$$\omega_B^P(A) = \frac{\omega^P(AB)}{\omega^P(B)} \quad .$$

As $\tau^P = \tau^\Lambda \otimes \tau^{\Lambda^c}$ the τ^P-KMS condition for ω^P implies that ω_B^P is a τ^Λ-KMS state. But ω_Λ is the unique such state by Example 5.3.31. Therefore, $\omega_B^P = \omega_\Lambda$ and

$$\omega^P(AB) = \omega_\Lambda(A)\omega^P(B)$$

for all $A \in \mathfrak{A}_\Lambda$ and $0 < B \in \mathfrak{A}_{\Lambda^c}$, i.e.,

$$\omega^P = \omega_\Lambda \otimes \omega^P|_{\mathfrak{A}_{\Lambda^c}} \quad .$$

Thus the Gibbs condition is valid.

The converse of this proposition is valid under slightly more stringent conditions on the interaction Φ. We first derive a result in which these conditions are stated in an implicit form and subsequently give alternative explicit assumptions which also imply the converse.

Theorem 6.2.18. *Let* Φ *be an interaction of a quantum spin system and* τ^Λ *the corresponding local automorphism group. Assume that:*

(1) τ^Λ *converges strongly to an automorphism group* τ*, i.e.,*

$$\lim_{\Lambda \to \infty} \|\tau_t^\Lambda(A) - \tau_t(A)\| = 0$$

for all $A \in \mathfrak{A}$ *and* $t \in \mathbb{R}$.

(2) *The surface energies* $W_\Phi(\Lambda)$ *are well-defined elements of* $\mathfrak{A}$ *for all* $\Lambda \subset L$,

(3)
$$D = \bigcup_{\Lambda \subset L} \mathfrak{A}_\Lambda$$

is a core for the generator δ *of* τ.

Then the following conditions are equivalent for each $\beta \in \mathbb{R}$:

(1) *ω satisfies the Gibbs condition with respect to $\beta\Phi$.*

(2) *ω is a (τ, β)-KMS state.*

Remark. If δ is a symmetric derivation defined on D, then one can always find an interaction Φ' such that $\delta = \delta_{\Phi'}$, and the surface energies $W_{\Phi'}(\Lambda)$ are well-defined elements of $\mathfrak{A}$. This follows from the Remark before Theorem 6.2.4. The surface energies are not well defined for all interactions defining δ, however. The same remark applies to later theorems on variational principles in this section.

PROOF. If $\beta = 0$, both conditions state that ω is a trace. Thus by rescaling it suffices to consider the case $\beta = -1$. Moreover, throughout the proof we identify $\pi_\omega(\mathfrak{A})$ and $\mathfrak{A}$.

(1) $\Rightarrow$ (2). By assumption, ω is separating. Let σ denote the corresponding modular automorphism group. Now for each $P = P^* \in \mathfrak{A}$ the perturbed state ω^P is also separating and has modular automorphism group σ^P where σ^P is the perturbation of σ introduced in Proposition 5.4.1. Choosing $P = -W_\Phi(\Lambda)$, the Gibbs condition implies that $\omega^P = \omega_\Lambda \otimes \tilde{\omega}$, where $\omega_\Lambda (= \omega_\Lambda^{-\Phi})$ is the local Gibbs state on $\mathfrak{A}_\Lambda$ and $\tilde{\omega}$ is a state on $\mathfrak{A}_{\Lambda^c}$. As ω^P is separating, it follows that both ω_Λ and $\tilde{\omega}$ must be separating. But the modular group of ω_Λ is the group τ^Λ and we let $\tilde{\tau}$ denote the modular group of $\tilde{\omega}$. Now $\omega^P = \omega_\Lambda \otimes \tilde{\omega}$ satisfies the modular ($(\tau, -1)$-KMS) condition with respect to $\tau = \tau^\Lambda \otimes \tilde{\tau}$ and therefore by the uniqueness of the modular group, Theorem 5.3.10, one has $\sigma^P = \tau^\Lambda \otimes \tilde{\tau}$. In particular $\sigma^P|_{\mathfrak{A}_\Lambda} = \tau^\Lambda$.

Next let δ_σ denote the generator of σ. It follows that the generator δ_{σ^P} of σ^P is given by $D(\delta_{\sigma^P}) = D(\delta_\sigma)$ and

$$\delta_\sigma(A) = \delta_{\sigma^P}(A) - i[P, A]$$

for all $A \in D(\delta_\sigma)$. Thus as σ^P and τ^Λ coincide on $\mathfrak{A}_\Lambda$ one concludes that $\mathfrak{A}_\Lambda \subset D(\delta_\sigma)$ and

$$\begin{aligned}\delta_\sigma(A) &= i[H_\Phi(\Lambda), A] + i[W_\Phi(\Lambda), A] \\ &= i \sum_{X \cap \Lambda \neq \varnothing} [\Phi(X), A] = \lim_{\Lambda' \to \infty} \delta_{\Lambda'}(A)\end{aligned}$$

for all $A \in \mathfrak{A}_\Lambda$, where we have introduced $\delta_{\Lambda'}$, by $D(\delta_{\Lambda'}) = D$ and

$$\delta_{\Lambda'}(A) = i \sum_{X \subset \Lambda'} [\Phi(X), A] \ ,$$

and the limit exists in the norm sense.

But if δ is the generator of τ, it follows from Theorem 3.1.28 that δ is the graph limit of $\delta_{\Lambda'}$ as $\Lambda' \to \infty$, hence $A \in D(\delta)$ and

$$\delta(A) = \delta_\sigma(A)$$

for all $A \in D$. But D is a core for δ. Hence D is a core for δ_σ and $\delta = \delta_\sigma$ by Theorem 3.1.19 and Proposition 3.2.52. It follows that $\tau = \sigma$, i.e., ω is a $(\tau, -1)$-KMS state.

(2) $\Rightarrow$ (1). This follows from Proposition 6.2.17.

If we combine this theorem with Theorem 6.2.4 we obtain a statement which involves the interaction in a much more explicit manner.

Corollary 6.2.19. *Let Φ be an interaction of a quantum spin system satisfying*

$$\|\Phi\|_\lambda = \sum_{n \geq 0} e^{\lambda n} \left(\sup_{x \in L} \sum_{\substack{X \ni x \\ |X| = n+1}} \|\Phi(X)\| \right) < +\infty$$

for some $\lambda > 0$ and let τ^Φ be the associated automorphism group (see Theorem 6.2.4).

The following conditions are equivalent:

(1) *ω satisfies the Gibbs condition with respect to $\beta\Phi$.*
(2) *ω is a (τ^Φ, β)-KMS state.*

PROOF. The restriction $\|\Phi\|_\lambda < +\infty$ is sufficient to ensure that $W_\Phi(\Lambda)$ is well defined. The other two hypotheses of Theorem 6.2.18 then follow from Theorem 6.2.4. Hence the two conditions are equivalent.

A similar result can be derived from the assumptions of Theorem 6.2.6.

EXAMPLE 6.2.20. Suppose L is homogeneous, the interaction Φ is of finite range and

$$\sup_{X \subset L} \|\Phi(X)\| < +\infty \ .$$

Then the assumptions of Corollary 6.2.19 are satisfied and a state ω is a (τ^Φ, β)-KMS state if, and only if, it satisfies the Gibbs condition with respect to $\beta\Phi$.

6.2.3. The Maximum Entropy Principle

The Gibbs states of isolated, i.e., closed, systems can be characterized by a principle of maximum entropy at fixed energy. This principle was outlined in Section 5.3.1 prior to Theorem 5.3.15 and it is often referred to as the principle of minimum free energy. Our intention is to give a more detailed description of this principle for quantum spin systems and to extend it to open systems.

The notion of entropy first arose in thermodynamics as a measure of the heat absorbed, or emitted, when external work is done on a system. In the subsequent development of classical statistical mechanics this quantity was related to the order, or disorder, of the microscopic particles which constitute the system. Thus, the principle of maximum entropy describes equilibrium as the state of maximum disorder compatible with a given energy or particle density, etc. The concept of entropy was then abstracted from statistical mechanics and used in both probability theory and information theory. In the former it constitutes a measure of the "uncertainty" and in the latter it measures the information content although a direct justification of these latter interpretations is difficult. Nevertheless, the entropy arises naturally in the

formalism of the law of large numbers and it is apparently this fact which leads to its general utility (see Notes and Remarks).

The relative entropy $S(\mu|\nu)$ of a probability measure $\mu \in M_1(X)$ with respect to a positive measure $\nu \in M_+(X)$ is usually defined by

$$\begin{aligned} S(\mu|\nu) &= -\int d\nu(\omega)\left(\frac{d\mu}{d\nu}\right)(\omega)\log\left(\frac{d\mu}{d\nu}\right)(\omega) \\ &= -\mu\left(\log\left(\frac{d\mu}{d\nu}\right)\right) \end{aligned}$$

if μ is absolutely continuous with respect to ν, and $-\infty$ if this is not the case. Thus if X is discrete with a finite number of points $\omega_1, \ldots, \omega_n$, and $\mu(\omega_i) = p_i$, $\nu(\omega_i) = q_i$, then

$$S(\mu|\nu) = -\sum_{i=1}^{n}(p_i \log p_i - p_i \log q_i) \ .$$

In particular the *entropy*, $S(\mu)$, of the measure μ with respect to the measure which gives unit weight to each point is given by

$$S(\mu) = -\sum_{i=1}^{n} p_i \log p_i \ .$$

In the sequel we need to generalize both these concepts, the entropy $S(\mu)$ and the relative entropy $S(\mu|\nu)$, to the states of quantum spin systems, and for the discussion of open subsystems it is also necessary to introduce a third concept, the conditional entropy. We begin by recalling the relevant description of a closed subsystem.

Each state ω of the local (matrix) subalgebra $\mathfrak{A}_\Lambda$ of the quantum spin system is determined by a unique density matrix ρ_Λ on $\mathfrak{H}_\Lambda$ in the form

$$\omega(A) = \mathrm{Tr}_{\mathfrak{H}_\Lambda}(\rho_\Lambda A)$$

for all $A \in \mathfrak{A}_\Lambda$, and the *entropy* $S_\Lambda(\omega)$ of ω is defined by

$$S_\Lambda(\omega) = -\mathrm{Tr}_{\mathfrak{H}_\Lambda}(\rho_\Lambda \log \rho_\Lambda) \ .$$

If $\{p_i\}_{1 \le i \le n}$ is a complete set of eigenvalues of ρ_Λ, this definition takes the classical form

$$S_\Lambda(\omega) = -\sum_{i=1}^{n} p_i \log p_i \ .$$

(The function $-x \log x$ is always defined by continuity to be zero at $x = 0$.) If φ is any other positive functional on $\mathfrak{A}_\Lambda$, then φ is also determined by a positive trace class operator σ_Λ, i.e.,

$$\varphi(A) = \mathrm{Tr}_{\mathfrak{H}_\Lambda}(\sigma_\Lambda A)$$

and one can define the *entropy of* ω *relative to* φ by

$$S(\omega|\varphi) = -\mathrm{Tr}_{\mathfrak{H}_\Lambda}(\rho_\Lambda \log \rho_\Lambda - \rho_\Lambda \log \sigma_\Lambda) \ .$$

Thus if ρ_Λ and σ_Λ commute,

$$S(\omega|\varphi) = -\sum_{i=1}^{n}(p_i \log p_i - p_i \log\ q_i)\ ,$$

where $\{q_i\}_{1\leq i\leq n}$ are the eigenvalues of σ_Λ. Therefore $S(\cdot|\cdot)$ is a natural extension of the classical relative entropy. The next lemma establishes that this generalized relative entropy is negative and the subsequent proposition demonstrates that this negativity is equivalent to the principle of maximum entropy, at fixed energy, for the Gibbs state of $\mathfrak{A}_\Lambda$.

Lemma 6.2.21. *Let A be a positive $n \times n$ matrix and B a strictly positive $n \times n$ matrix.*

It follows that

$$-\mathrm{Tr}(A \log A - A \log B) \leq \mathrm{Tr}(B - A)$$

with equality if, and only if, $A = B$.

Proof. Let $\{a_i\}_{1\leq i\leq n}$ and $\{b_i\}_{1\leq i\leq n}$ be complete sets of eigenvalues of A and B with corresponding orthonormal eigenvectors $\{\psi_i^A\}_{1\leq i\leq n}$ and $\{\psi_i^B\}_{1\leq i\leq n}$. One has

$$-\mathrm{Tr}(A \log A - A \log B) = -\sum_{i=1}^{n} a_i \log a_i + \sum_{i=1}^{n}\sum_{j=1}^{n} a_i |(\psi_i^A, \psi_j^B)|^2 \log b_j\ .$$

But

$$\sum_{j=1}^{n} |(\psi_i^A, \psi_j^B)|^2 \log b_j \leq \log \sum_{j=1}^{n} |(\psi_i^A, \psi_j^B)|^2 b_j = \log(\psi_i^A, B\psi_i^A)$$

by convexity of $x \to \log x$. Therefore,

$$\begin{aligned} -\mathrm{Tr}(A \log A - A \log B) &\leq \sum_{i=1}^{n}(\psi_i^A, B\psi_i^A)\left\{-\frac{a_i}{(\psi_i^A, B\psi_i^A)} \log \frac{a_i}{(\psi_i^A, B\psi_i^A)}\right\} \\ &\leq \sum_{i=1}^{n}(\psi_i^A, B\psi_i^A)\left\{1 - \frac{a_i}{(\psi_i^A, B\psi_i^A)}\right\} = \mathrm{Tr}(B - A)\ , \end{aligned}$$

where the second inequality follows from the convexity of $x \to -x \log x$ in the form

$$-x \log x \leq 1 - x\ .$$

This gives the desired inequality. But we have used two estimates and equality occurs in the first if, and only if, there is a relabeling $j \to j(i)$ such that ψ_i^A is proportional to $\psi_{j(i)}^B$ and equality occurs in the second if, and only if, $a_i = b_{j(i)}$. Hence equality occurs in the total estimate if, and only if, $A = B$.

Proposition 6.2.22. *Let ω and φ be states over the local subalgebra $\mathfrak{A}_\Lambda$ of the quantum spin system with corresponding density matrices ρ_Λ and σ_Λ.*

It follows that the relative entropy $S_\Lambda(\omega|\varphi)$ is negative, i.e.,

$$S_\Lambda(\omega|\varphi) = -\mathrm{Tr}_{\mathfrak{H}_\Lambda}(\rho_\Lambda \log \rho_\Lambda - \rho_\Lambda \log \sigma_\Lambda) \leq 0$$

and $S_\Lambda(\omega|\varphi) = 0$ if, and only if, $\omega = \varphi$.

Moreover if ω_Λ^Φ is the Gibbs state of $\mathfrak{A}_\Lambda$ corresponding to the interaction Φ, then

$$S_\Lambda(\omega|\omega_\Lambda^\Phi) = S_\Lambda(\omega) - \omega(H_\Phi(\Lambda)) + \log \mathrm{Tr}_{\mathfrak{H}_\Lambda}(e^{-H_\Phi(\Lambda)}) \ ,$$

where the entropy $S_\Lambda(\omega)$ is given by

$$S_\Lambda(\omega) = -\mathrm{Tr}_{\mathfrak{H}_\Lambda}(\rho_\Lambda \log \rho_\Lambda) \ .$$

Consequently ω_Λ^Φ is the unique state which maximizes the functional

$$\omega \in E_{\mathfrak{A}_\Lambda} \ \rightarrow \ F_\Lambda(\omega) = S_\Lambda(\omega) - \omega(H_\Phi(\Lambda))$$

and the maximal value is given by

$$\log \mathrm{Tr}_{\mathfrak{H}_\Lambda}(e^{-H_\Phi(\Lambda)}) \ .$$

Proof. The first statement follows from Lemma 6.2.21 with the choice $A = \rho_\Lambda$ and $B = \sigma_\Lambda$ because

$$\mathrm{Tr}(A - B) = \mathrm{Tr}_{\mathfrak{H}_\Lambda}(\rho_\Lambda - \sigma_\Lambda) = 1 - 1 = 0 \ .$$

The other statements follow from the first by noting that the Gibbs state is determined by the density matrix

$$\sigma_\Lambda = \frac{e^{-H_\Phi(\Lambda)}}{\mathrm{Tr}_{\mathfrak{H}_\Lambda}(e^{-H_\Phi(\Lambda)})} \ .$$

Remark. The function

$$\omega \in E_{\mathfrak{A}_\Lambda} \mapsto \omega(H_\Phi(\Lambda)) - \beta^{-1} S_\Lambda(\omega)$$

is often called the *free energy* of the spin system at inverse temperature β. Thus, the Gibbs state $\omega^{\beta\Phi}$ is the unique state which minimizes this energy. The term free energy is also used for the minimum value

$$F_\Lambda(\beta\Phi) = -\beta^{-1} \log \mathrm{Tr}_{\mathfrak{H}_\Lambda}(e^{-\beta H_\Phi(\Lambda)})$$

of this function. In the lattice gas interpretation this latter quantity corresponds to the pressure.

In order to extend the maximum entropy principle to open systems it is necessary to analyze properties of the entropy $S_\Lambda(\omega)$ both as a function of the finite subsets $\Lambda \subset L$ and of the state $\omega \in E_{\mathfrak{A}_\Lambda}$. Moreover, one must extend the notion of relative entropy to pairs of states of the total spin system. We begin by analyzing the entropy.

First, remark that as $x \in [0, 1] \mapsto -x \log x$ is positive, the entropy must be positive. Next, note that if ν is chosen to be the (normalized) trace-state over $\mathfrak{A}_\Lambda$, then $S_\Lambda(\omega|\nu) \leq 0$ implies that

$$S_\Lambda(\omega) \leq \log\{(N+1)^{|\Lambda|}\} \ .$$

Thus

$$0 \ \leq \ S_\Lambda(\omega) \ \leq \ |\Lambda| \log(N+1) \ .$$

Moreover, $S(\omega|\nu) = 0$ if, and only if, $\omega = \nu$ and hence $S_\Lambda(\omega)$ attains its upper bound if, and only if, ω is the trace-state.

It should be emphasized that $S_\Lambda(\omega)$ is an extensive quantity, i.e., it is essentially proportional to $|\Lambda|$, and hence the total entropy

$$\lim_{\Lambda \to \infty} S_\Lambda(\omega)$$

of a state ω is only finite under exceptional circumstances. A more suitable global measurement of entropy is the entropy per unit volume

$$\lim_{\Lambda \to \infty} \frac{S_\Lambda(\omega)}{|\Lambda|}$$

of ω and we will examine this quantity for translationally invariant states in the next subsection.

EXAMPLE 6.2.23. Let ω be a product state over $\mathfrak{A}$, i.e., if $\rho_{\{x\}}$ denotes the density matrix determining $\omega|_{\mathfrak{A}_{\{x\}}}$, then the density matrix ρ_Λ which determines $\omega|_{\mathfrak{A}_\Lambda}$ is given by

$$\rho_\Lambda = \prod_{x \in \Lambda}{}^{\otimes} \rho_{(x)} \ .$$

It follows immediately that

$$S_\Lambda(\omega) = \sum_{x \in \Lambda} S_{\{x\}}(\omega) \ .$$

Hence $\Lambda \to S_\Lambda(\omega)$ is monotonically increasing and the total entropy

$$\lim_{\Lambda \to \infty} S_\Lambda(\omega) = \sum_{x \in L} S_{\{x\}}(\omega)$$

is well defined but it is only finite if $x \mapsto S_{\{x\}}(\omega)$ is summable. But $S_{\{x\}}(\omega) = 0$ if, and only if, $\omega|_{\mathfrak{A}_{\{x\}}}$ is pure and $S_{\{x\}}(\omega)$ is small if, and only if, $\omega|_{\mathfrak{A}_{\{x\}}}$ is "almost pure" in the sense that one eigenvalue of $\rho_{\{x\}}$ is close to one and the others are close to zero. Thus, for ω to have finite entropy the restrictions $\omega|_{\mathfrak{A}_{\{x\}}}$ must be predominantly "almost pure." Thus, finite entropy is only possible for states which are pure in this very strong sense.

Probably the most important property of $\Lambda \mapsto S_\Lambda(\omega)$ is *strong sub-additivity*.

Proposition 6.2.24. *The entropy $\Lambda \subset L \mapsto S_\Lambda(\omega) \in \mathbb{R}$ of each state ω over $\mathfrak{A}_\Lambda$ satisfies the strong subadditivity inequality*

$$S_{\Lambda_1 \cup \Lambda_2 \cup \Lambda_3}(\omega) - S_{\Lambda_1 \cup \Lambda_2}(\omega) \leq S_{\Lambda_1 \cup \Lambda_3}(\omega) - S_{\Lambda_1}(\omega)$$

for all mutually disjoint $\Lambda_1, \Lambda_2, \Lambda_3 \subset L$.

The proof of this proposition consists of a rather long, but elementary, series of arguments based upon convexity and positivity or convexity combined with complex analysis. As this proof is not very illuminating we omit the details

(see Notes and Remarks) and satisfy ourselves with comments on two special cases.

Note that $S_\emptyset(\omega) = 0$ by definition and hence setting $\Lambda_1 = \emptyset$ in the strong subadditivity inequality one finds the usual subadditivity property

$$S_{\Lambda_2 \cup \Lambda_3}(\omega) \leq S_{\Lambda_2}(\omega) + S_{\Lambda_3}(\omega)$$

for $\Lambda_2 \cap \Lambda_3 = \emptyset$. This explains the terminology strong subadditivity. Moreover, the ordinary subadditivity follows directly from Lemma 6.2.21 by choosing $A = \rho_{\Lambda_2 \cup \Lambda_3}$ and $B = \rho_{\Lambda_2} \otimes \rho_{\Lambda_3}$.

Strong subadditivity is also easy to derive whenever the various ρ_Λ commute. For example, if ω is faithful, the ρ_Λ are invertible and

$$\begin{aligned}(S_{\Lambda_1 \cup \Lambda_2 \cup \Lambda_3}(\omega) - S_{\Lambda_1 \cup \Lambda_2}(\omega)) - (S_{\Lambda_1 \cup \Lambda_3}(\omega) - S_{\Lambda_1}(\omega)) \\ = -\operatorname{Tr}_{\mathfrak{H}_{\Lambda_1 \cup \Lambda_2 \cup \Lambda_3}}(\rho_{\Lambda_1 \cup \Lambda_2 \cup \Lambda_3} \log X) \ ,\end{aligned}$$

where

$$X = \rho_{\Lambda_1 \cup \Lambda_2 \cup \Lambda_3} \rho_{\Lambda_1} \rho^{-1}_{\Lambda_1 \cup \Lambda_2} \rho^{-1}_{\Lambda_1 \cup \Lambda_3} \ .$$

But convexity of $x \to -x \log x$ gives $-x \log x \leq 1 - x$. Hence

$$-\log X \leq X^{-1} - \mathbb{1}$$

and strong subadditivity follows immediately. Nonfaithful ω can be handled by approximation.

The next proposition summarizes various properties of the function $\Lambda, \omega \mapsto S_\Lambda(\omega)$. Some of these properties will only be relevant in the following subsection when we discuss translationally invariant states and interactions.

Proposition 6.2.25. *For each $\Lambda \subset L$ the function*

$$\omega \in E_{\mathfrak{A}} \mapsto S_\Lambda(\omega) \in \mathbb{R}$$

is continuous, when $E_{\mathfrak{A}}$ is equipped with the weak topology, and concave, i.e.,*

$$S_\Lambda(\lambda\omega_1 + (1-\lambda)\omega_2) \geq \lambda S_\Lambda(\omega_1) + (1-\lambda) S_\Lambda(\omega_2) \ .$$

Further it satisfies the "convexity" relation

$$\begin{aligned}&S_\Lambda(\lambda\omega_1 + (1-\lambda)\omega_2) \\ &\qquad \leq \lambda S_\Lambda(\omega_1) + (1-\lambda) S_\Lambda(\omega_2) - \lambda \log \lambda - (1-\lambda)\log(1-\lambda)\end{aligned}$$

and the triangle inequality

$$|S_{\Lambda_1}(\omega) - S_{\Lambda_2}(\omega)| \leq S_{\Lambda_1 \cup \Lambda_2}(\omega) \leq S_{\Lambda_1}(\omega) + S_{\Lambda_2}(\omega)$$

for all disjoint $\Lambda_1, \Lambda_2 \subset L$.

Proof. If $\omega_\alpha \to \omega$ in the weak* topology on $E_{\mathfrak{A}}$, then $\omega_\alpha|_{\mathfrak{A}_\Lambda} \to \omega|_{\mathfrak{A}_\Lambda}$ in the weak* topology on $E_{\mathfrak{A}_\Lambda}$. But $\mathfrak{A}_\Lambda$ is a matrix algebra and hence $\omega_\alpha|_{\mathfrak{A}_\Lambda} \to \omega|_{\mathfrak{A}_\Lambda}$ in the uniform topology. In particular, the density matrices ρ^α_Λ corresponding to $\omega_\alpha|_{\mathfrak{A}_\Lambda}$ converge in norm to ρ_Λ. Thus, if $\{\lambda^\alpha_i\}$ and $\{\lambda_i\}$ denote the eigenvalues of ρ^α_Λ and ρ_Λ, arranged in

decreasing order and repeated according to multiplicity, perturbation theory implies that $\lambda_i^\alpha \to \lambda_i$. Therefore

$$S_\Lambda(\omega_\alpha) = -\sum_i \lambda_i^\alpha \log \lambda_i^\alpha \to -\sum_i \lambda_i \log \lambda_i = S_\Lambda(\omega) \ ,$$

i.e., S_Λ is continuous.

To prove concavity let $\rho_\Lambda^{(1)}$ and $\rho_\Lambda^{(2)}$ denote the density matrices corresponding to ω_1 and ω_2 over $\mathfrak{A}_\Lambda$. Let E_1 and E_2 be two mutually orthogonal rank-one projections in $\mathfrak{A}_{\Lambda'}$ for some Λ' with $\Lambda \cap \Lambda' = \varnothing$ and define ω as the state over $\mathfrak{A}_{\Lambda \cup \Lambda'}$ with density matrix

$$\rho = \lambda \rho_\Lambda^{(1)} \otimes E_1 + (1-\lambda)\rho_\Lambda^{(2)} \otimes E_2 \ .$$

One has

$$S_\Lambda(\omega) = S_\Lambda(\lambda\omega_1 + (1-\lambda)\omega_2)$$

and

$$S_{\Lambda\cup\Lambda'}(\omega) - S_{\Lambda'}(\omega) = \lambda S_\Lambda(\omega_1) + (1-\lambda)S_\Lambda(\omega_2) \ .$$

Thus concavity follows from subadditivity.

Next note that

$$\lambda\rho_\Lambda^{(1)} + (1-\lambda)\rho_\Lambda^{(2)} \geq \lambda\rho_\Lambda^{(1)} \geq 0$$

and hence

$$\log(\lambda\rho_\Lambda^{(1)} + (1-\lambda)\rho_\Lambda^{(2)}) \geq \log \lambda\rho_\Lambda^{(1)} \ .$$

(This last conclusion follows from the representation

$$\log A - \log B = \int_0^\infty d\lambda \left(\frac{1}{B+\lambda\mathbb{1}} - \frac{1}{A+\lambda\mathbb{1}} \right)$$

for $A, B > 0$ and Proposition 2.2.13.) Therefore

$$\begin{aligned} -\lambda \mathrm{Tr}_{\mathfrak{H}_\Lambda}(\rho_\Lambda^{(1)} \log(\lambda\rho_\Lambda^{(1)} + (1-\lambda)\rho_\Lambda^{(2)})) &\leq -\lambda \mathrm{Tr}_{\mathfrak{H}_\Lambda}(\rho_\Lambda^{(1)} \log \lambda\rho_\Lambda^{(1)}) \\ &= -\lambda \log \lambda + \lambda S_\Lambda(\omega_1) \ . \end{aligned}$$

Similarly

$$\begin{aligned} &-(1-\lambda)\mathrm{Tr}_{\mathfrak{H}_\Lambda}(\rho_\Lambda^{(2)} \log(\lambda\rho_\Lambda^{(1)} + (1-\lambda)\rho_\Lambda^{(2)})) \\ &\qquad \leq -(1-\lambda)\log(1-\lambda) + (1-\lambda)S_\Lambda(\omega_2) \ . \end{aligned}$$

The "convexity" relation follows by addition.

The right-hand side of the triangle inequality is subadditivity which results from Proposition 6.2.24. To establish the left-hand side we proceed as follows.

Let ρ be a density matrix on the n-dimensional space $\mathfrak{H}$ with eigenvalues $\{\lambda_i\}_{1 \leq i \leq n}$ and corresponding orthonormal eigenvectors $\{\psi_i\}_{1 \leq i \leq n}$. Further let $\mathfrak{H}'$ be an m-dimensional space with an orthonormal basis $\{\varphi_i\}_{1 \leq i \leq m}$, where $m \geq n$ If E is the one-dimensional projection on $\mathfrak{H} \otimes \mathfrak{H}'$ with range

$$\psi_E = \sum_{i=1}^n \lambda_i^{1/2} \psi_i \otimes \varphi_i \ ,$$

it follows that

$$\mathrm{Tr}_{\mathfrak{H}\otimes\mathfrak{H}'}(E(A\otimes\mathbb{1}))=\mathrm{Tr}_{\mathfrak{H}}(\rho A)\ ,$$

$$\mathrm{Tr}_{\mathfrak{H}\otimes\mathfrak{H}'}(E(\mathbb{1}\otimes B))=\mathrm{Tr}_{\mathfrak{H}'}(\rho' B)\ ,$$

where ρ' denotes the density matrix on $\mathfrak{H}'$ whose first n eigenvalues are λ_i, with corresponding eigenvectors φ_i, and whose remaining eigenvalues are zero.

Thus it follows from these observations that if ω is a state over $\mathfrak{A}_\Lambda$, then one can find Λ' with $\Lambda\cap\Lambda'=\varnothing$ and a state $\tilde\omega$ over $\mathfrak{A}_{\Lambda\cup\Lambda'}$ such that (1) $\tilde\omega|_{\mathfrak{A}_\Lambda}=\omega$, (2) the density matrix corresponding to $\tilde\omega$ is one-dimensional, i.e., $\tilde\omega$ is a pure state, and (3) $S_\Lambda(\tilde\omega)=S_\Lambda(\omega)=S_{\Lambda'}(\tilde\omega)$. By a similar argument it follows that if $\tilde\omega$ is any pure state on $\mathfrak{A}_{\Lambda\cup\Lambda'}=\mathfrak{A}_\Lambda\otimes\mathfrak{A}_{\Lambda'}$, then $S_\Lambda(\tilde\omega)=S_{\Lambda'}(\tilde\omega)$.

Therefore, replacing Λ by $\Lambda\cup\Lambda'$, we can consider ω, over $\mathfrak{A}_{\Lambda\cup\Lambda'}$, to be the restriction of a pure state $\tilde\omega$ over $\mathfrak{A}_{\Lambda\cup\Lambda'\cup\Lambda''}$ for some $\Lambda''\subset L$. It follows from purity that $S_{\Lambda\cup\Lambda'\cup\Lambda''}(\tilde\omega)=0$ and $S_{\Lambda'\cup\Lambda''}(\tilde\omega)=S_\Lambda(\tilde\omega)=S_\Lambda(\omega)$. Finally an application of Proposition 6.2.24 with the identifications $\Lambda_1=\Lambda'$, $\Lambda_2=\Lambda$, $\Lambda_3=\Lambda''$, and $\omega=\tilde\omega$ gives

$$-S_{\Lambda\cup\Lambda'}(\omega)\le S_\Lambda(\omega)-S_{\Lambda'}(\omega)\ .$$

Thus by interchange of Λ and Λ' one concludes that

$$S_{\Lambda\cup\Lambda'}(\omega)\ge|S_\Lambda(\omega)-S_{\Lambda'}(\omega)|\ .$$

Proposition 6.2.24 is basically a statement concerning the difference $S_{\Lambda\cup\Lambda'}(\omega)-S_{\Lambda'}(\omega)$ and Proposition 6.2.25 gives further information concerning this difference which we summarize in the following.

Proposition 6.2.26. *For $\Lambda\subset L$ consider the functional*

$$(\Lambda',\omega)\in\Lambda^c\times E_{\mathfrak{A}}\mapsto S_{\Lambda,\Lambda'}(\omega)=S_{\Lambda\cup\Lambda'}(\omega)-S_{\Lambda'}(\omega)\ .$$

It follows that:

(1) *For $\omega\in E_{\mathfrak{A}}$ fixed, $\Lambda'\subset\Lambda^c\mapsto S_{\Lambda,\Lambda'}(\omega)$ is decreasing.*

(2) $|S_{\Lambda,\Lambda}(\omega)|\le S_\Lambda(\omega)\le|\Lambda|\log(N+1)$.

(3) *For Λ and Λ' fixed $\omega\mapsto S_{\Lambda,\Lambda'}(\omega)$ is continuous if $E_{\mathfrak{A}}$ is equipped with the weak* topology.*

(4) *For Λ and Λ' fixed $\omega\mapsto S_{\Lambda,\Lambda'}(\omega)$ is concave, i.e.,*

$$S_{\Lambda,\Lambda'}(\lambda\omega_1+(1-\lambda)\omega_2)\ge\lambda S_{\Lambda,\Lambda'}(\omega_1)+(1-\lambda)S_{\Lambda,\Lambda'}(\omega_2)$$

and satisfies the "convexity" relation

$$\begin{aligned}S_{\Lambda,\Lambda'}(\lambda\omega_1+(1-\lambda)\omega_2)\le{}&\lambda S_{\Lambda,\Lambda'}(\omega_1)+(1-\lambda)S_{\Lambda,\Lambda'}(\omega_2)\\&-\lambda\log\lambda-(1-\lambda)\log(1-\lambda)\end{aligned}$$

for $0\le\lambda\le1$ and $\omega_1,\omega_2\in E_{\mathfrak{A}}$.

Proof. (1) This is a reformulation of Proposition 6.2.24.

(2) This follows from the triangle inequality of Proposition 6.2.25.

(3) Again this follows from the continuity of $S_\Lambda(\omega)$ given in Proposition 6.2.25.

(4) Let ω_1 and ω_2, be states $\mathfrak{A}_{\Lambda\cup\Lambda'}$ with corresponding density matrices $\rho^{(1)}_{\Lambda\cup\Lambda'}$ and $\rho^{(2)}_{\Lambda\cup\Lambda'}$. Next let E_1 and E_2 be mutually orthogonal rank-one projections in $\mathfrak{A}_{\Lambda''}$ for some Λ'' with $\Lambda''\cap(\Lambda\cup\Lambda')=\varnothing$. Now define ω as the state over $\mathfrak{A}_{\Lambda\cup\Lambda'\cup\Lambda''}$ with density matrix

$$\rho = \lambda\rho^{(1)}_{\Lambda\cup\Lambda'}\otimes E_1 + (1-\lambda)\rho^{(2)}_{\Lambda\cup\Lambda'}\otimes E_2 \ .$$

Thus

$$S_{\Lambda\cup\Lambda'}(\omega) - S_{\Lambda'}(\omega) = S_{\Lambda,\Lambda'}(\lambda\omega_1 + (1-\lambda)\omega_2)$$

and

$$S_{\Lambda\cup\Lambda'\cup\Lambda''}(\omega) - S_{\Lambda'\cup\Lambda''}(\omega) = \lambda S_{\Lambda,\Lambda'}(\omega_1) + (1-\lambda)S_{\Lambda,\Lambda'}(\omega_2) \ .$$

Concavity of $S_{\Lambda,\Lambda'}$, now follows from Proposition 6.2.24.

The convexity relation for $S_{\Lambda,\Lambda'}$ is a consequence of the concavity of S_Λ, and the convexity relation for S_Λ, established in Proposition 6.2.25.

The difference $S_{\Lambda\cup\Lambda'}(\omega) - S_{\Lambda'}(\omega)$ measures the entropy of the spin system on $\Lambda\cup\Lambda'$, in the state ω, minus the entropy of the system on Λ'. Thus, it measures the entropy of the Λ-subsystem in interaction with the Λ'-subsystem. Therefore, the entropy of the Λ-subsystem in interaction with the remainder of the lattice system is given by the limit of this difference as $\Lambda'\to\Lambda^c$. The limit exists because $\Lambda'\mapsto S_{\Lambda,\Lambda'}(\omega)$ is decreasing by Proposition 6.2.26 (1) and this limit is often called the conditional entropy. It represents the entropy of the Λ-subsystem conditioned by interaction with the exterior.

It is also referred to as the entropy of the open Λ-subsystem in contradistinction to $S_\Lambda(\omega)$ which measures the entropy of the isolated, or closed, subsystem.

Definition 6.2.27. Let $S_\Lambda(\omega)$ denote the entropy of the subsystem Λ of the quantum spin system in the state $\omega\in E_{\mathfrak{A}}$. The corresponding *conditional entropy* $\tilde{S}_\Lambda(\omega)$ is defined by

$$\begin{aligned}\tilde{S}_\Lambda(\omega) &= \inf_{\Lambda'\subset\Lambda^c}(S_{\Lambda\cup\Lambda'}(\omega) - S_{\Lambda'}(\omega))\\ &= \lim_{\Lambda'\to\Lambda^c}(S_{\Lambda\cup\Lambda'}(\omega) - S_{\Lambda'}(\omega)) \ .\end{aligned}$$

The conditional entropy $\tilde{S}_\Lambda(\omega)$ is again an extensive quantity, i.e., essentially proportional to $|\Lambda|$. In fact, if ω is a product state, then $\tilde{S}_\Lambda(\omega) = S_\Lambda(\omega)$ and we have already argued that $S_\Lambda(\omega)$ is extensive (see Example 6.2.23). Several basic properties of $\tilde{S}_\Lambda(\omega)$ follow immediately from Propositions 6.2.24–6.2.26.

Proposition 6.2.28. *The conditional entropy $\tilde{S}_\Lambda(\omega)$ has the following properties:*

(1) *For $\omega\in E_{\mathfrak{A}}$ fixed, the function $\Lambda\subset L\mapsto\tilde{S}_\Lambda(\omega)\in\mathbb{R}$ satisfies*

(a) (*Strong superadditivity*)

$$\tilde{S}_{\Lambda_1\cup\Lambda_2\cup\Lambda_3}(\omega) - \tilde{S}_{\Lambda_1\cup\Lambda_2}(\omega) \geq \tilde{S}_{\Lambda_1\cup\Lambda_3}(\omega) - \tilde{S}_{\Lambda_1}(\omega)$$

for Λ_1, Λ_2, and Λ_3 mutually disjoint.

(b) $$|\tilde{S}_\Lambda(\omega)| \leq S_\Lambda(\omega) \ .$$

(2) *For $\Lambda \subset L$ fixed, the function $\omega \in E_{\mathfrak{A}} \mapsto \tilde{S}_\Lambda(\omega) \in \mathbb{R}$ is upper semi-continuous if $E_{\mathfrak{A}}$ is equipped with the weak* topology and*

$$\lambda\tilde{S}_\Lambda(\omega_1) + (1-\lambda)\tilde{S}_\Lambda(\omega_2) - \lambda\log\lambda - (1-\lambda)\log(1-\lambda)$$
$$\geq \tilde{S}_\Lambda(\lambda\omega_1 + (1-\lambda)\omega_2) \geq \lambda\tilde{S}_\Lambda(\omega_1) + (1-\lambda)\tilde{S}_\Lambda(\omega_2)$$

for $0 \leq \lambda \leq 1$ and $\omega_1, \omega_2 \in E_{\mathfrak{A}}$.

PROOF.

(1a) By definition

$$\begin{aligned}
&\tilde{S}_{\Lambda_1\cup\Lambda_2\cup\Lambda_3}(\omega) - \tilde{S}_{\Lambda_1\cup\Lambda_2}(\omega) - \tilde{S}_{\Lambda_1\cup\Lambda_3}(\omega) + \tilde{S}_{\Lambda_1}(\omega) \\
&\quad = \lim_{\Lambda_0 \to (\Lambda_1\cup\Lambda_2\cup\Lambda_3)^c} \{(S_{\Lambda_0\cup\Lambda_1\cup\Lambda_2\cup\Lambda_3}(\omega) - S_{\Lambda_0}(\omega)) \\
&\qquad - (S_{\Lambda_0\cup\Lambda_1\cup\Lambda_2\cup\Lambda_3}(\omega) - S_{\Lambda_0\cup\Lambda_3}(\omega)) - (S_{\Lambda_0\cup\Lambda_1\cup\Lambda_2\cup\Lambda_3}(\omega) - S_{\Lambda_0\cup\Lambda_2}(\omega)) \\
&\qquad + (S_{\Lambda_0\cup\Lambda_1\cup\Lambda_2\cup\Lambda_3}(\omega) - S_{\Lambda_0\cup\Lambda_2\cup\Lambda_3}(\omega))\} \\
&\quad = \lim_{\Lambda_0 \to (\Lambda_1\cup\Lambda_2\cup\Lambda_3)^c} \{-S_{\Lambda_0\cup\Lambda_2\cup\Lambda_3}(\omega) + S_{\Lambda_0\cup\Lambda_3}(\omega) + S_{\Lambda_0\cup\Lambda_2}(\omega) - S_{\Lambda_0}(\omega)\} \\
&\quad \geq 0
\end{aligned}$$

where the inequality follows from the strong subadditivity of $S_\Lambda(\omega)$.

(1b) This is an immediate consequence of (2) of Proposition 6.2.26.

(2) By definition $\tilde{S}_\Lambda$ is the infimum over the family of functions $S_{\Lambda\cup\Lambda'} - S_\Lambda$. But these are continuous by Proposition 6.2.26 (3) and hence $\tilde{S}_\Lambda$ is upper semi-continuous. The concavity-convexity relations follow directly from (4) of Proposition 6.2.26.

Proposition 6.2.22 established that the Gibbs states of a closed subsystem are given by maximizing the entropy at fixed energy. But the conditional entropy measures the entropy of an open subsystem of the infinite system and our aim is to demonstrate that the states satisfying the Gibbs condition are exactly those which maximize the conditional entropy with the conditional energy fixed. By *conditional energy* we now mean the energy of the open subsystem, i.e., the subsystem in interaction with its surroundings. This principle of maximal conditional entropy is also referred to as *local thermodynamic stability*.

If one refers to Proposition 6.2.22 one sees that the maximum entropy principle for closed systems follows from the negativity of the relative entropy of finite systems. The same is basically true for the infinite spin system but in order to establish this it is first necessary to generalize the notion of relative entropy. We next extend this notion to pairs of faithful states of $\mathfrak{A}$, i.e., states ω such that Ω_ω is separating for $\pi_\omega(\mathfrak{A})''$. In fact we define relative entropy for pairs of faithful normal states of a von Neumann algebra and then use this to discuss the corresponding notion for states of a C^*-algebra. (It is possible to introduce the relative entropy of nonfaithful states but this is not directly relevant to the discussion of equilibrium states.)

Let $\mathfrak{M}$ be a von Neumann algebra acting on a Hilbert space $\mathfrak{H}$ and let $\xi_1, \xi_2 \in \mathfrak{H}$ be two vectors which are both cyclic and separating for $\mathfrak{M}$. Next reintroduce S_{ξ_1,ξ_2} as the closure of the operator defined on $\mathfrak{M}\xi_2$ by

$$S_{\xi_1,\xi_2} A\xi_2 = A^*\xi_1 \ .$$

This operator was already discussed in Chapter 2 and in particular Lemma 2.5.33 established closability. Let

$$S_{\xi_1,\xi_2} = J_{\xi_1,\xi_2}\Delta^{1/2}_{\xi_1,\xi_2}$$

denote the polar decomposition of S_{ξ_1,ξ_2}. The selfadjoint operator

$$\Delta_{\xi_1,\xi_2} = S^*_{\xi_1,\xi_2} S_{\xi_1,\xi_2}$$

is called *the relative modular operator* of $(\mathfrak{M}, \xi_1, \xi_2)$. It is instrumental in the following, useful, definition of relative entropy.

Definition 6.2.29. Let ω_1 and ω_2 be two faithful normal positive linear functionals over a von Neumann algebra $\mathfrak{M}$, and Ω_1 and Ω_2 the unique vector representatives of ω_1 and ω_2 in the natural positive cone $\mathscr{P} = \mathscr{P}_{\Omega_1} = \mathscr{P}_{\Omega_2}$. The *relative entropy* of ω_1 and ω_2 is defined by

$$S(\omega_1|\omega_2) = \int_0^\infty d(\Omega_1, E(\lambda)\Omega_1)\log\lambda \ ,$$

where E is the spectral family of the relative modular operator $\Delta_{\Omega_2,\Omega_1}$, i.e.,

$$\Delta_{\Omega_2,\Omega_1} = \int_0^\infty dE(\lambda)\lambda \ .$$

Let ω_1 and ω_2 be two positive forms over a C^*-algebra such that their unique normal extensions $\tilde{\omega}_1$ and $\tilde{\omega}_2$ to $\mathfrak{M} = (\pi_{\omega_1} \oplus \pi_{\omega_2}(\mathfrak{A}))''$ are faithful. The *relative entropy* of ω_1 and ω_2 is then defined by

$$S(\omega_1|\omega_2) = S(\tilde{\omega}_1|\tilde{\omega}_2) \ .$$

We now analyze various basic properties of the relative entropy.

First note that $\Delta_{\sqrt{\lambda_2}\Omega_2,\sqrt{\lambda_1}\Omega_1} = (\lambda_2/\lambda_1)\Delta_{\Omega_2,\Omega_1}$ and hence

$$S(\lambda_1\omega_1|\lambda_2\omega_2) = \lambda_1 S(\omega_1|\omega_2) + \lambda_1\log(\lambda_2/\lambda_1)\omega_1(\mathbb{1}) \ ,$$

and in particular

$$S(\lambda\omega_1|\lambda\omega_2) = \lambda S(\omega_1|\omega_2) \ ,$$

i.e., $(\omega_1, \omega_2) \mapsto S(\omega_1|\omega_2)$ is homogeneous of order one.

Next remark that $\log\lambda \leq \lambda - 1$ and hence

$$\begin{aligned} S(\omega_1|\omega_2) &\leq \int_0^\infty d(\Omega_1, E(\lambda)\Omega_1)(\lambda - 1) \\ &= (\Omega_1, \Delta_{\Omega_2,\Omega_1}\Omega_1) - (\Omega_1,\Omega_1) = (\Omega_2,\Omega_2) - (\Omega_1,\Omega_1) \ . \end{aligned}$$

Thus if ω_1 and ω_2 are states, $(\Omega_2,\Omega_2) = 1 = (\Omega_1,\Omega_1)$, and one concludes that $S(\omega_1|\omega_2)$ is negative. Moreover, $S(\omega_1|\omega_2) = 0$ if, and only if, $E(\lambda)$ is con-

centrated at the point $\lambda = 1$. But this only occurs if $\Delta_{\Omega_2,\Omega_1} = \mathbb{1}$ and hence $S(\omega_1|\omega_2) = 0$ if, and only if, $\omega_1 = \omega_2$.

In contrast to the entropy and conditional entropy the relative entropy of states of a spin system is a global quantity. Nevertheless, one can argue that $S(\omega_1|\omega_2)$ takes finite values only for pairs of states which are globally similar. This qualitative notion will be illustrated in Example 6.2.31. It motivates the following examination of the entropy of a state ω relative to a perturbed state ω^P.

Let ω be a faithful state on the von Neumann algebra $\mathfrak{M}$ with corresponding cyclic and separating vector Ω. For each selfadjoint $P \in \mathfrak{M}$ we can define the perturbed vector Ω^P, and the corresponding perturbed positive form

$$\hat{\omega}^P(A) = (\Omega^P, A\Omega^P) \ , \quad A \in \mathfrak{A} \ .$$

as in Theorem 5.4.4. Note that $\hat{\omega}^P$ is not normalized and $\hat{\omega}^P = \|\Omega^P\|^2\omega^P$, where ω^P is the perturbed state given in Theorem 5.4.4. Now let us recall some of the basic facts derived in Section 5.4.1.

First one has

$$\Omega^P = \Gamma^P_{-i/2}\Omega \ ,$$

where $\Gamma^P_{-i/2}$ is the analytic continuation to the point $-i/2$ of the unitary cocycle which intertwines the modular group σ associated with $(\mathfrak{M}, \Omega)$ and the perturbed modular group σ^P which corresponds to $(\mathfrak{M}, \Omega^P)$. If Δ_Ω denotes the modular operator corresponding to $(\mathfrak{M}, \Omega)$ and $H = \log \Delta_\Omega$ is the infinitesimal generator of σ, then

$$\Gamma^P_{-i/2} = e^{(H+P)/2}e^{-H/2} \ .$$

Now assuming for simplicity that P is analytic with respect to σ one has $\Gamma^P_{-i/2} \in \mathfrak{M}$. Therefore,

$$S_\Omega\, \Gamma^P_{-i/2}{}^* A\Omega = A^*\Gamma^P_{-i/2}\Omega = A^*\Omega^P = S_{\Omega^P,\,\Omega}A\Omega \ .$$

But $\mathfrak{M}\Omega$ is a core for both S_Ω and $S_{\Omega^P,\Omega}$. Moreover, $\Gamma^P_{-i/2}$ is invertible and hence $\Gamma^P_{-i/2}{}^*\mathfrak{M}\Omega$ is a core for S_Ω. It follows immediately that

$$S_\Omega\, \Gamma^P_{-i/2}{}^* = S_{\Omega^P,\Omega} \ .$$

Consequently

$$\begin{aligned}\Delta_{\Omega^P,\Omega} &= \Gamma^P_{-i/2}\, \Delta_\Omega\, \Gamma^P_{-i/2}{}^* \\ &= (e^{(H+P)/2}e^{-H/2})e^H(e^{-H/2}e^{(H+P)/2}) = e^{(H+P)}\end{aligned}$$

and

$$\log \Delta_{\Omega^P,\,\Omega} = \log \Delta_\Omega + P \ .$$

These relations then extend to general $P = P^* \in \mathfrak{M}$ by approximation in the strong topology with sequences of analytic elements P_n. One uses, for example $\|\Omega^{P_n} - \Omega^P\| \to 0$. Thus we have deduced that

$$\begin{aligned} S(\omega|\hat{\omega}^P) &= (\Omega, \log \Delta_{\Omega^P,\Omega}\Omega) \\ &= (\Omega, \log \Delta_\Omega \Omega) + (\Omega, P\Omega) = \omega(P) \end{aligned}$$

where the last step follows because $\Delta_\Omega \Omega = \Omega$. By rescaling one also obtains the identity

$$S(\omega|\omega^P) = \omega(P) - \log \|\Omega^P\|^2 \ .$$

But it follows from Corollary 5.4.5 that $(\omega^P)^{-P} = \omega$ and $(\Omega^P)^{-P} = \Omega$. Thus interchanging ω and ω^P one finds

$$S(\omega^P|\omega) = -\omega^P(P) + \log \|\Omega^P\|^2 \ .$$

Combination of these two relations then provides a lower bound for the relative entropy. One has

$$0 \geq S(\omega|\omega^P) \geq S(\omega|\omega^P) + S(\omega^P|\omega) = \omega(P) - \omega^P(P) \geq -2\|P\| \ .$$

Thus both $S(\omega|\omega^P)$ and $S(\omega^P|\omega)$ take values in the interval $[0, -2\|P\|]$.
It is of interest to remark that the nonpositivity of $S(\omega|\omega^P)$ combined with the above expression yields the bound

$$\|\Omega^P\|^2 \geq e^{\omega(P)} \ .$$

This is a generalization of the inequality

$$\frac{\mathrm{Tr}(e^{H+P})}{\mathrm{Tr}(e^H)} \geq \exp\left\{\frac{\mathrm{Tr}(e^H P)}{\mathrm{Tr}(e^H)}\right\}$$

which is valid for matrices $H = H^*$ and $P = P^*$ and is known as the *Peierls–Bogoliubov inequality*. (One can also derive the upper bound $\omega(e^P) \geq \|\Omega^P\|^2$ corresponding to the *Golden–Thompson inequality* $\mathrm{Tr}(e^H e^P) \geq \mathrm{Tr}(e^{H+P})$).

These relations and bounds will be of importance in the sequel.

EXAMPLE 6.2.30. Let ω_1 be a faithful state over the algebra $\mathfrak{M}_n$ of $n \times n$ matrices and ρ_1 the density matrix determining ω_1. Furthermore, let ω_2 be a positive faithful form determined by the positive matrix ρ_2. Faithfulness implies that ρ_1 and ρ_2 are invertible and hence one can define H_1 and H_2 by

$$H_i = \log \rho_i \ .$$

One then has $\omega_2 = \hat{\omega}_1^P$ where $P = H_2 - H_1$. Thus the relation

$$S(\omega|\hat{\omega}^P) = \omega(P)$$

gives

$$S(\omega_1|\omega_2) = \omega_1(H_2 - H_1) = -\mathrm{Tr}(\rho_1 \log \rho_1 - \rho_1 \log \rho_2) \ .$$

Thus the general definition of the relative entropy coincides with the previous definition for matrix algebras.

EXAMPLE 6.2.31. Let ω_1 and ω_2 be product states over the quantum spin algebra, as in Example 6.2.23, and assume they are both faithful. The representations $(\mathfrak{H}_{\omega_i}, \pi_{\omega_i}, \Omega_{\omega_i})$ can be realized as tensor products of the representations $(\mathfrak{H}_{\omega_{i,x}}, \pi_{\omega_{i,x}}, \Omega_{\omega_{i,x}})$ associated with $\omega_{i,x} = \omega_i|_{\mathfrak{A}_{\{x\}}}$. The relative modular operator is

expressible as a tensor product of the corresponding one-point relative operators and consequently

$$S(\omega_1|\omega_2) = \sum_{x\in L} S(\omega_{1,x}|\omega_{2,x}) = \sum_{x\in L} -\mathrm{Tr}_{\mathfrak{H}_{\{x\}}}(\rho_x^{(1)}(\log\rho_x^{(1)} - \log\rho_x^{(2)}))\ .$$

In this last expression $\rho_x^{(i)}$ denotes the density matrix which determines $\omega_{i,x}$ and the identification follows from Example 6.2.30. Thus for finite relative entropy the function $x \in L \mapsto S(\omega_{1,x}|\omega_{2,x}) \leq 0$ must be summable. Now if $L = \mathbb{Z}^\nu$ this means that

$$x \in \mathbb{Z}^\nu \to -\mathrm{Tr}_{\mathfrak{H}_{\{x\}}}(\rho_x^{(1)}(\log\rho_x^{(1)} - \log\rho_x^{(2)})) \leq 0$$

must vanish sufficiently fast as $|x| \to \infty$. But this function is a continuous function of $\rho_x^{(1)}$ and $\rho_x^{(2)}$, because $\mathfrak{H}_{\{x\}}$ has dimension $N+1$, and it vanishes only if $\rho_x^{(1)} = \rho_x^{(2)}$. Thus for finite relative entropy one must have $\|\rho_x^{(1)} - \rho_x^{(2)}\| \to 0$ as $|x| \to \infty$. But this implies $\|\omega_{1,x} - \omega_{2,x}\| \to 0$ as $|x| \to \infty$, i.e., the restrictions $\omega_{1,x}$ and $\omega_{2,x}$ must be asymptotically equal.

If ω_1 is $\mathbb{Z}^\nu$-invariant it is possible to estimate the rate of decrease of $\|\rho_x^{(1)} - \rho_x^{(2)}\|$ sufficient to ensure that $S(\omega_1|\omega_2)$ is finite. Again we use the representation

$$\log A - \log B = \int_0^\infty d\lambda \left(\frac{1}{B+\lambda\mathbb{1}} - \frac{1}{A+\lambda\mathbb{1}}\right)$$

for positive matrices A and B to deduce that

$$\begin{aligned}
|S(\omega_{1,x}|\omega_{2,x})| &= \left|\mathrm{Tr}_{\mathfrak{H}_{\{x\}}}\left(\rho_x^{(1)}\int_0^\infty d\lambda(\rho_x^{(2)}+\lambda\mathbb{1})^{-1}(\rho_x^{(1)}-\rho_x^{(2)})(\rho_x^{(1)}+\lambda\mathbb{1})^{-1}\right)\right| \\
&\leq \int_0^\infty d\lambda\, \|\,(\rho_x^{(1)}+\lambda\mathbb{1})^{-1}\,\|\|\,(\rho_x^{(2)}+\lambda\mathbb{1})^{-1}\,\|\|\,\rho_x^{(1)}-\rho_x^{(2)}\,\| \\
&= \int_0^\infty d\lambda\{(\|\,\rho_x^{(2)-1}\,\|^{-1}+\lambda)^{-1} - (\|\,\rho_x^{(1)-1}\,\|^{-1}+\lambda)\} \\
&\quad \times \frac{\|\,\rho_x^{(1)}-\rho_x^{(2)}\,\|}{\|\,\rho_x^{(1)-1}\,\|^{-1} - \|\,\rho_x^{(2)-1}\,\|^{-1}} \\
&= \log\left(\frac{\|\,\rho_x^{(2)-1}\,\|}{\|\,\rho_x^{(1)-1}\,\|}\right)(\|\,\rho_x^{(1)-1}\,\|^{-1} - \|\,\rho_x^{(2)-1}\,\|^{-1})^{-1}\,\|\,\rho_x^{(1)}-\rho_x^{(2)}\,\| \\
&\leq \|\,\rho_x^{(2)-1}\,\|\|\,\rho_x^{(1)}-\rho_x^{(2)}\,\|\ .
\end{aligned}$$

But $\|\,\rho_x^{(1)}-\rho_x^{(2)}\,\| \to 0$ as $|x| \to \infty$ and $\|\,\rho_x^{(1)-1}\,\| = \|\,\rho_0^{(1)-1}\,\|$ by $\mathbb{Z}^\nu$-invariance. Therefore, $\|\,\rho_x^{(2)-1}\,\| \to \|\,\rho_0^{(1)-1}\,\|$ as $|x| \to \infty$, and we conclude that

$$|S(\omega_1|\omega_2)| \leq \|\,\rho_0^{(1)-1}\,\| \sum_{x\in\mathbb{Z}^\nu} \|\,\rho_x^{(1)}-\rho_x^{(2)}\,\|\ .$$

Next we derive an extension of the rule before Example 6.2.30 for the entropy of a state ω relative to the perturbed state ω^P.

Proposition 6.2.32. *Let ω_1 and ω_2 be faithful states over the von Neumann algebra $\mathfrak{M}$ and for each selfadjoint $P \in \mathfrak{M}$ introduce the perturbed form*

$$\hat{\omega}_2^P(A) = (\Omega_2^P, A\Omega_2^P)$$

where Ω_2^P is the perturbation of the cyclic and separating vector associated with ω_2.

It follows that

$$S(\omega_1|\hat{\omega}_2^P) = S(\omega_1|\omega_2) + \omega_1(P) \ .$$

PROOF. The proof combines the argument used to derive the relation

$$S(\omega_1|\hat{\omega}_1^P) = \omega_1(P)$$

and the 2×2 matrix arguments used in Section 2.5.4.

Adopt the notation of Lemma 2.5.33, and perturb the vector $\Omega_0 = \Omega_0(\xi_1, \xi_2) = \xi_1 \otimes \eta_{11} + \xi_2 \otimes \eta_{22}$ by an operator of the form

$$P \otimes E_{22} = U_{21} P U_{21}^* + U_{22} P U_{22}^* \ .$$

By Lemma 2.5.34 one has that

$$\log \Delta_{\Omega_0} = \sum_{i,j=1}^{2} U_{ij} \log(\Delta_{\xi_i, \xi_j}) U_{ij}^*$$

and hence

$$\begin{aligned} \Omega_0(\xi_1, \xi_2)^{P \otimes E_{22}} &= e^{(\log \Delta_{\Omega_0} + P \otimes E_{22})/2} e^{-\log \Delta_{\Omega_0}/2} \Omega_0(\xi_1, \xi_2) \\ &= \xi_1 \otimes \eta_{11} + \xi_2^P \otimes \eta_{22} = \Omega_0(\xi_1, \xi_2^P) \ . \end{aligned} \tag{*}$$

But if $\Delta = \exp H$ and J are the modular operator and conjugation associated with $(\mathfrak{M}, \Omega_0)$ then

$$\Delta_{P'} = \exp\{H + P' - JP'J\}$$

is the modular operator associated with $(\mathfrak{M}, \Omega_0^{P'})$. (A proof of this appears prior to Corollary 5.4.5.) Also by Lemma 2.5.34 one has

$$J = \sum_{i,j=1}^{2} U_{ij} J_{\xi_j, \xi_i} U_{ji}^*$$

and hence

$$J(P \otimes E_{22})J = U_{12} J_{\xi_2, \xi_1} P J_{\xi_1, \xi_2} U_{12}^* + U_{22} J_{\xi_2} P J_{\xi_2} U_{22}^* \ .$$

It follows, using $P' = P \otimes E_{22}$, that

$$\begin{aligned} \log \Delta_{\Omega_0(\xi_1, \xi_2^P)} &= \log \Delta_{\Omega_0(\xi_1, \xi_2)} P \otimes E_{22} \\ &= \log \Delta_{\Omega_0(\xi_1, \xi_2)} + U_{21} P U_{21}^* + U_{22} P U_{22}^* \\ &\quad - U_{12} J_{\xi_2, \xi_1} P J_{\xi_1, \xi_2} U_{12}^* - U_{22} J_{\xi_2} P J_{\xi_2} U_{22}^* \ , \end{aligned}$$

where the first equality is a consequence of (*). Taking the (2, 1) component of this equation we obtain

$$\log \Delta_{\xi_2^P, \xi_1} = \log \Delta_{\xi_2, \xi_1} + P$$

and applying this to $\xi_1 = \Omega_1$ and $\xi_2 = \Omega_2$ one deduces

$$S(\omega_1|\hat{\omega}_2^P) = S(\omega_1|\omega_2) + \omega_1(P) \ .$$

Next we examine the connection between the relative entropy and the conditional entropy.

Let ω_1 and ω_2 be states over the quantum spin algebra and $\{\rho_\Lambda^{(1)}\}_{\Lambda\subset L}$ and $\{\rho_\Lambda^{(2)}\}_{\Lambda\subset L}$ the corresponding families of density matrices. If $\Lambda' \subset \Lambda^c$, then

$$\begin{aligned} S_{\Lambda\cup\Lambda'}(\omega_1) - S_{\Lambda'}(\omega_1) &= -\operatorname{Tr}(\rho^{(1)}_{\Lambda\cup\Lambda'} \log \rho^{(1)}_{\Lambda\cup\Lambda'}) + \operatorname{Tr}(\rho^{(1)}_{\Lambda'} \log \rho^{(1)}_{\Lambda'}) \\ &= -\operatorname{Tr}(\rho^{(1)}_{\Lambda\cup\Lambda'}(\log \rho^{(1)}_{\Lambda\cup\Lambda'} - \log(\mathbb{1} \otimes \rho^{(2)}_{\Lambda'}))) \\ &\quad + \operatorname{Tr}(\rho^{(1)}_{\Lambda'}(\log \rho^{(1)}_{\Lambda'} - \log \rho^{(2)}_{\Lambda'})) \\ &= S(\omega_1|_{\mathfrak{A}_{\Lambda\cup\Lambda'}}|\tau_\Lambda \otimes \omega_2|_{\mathfrak{A}_{\Lambda'}}) - S(\omega_1|_{\mathfrak{A}_{\Lambda'}}|\omega_2|_{\mathfrak{A}_{\Lambda'}}) \ , \end{aligned}$$

where we have used the identification of the relative entropy established in Example 6.2.30 and τ_Λ denotes the (unnormalized) trace on $\mathfrak{A}_\Lambda$, i.e.,

$$\tau_\Lambda(A) = \operatorname{Tr}_{\mathfrak{H}_\Lambda}(A) \ , \quad A \in \mathfrak{A}_\Lambda \ .$$

This relation can be translated to a relation between the conditional and relative entropies by taking the limit $\Lambda' \to \Lambda^c$. But this requires knowledge of continuity properties of the relative entropy.

Proposition 6.2.33. *Let $\mathfrak{M}$ be a von Neumann algebra with an increasing net of finite-dimensional subalgebras $\mathfrak{M}_\alpha$ such that $\bigcup_\alpha \mathfrak{M}_\alpha$ is dense in $\mathfrak{M}$. Let ω_1, ω_2 be two faithful, normal, positive, linear functionals over $\mathfrak{M}$ and $\omega_{1,\alpha}, \omega_{2,\alpha}$, their restrictions to $\mathfrak{M}_\alpha$.*

It follows that $\alpha \mapsto S(\omega_{1,\alpha}|\omega_{2,\alpha})$ is monotonically decreasing and

$$\lim_\alpha S(\omega_{1,\alpha}|\omega_{2,\alpha}) = S(\omega_1|\omega_2) \ .$$

Although this is a key result, the proof is rather long and so we choose to omit it (see Notes and Remarks). Combination of this result and the discussion preceding it gives a relation between the conditional entropy and the relative entropy which is fundamental for the derivation of the maximum entropy principle from the Gibbs condition.

Corollary 6.2.34. *Let ω_1 and ω_2 be states over the quantum spin algebra $\mathfrak{A}$ and let τ_Λ denote the (unnormalized) trace over $\mathfrak{A}_\Lambda$.*

It follows that

$$\tilde{S}_\Lambda(\omega_1) = S(\omega_1|\tau_\Lambda \otimes \omega_2|_{\mathfrak{A}_{\Lambda^c}}) - S(\omega_1|_{\mathfrak{A}_{\Lambda^c}}|\omega_2|_{\mathfrak{A}_{\Lambda^c}}) \ .$$

This follows from the relation preceding Proposition 6.2.33 by taking the limit $\Lambda' \mapsto \Lambda^c$.

Proposition 6.2.35. *Let Φ be an interaction of a quantum spin system such that the surface energy $W_\Phi(\Lambda)$ is a well-defined element of $\mathfrak{A}$ for all $\Lambda \subset L$. Furthermore, let ω be a state which satisfies the Gibbs condition with respect to Φ.*

It follows that

$$\tilde{S}_\Lambda(\omega) - \beta\omega(\tilde{H}_\Phi(\Lambda)) = \sup_{\omega' \in C^\omega_\Lambda} \{\tilde{S}_\Lambda(\omega') - \beta\omega'(\tilde{H}_\Phi(\Lambda))\}$$

for each $\Lambda \subset L$, where $\tilde{S}_\Lambda$ is the conditional entropy, $\tilde{H}_\Phi(\Lambda) = H_\Phi(\Lambda) + W_\Phi(\Lambda)$ the conditional energy, and

$$C_\Lambda^\omega = \{\omega'; \omega' \in E_{\mathfrak{A}}, \omega'|_{\mathfrak{A}_{\Lambda^c}} = \omega|_{\mathfrak{A}_{\Lambda^c}}\} \ .$$

PROOF. The Gibbs condition states that

$$\omega^{\beta W_\Phi(\Lambda)} = \omega_\Lambda \otimes \omega|_{\mathfrak{A}_{\Lambda^c}} \ ,$$

where ω_Λ is the finite-volume Gibbs state. This is equivalent to

$$\omega^{\beta \tilde{H}_\Phi(\Lambda)} = \tau_\Lambda^0 \otimes \omega|_{\mathfrak{A}_{\Lambda^c}} \ ,$$

where τ_Λ^0 is the (normalized) trace state on $\mathfrak{A}_\Lambda$, i.e.,

$$\tau_\Lambda^0(A) = \frac{\mathrm{Tr}_{\mathfrak{H}_\Lambda}(A)}{\mathrm{Tr}_{\mathfrak{H}_\Lambda}(\mathbb{1})}, \qquad A \in \mathfrak{A}_\Lambda \ .$$

It follows from Proposition 6.2.32 and rescaling that

$$S(\omega_1|\omega^{\beta\tilde{H}_\Phi(\Lambda)}) = S(\omega_1|\omega) + \beta\omega_1(\tilde{H}_\Phi(\Lambda)) + \log(\Omega_\omega^{\beta\tilde{H}_\Phi(\Lambda)}, \Omega_\omega^{\beta\tilde{H}_\Phi(\Lambda)}) \ .$$

But then the Gibbs condition, Definition 6.2.16, and Corollary 6.2.34 give

$$\begin{aligned} S(\omega_1|\omega^{\beta\tilde{H}_\Phi(\Lambda)}) &= S(\omega_1|\tau_\Lambda^0 \otimes \omega|_{\mathfrak{A}_{\Lambda^c}}) \\ &= S(\omega_1|\tau_\Lambda \otimes \omega|_{\mathfrak{A}_{\Lambda^c}}) - \log \mathrm{Tr}_{\mathfrak{H}_\Lambda}(\mathbb{1}) \\ &= S(\omega_1|_{\mathfrak{A}_{\Lambda^c}}|\omega|_{\mathfrak{A}_{\Lambda^c}}) + \tilde{S}_\Lambda(\omega_1) - \log \mathrm{Tr}_{\mathfrak{H}_\Lambda}(\mathbb{1}) \ . \end{aligned}$$

Combining these relations one finds

$$\begin{aligned} \tilde{S}_\Lambda(\omega_1) = S(\omega_1|\omega) - S(\omega_1|_{\mathfrak{A}_{\Lambda^c}}|\omega|_{\mathfrak{A}_{\Lambda^c}}) + \beta\omega_1(\tilde{H}_\Phi(\Lambda)) \\ + \log\{(\Omega_\omega^{\beta\tilde{H}_\Phi(\Lambda)}, \Omega_\omega^{\beta\tilde{H}_\Phi(\Lambda)})\mathrm{Tr}_{\mathfrak{H}_\Lambda}(\mathbb{1})\} \ . \end{aligned}$$

Now setting $\omega_1 = \omega$ this gives

$$\tilde{S}_\Lambda(\omega) = \beta\omega(\tilde{H}_\Phi(\Lambda)) + \log\{(\Omega_\omega^{\beta\tilde{H}_\Phi(\Lambda)}, \Omega_\omega^{\beta\tilde{H}_\Phi(\Lambda)})\mathrm{Tr}_{\mathfrak{H}_\Lambda}(\mathbb{1})\}$$

and hence, by subtraction,

$$\tilde{S}_\Lambda(\omega) - \beta\omega(\tilde{H}_\Phi(\Lambda)) = \tilde{S}_\Lambda(\omega_1) - \beta\omega_1(\tilde{H}_\Phi(\Lambda)) - S(\omega_1|\omega) + S(\omega_1|_{\mathfrak{A}_{\Lambda^c}}|\omega|_{\mathfrak{A}_{\Lambda^c}}) \ .$$

Therefore, if $\omega_1 \in C_\Lambda^\omega$

$$\begin{aligned} \tilde{S}_\Lambda(\omega) - \beta\omega(\tilde{H}_\Phi(\Lambda)) &= \tilde{S}_\Lambda(\omega_1) - \beta\omega_1(\tilde{H}_\Phi(\Lambda)) - S(\omega_1|\omega) \\ &\geq \tilde{S}_\Lambda(\omega_1) - \beta\omega_1(\tilde{H}_\Phi(\Lambda)) \ , \end{aligned}$$

where the inequality follows from the negativity of the relative entropy. As equality is achieved if $\omega = \omega_1$, the proof is complete.

Note that $S(\omega_1|\omega) = 0$ if, and only if, $\omega_1 = \omega$ and hence the state ω is the unique state in C_Λ^ω for which the supremum is attained.

Next we establish a converse of Proposition 6.2.35 under stronger assumptions on the interaction. In fact, we use the assumptions that sufficed to establish the equivalence of the Gibbs condition and the τ-KMS condition,

Theorem 6.2.18. This is slightly unsatisfactory because the Gibbs condition and the maximum entropy principle can both be defined when the surface energies $W_\Phi(\Lambda)$ make sense and it is not essential that the dynamics are determined by a strongly continuous one-parameter group of *-automorphisms τ of $\mathfrak{A}$. Thus, this hypothesis in the following theorem appears redundant. (See also the Remark after Theorem 6.2.18.)

Theorem 6.2.36. *Let Φ be an interaction of a quantum spin system and τ^Λ the corresponding local automorphism group. Assume that*

(1) *τ^Λ converges strongly to an automorphism group τ, i.e.,*

$$\lim_{\Lambda\to\infty} \|\tau_t^\Lambda(A) - \tau_t(A)\| = 0$$

for all $A \in \mathfrak{A}, t \in \mathbb{R}$.

(2) *The surface energies $W_\Phi(\Lambda)$ are well-defined elements of $\mathfrak{A}$ for all $\Lambda \subset L$.*

(3)
$$D = \bigcup_{\Lambda \subset L} \mathfrak{A}_\Lambda$$

is a core for the generator δ of τ

The following conditions are equivalent, for $\beta \in \mathbb{R}$ and for a state $\omega \in E_\mathfrak{A}$.

(1)
$$\tilde{S}_\Lambda(\omega) - \beta\omega(\tilde{H}_\Phi(\Lambda)) = \sup_{\omega' \in C_\Lambda^\omega} \{\tilde{S}_\Lambda(\omega') - \beta\omega'(\tilde{H}_\Phi(\Lambda))\}$$

for all $\Lambda \subset L$, where $\tilde{S}_\Lambda$ is the conditional entropy, $\tilde{H}_\Phi(\Lambda) = H_\Phi(\Lambda) + W_\Phi(\Lambda)$ the conditional energy, and

$$C_\Lambda^\omega = \{\omega'; \omega' \in E_\mathfrak{A}, \omega'|_{\mathfrak{A}_{\Lambda^c}} = \omega|_{\mathfrak{A}_{\Lambda^c}}\} \ .$$

(2) *ω is a (τ, β)-KMS state.*

Proof. (1) $\Rightarrow$ (2) : If $\beta = 0$ and τ_Λ^0 denotes the (normalized) trace state on $\mathfrak{A}_\Lambda$, it follows by choosing $\omega' = \tau_\Lambda^0 \otimes \omega|_{\mathfrak{A}_{\Lambda^c}}$ in the maximum principle and also invoking the bound given in Proposition 6.2.28 that

$$S_\Lambda(\tau_\Lambda^0) \le \tilde{S}_\Lambda(\omega') \le S_\Lambda(\omega) \ .$$

Thus $S_\Lambda(\omega)$ achieves its maximum value $S_\Lambda(\tau_\Lambda^0)$. Hence $\omega|_{\mathfrak{A}_\Lambda} = \tau_\Lambda^0$ and ω is a trace.

If $\beta \neq 0$, the proof is indirect. We argue that condition (1) implies that ω satisfies the autocorrelation lower bound and then appeal to Theorem 5.3.15.

First note that if δ denotes the generator of τ, then

$$\delta(A) = i[\tilde{H}_\Phi(\Lambda), A]$$

for all $A \in \mathfrak{A}_\Lambda$ by the argument given in the proof of Theorem 6.2.18. But if ω_t is defined by

$$\omega_t(B) = \omega(e^{itA} B e^{-itA})$$

for all $B \in \mathfrak{A}$, then condition (1) implies that

$$\beta\{\omega_t(\tilde{H}_\Phi(\Lambda)) - \omega(\tilde{H}_\Phi(\Lambda))\} \geq \tilde{S}_\Lambda(\omega_t) - \tilde{S}_\Lambda(\omega)$$

whenever $A = A^* \in \mathfrak{A}_\Lambda$. But it follows from the definition of $\tilde{S}_\Lambda$ and properties of the trace that

$$\tilde{S}_\Lambda(\omega_t) = \tilde{S}_\Lambda(\omega)$$

and consequently

$$\beta\{\omega_t(\tilde{H}_\Phi(\Lambda)) - \omega(\tilde{H}_\Phi(\Lambda))\} \geq 0 \ .$$

Thus, $t \mapsto \beta\omega_t(\tilde{H}_\Phi(\Lambda))$ has a minimum at $t = 0$ and hence its first derivative vanishes at this point. Therefore

$$\beta\omega(\delta(A)) = 0$$

for all $A \in \mathfrak{A}_\Lambda$ and $\Lambda \subset L$ and since $\beta \neq 0$ this shows that ω is invariant under δ.

Next consider the operator $\gamma_B; \mathfrak{A} \mapsto \mathfrak{A}$, introduced prior to Theorem 5.3.15, i.e.,

$$\gamma_B(A) = B^*AB - \{B^*B, A\}/2 \ .$$

If we choose $B \in \mathfrak{A}_\Lambda$, it follows that $\gamma_B(A) = 0$ for all $A \in \mathfrak{A}_{\Lambda^c}$. Therefore, $\mathfrak{A}_{\Lambda^c}$ is pointwise invariant under the semigroup $t \geq 0 \mapsto T_t = \exp\{t\gamma_B\}$, and hence

$$T_t^*\omega|_{\mathfrak{A}_{\Lambda^c}} = \omega|_{\mathfrak{A}_{\Lambda^c}} \ .$$

We already argued in Section 5.3 that $T_t^* E_{\mathfrak{A}} \subseteq E_{\mathfrak{A}}$, $t \geq 0$. Thus it follows from condition (1) that

$$\beta\{(T_t^*\omega)(\tilde{H}_\Phi(\Lambda)) - \omega(\tilde{H}_\Phi(\Lambda))\} \geq \tilde{S}_\Lambda(T_t^*\omega) - \tilde{S}_\Lambda(\omega) \ .$$

Next by the invariance of ω under δ one has

$$\begin{aligned} -i\beta\omega(B^*\delta(B)) &= -i\beta\{\omega(B^*\delta(B)) - \omega(\delta(B^*)B) + \omega(\delta(B^*B))\}/2 \\ &= -i\beta\{\omega(B^*\delta(B)) - \omega(\delta(B^*)B)\}/2 = \beta\omega(\gamma_B(\tilde{H}_\Phi(\Lambda))) \ . \end{aligned}$$

Thus, the previous estimate gives

$$\begin{aligned} -i\beta\omega(B^*\delta(B)) &= \lim_{t\to 0+} \beta\{(T_t^*\omega)(\tilde{H}_\Phi(\Lambda)) - \omega(\tilde{H}_\Phi(\Lambda))\}/t \\ &\geq \lim_{t\to 0+} \{\tilde{S}_\Lambda(T_t^*\omega) - \tilde{S}_\Lambda(\omega)\}/t \ . \end{aligned}$$

Next note that as $T_t^*\omega|_{\mathfrak{A}_{\Lambda^c}} = \omega|_{\mathfrak{A}_{\Lambda^c}}$ one has

$$S_{\Lambda'}(T_t^*\omega) = S_{\Lambda'}(\omega)$$

for all $\Lambda' \subset \Lambda^c$. Therefore,

$$\tilde{S}_\Lambda(T_t^*\omega) - \tilde{S}_\Lambda(\omega) = \lim_{\Lambda'\to\Lambda^c} (S_{\Lambda\cup\Lambda'}(T_t^*\omega) - S_{\Lambda\cup\Lambda'}(\omega)) \ .$$

But if $\Lambda'' = \Lambda \cup \Lambda'$, then

$$S_{\Lambda''}(T_t^*\omega) - S_{\Lambda''}(\omega) = -\int_0^t ds \frac{d}{ds} \mathrm{Tr}_{\mathfrak{H}_{\Lambda''}}(\rho^s_{\Lambda''} \log \rho^s_{\Lambda''}) \ ,$$

where $\rho^s_{\Lambda''}$ denotes the density matrix which determines the restriction of $T_s^*(\omega)$ to $\mathfrak{A}_{\Lambda''}$. But each $\rho^s_{\Lambda''}$ is a positive invertible matrix, and hence the expansion

$$\log \rho^s_{\Lambda''} = \int_0^\infty d\lambda \left(\frac{1}{\lambda + \mathbb{1}} - \frac{1}{\lambda + \rho^s_{\Lambda''}} \right)$$

is valid. It follows that

$$\begin{aligned}
\frac{d}{ds}\mathrm{Tr}(\rho^s \log \rho^s) &= \int_0^\infty d\lambda \frac{d}{ds}\mathrm{Tr}\left(\rho^s \left(\frac{1}{\lambda + \mathbb{1}} - \frac{1}{\lambda + \rho^s} \right) \right) \\
&= \int_0^\infty d\lambda \, \mathrm{Tr}\left\{ \frac{d\rho^s}{ds} \left(\frac{1}{\lambda + \mathbb{1}} - \frac{1}{\lambda + \rho^s} \right) \right. \\
&\quad \left. + \rho^s \frac{1}{\lambda + \rho^s} \frac{d\rho^s}{ds} \frac{1}{\lambda + \rho^s} \right\} \\
&= \int_0^\infty d\lambda \, \mathrm{Tr}\left(\frac{d\rho^s}{ds} \left(\frac{1}{\lambda + \mathbb{1}} - \frac{1}{\lambda + \rho^s} + \rho^s \frac{1}{(\lambda + \rho^s)^2} \right) \right) ,
\end{aligned}$$

where we have used the cyclicity of the trace and dropped the subscript Λ''.

Using the expansion

$$\mathbb{1} = \int_0^\infty d\lambda \, \rho^s \frac{1}{(\lambda + \rho^s)^2}$$

one then derives

$$\begin{aligned}
\frac{d}{ds}\mathrm{Tr}(\rho^s \log \rho^s) &= \mathrm{Tr}\left(\frac{d\rho^s}{ds} (\log \rho^s + \mathbb{1}) \right) \\
&= \frac{d}{dr} (T^*_r \omega)(\log \rho^s + \mathbb{1})|_{r=s} \\
&= \gamma^*_B (T^*_s \omega)(\log \rho^s + \mathbb{1}) \\
&= (T^*_s \omega)(\gamma_B(\log \rho^s + \mathbb{1})) = (T^*_s \omega)(\gamma_B \log \rho^s) \ .
\end{aligned}$$

Therefore,

$$S_{\Lambda''}(T^*_t \omega) - S_{\Lambda''}(\omega) = - \int_0^t ds (T^*_s \omega)(\gamma_B(\log \rho^s_{\Lambda''})) \ .$$

The next step is to bound the integrand. Let

$$\rho_{\Lambda''} = \sum_{j=1}^n \lambda_j E_j$$

denote the spectral decomposition of $\rho_{\Lambda''}$. A straightforward calculation shows that

$$-\omega(\gamma_B(\log \rho_{\Lambda''})) = \sum_{j,k=1}^n S(\lambda_j \, ; \lambda_k) C_{jk}$$

where

$$c_{jk} = \mathrm{Tr}_{\mathfrak{H}_{\Lambda''}}((E_k B E_j)(E_k B E_j)^*)$$

and the function $S(u \, ; v) = u \log(u/v)$ is defined as in Theorem 5.3.15. Now S is jointly convex in its two arguments and also homogeneous of first order. Therefore,

$$\sum_{j,k=1}^n S(\lambda_j \, ; \lambda_k) c_{jk} \geq S\left(\sum_{j,k=1}^n c_{jk} \lambda_j \, ; \sum_{j,k=1}^n c_{jk} \lambda_k \right) = S(\omega(B^* B) \, ; \omega(BB^*)) \ .$$

Finally combination of all these estimates together with lower semi-continuity of S gives

$$\begin{aligned} -i\beta\omega(B^*\delta(B)) &\geq \lim_{t\to 0+}\int_0^1 ds\, S((T_s^*\omega)(B^*B)\,;(T_s^*\omega)(BB^*))/t \\ &= S(\omega(B^*B)\,;\omega(BB^*)) \end{aligned}$$

for all $B \in \mathfrak{A}_\Lambda$. But the union of the $\mathfrak{A}_\Lambda$ is a core for δ and hence this inequality extends by lower semi-continuity to all $B \in D(\delta)$, i.e., the auto-correlation lower bound is valid. Condition (2) then follows from Theorem 5.3.15.

(2) $\Rightarrow$ (1) : If $\beta = 0$, then ω is the unique trace-state on $\mathfrak{A}$. Thus ω is a product state and $\tilde{S}_\Lambda(\omega) = S_\Lambda(\omega)$ achieves its maximum value. If $\beta \neq 0$, then the implication follows by combination of Propositions 6.2.17 and 6.2.35.

Corollary 6.2.37. *Let Φ be an interaction of a quantum spin system satisfying*

$$\|\Phi\|_\lambda = \sum_{n\geq 0} e^{\lambda n}\left(\sup_{x\in L}\sum_{\substack{X\ni x\\ |X|=n+1}}\|\Phi(X)\|\right) < +\infty$$

for some $\lambda > 0$ and let τ^Φ be the associated automorphism group (see Theorem 6.2.4).

The following conditions are equivalent for each $\beta \in \mathbb{R}$:

(1) *ω satisfies the Gibbs condition with respect to $\beta\Phi$,*
(2) *ω is a (τ^Φ, β)-*KMS *state,*
(3) *ω satisfies the maximum entropy principle,*

$$\tilde{S}_\Lambda(\omega) - \beta\omega(\tilde{H}_\Phi(\Lambda)) = \sup_{\omega'\in C_\Lambda^\omega}\{\tilde{S}_\Lambda(\omega') - \beta\omega'(\tilde{H}_\Phi(\Lambda))\}$$

for all $\Lambda \subset L$, given in Theorem 6.2.36.

This is an elaboration of Corollary 6.2.19. The restriction $\|\Phi\|_\lambda < +\infty$ ensures that the hypotheses of Theorems 6.2.18 and 6.2.36 are fulfilled (see Theorem 6.2.4).

Note that if L is a homogeneous lattice, as defined at the beginning of Section 6.2.1, then one has a concept of finite range interactions. For such interactions Corollary 6.2.37 establishes the equivalence of the Gibbs condition, the KMS condition and the maximum entropy principle whenever $\sup_{X\subset L}\|\Phi(X)\| < \infty$.

6.2.4. Translationally Invariant States

Homogeneity of the quantum spin system was unimportant in the foregoing discussion of equilibrium states. Nevertheless many physical systems exhibit spatial homogeneity and symmetry and it is worthwhile analyzing such features in more detail. Throughout this section we assume that $L = \mathbb{Z}^\nu$ and examine $\mathbb{Z}^\nu$-

invariant states and interactions. The particular choice $L = \mathbb{Z}^\nu$ is not of paramount importance and most of the subsequent arguments could be modified to cover systems associated with other periodic sublattices of $\mathbb{R}^\nu$. Some of the results are also valid for appropriate non-invariant interactions or even for aperiodic lattices. We return to a discussion of these points at the end of the section. We derive results of two types. First, we establish a global variant of the maximum entropy principle for $\mathbb{Z}^\nu$-invariant states and, second, we deduce some general statements concerning uniqueness and lack of uniqueness of equilibrium states.

Let $E_{\mathfrak{A}}^{\mathbb{Z}^\nu}$ denote the states invariant under the action τ of the group $\mathbb{Z}^\nu$ of space translations of the quantum spin system on the lattice $\mathbb{Z}^\nu$. If $\omega \in E_{\mathfrak{A}}^{\mathbb{Z}^\nu}$, it follows that the local entropy $S_\Lambda(\omega)$ has the invariance properties

$$S_{\Lambda+a}(\omega) = S_\Lambda(\omega)$$

for all $a \in \mathbb{Z}^\nu$, and $\Lambda \subset \mathbb{Z}^\nu$. But $S_\Lambda(\omega)$ is also extensive, i.e., proportional to $|\Lambda|$, and we aim to examine its mean value as $\Lambda \to \infty$. In order to establish the existence of the mean it appears necessary to restrict the manner in which $\Lambda \to \infty$.

If $a = (a_1, \ldots, a_\nu) \in \mathbb{Z}^\nu$ and $a_i > 0$, we define Λ_a as the parallelepiped with edges of length $a_i - 1$:

$$\Lambda_a = \{x;\ x \in \mathbb{Z}^\nu, 0 \le x_i < a_i,\ i = 1, \ldots, \nu\}\ .$$

The translates of Λ_a by vectors $na = (n_1 a_1, \ldots, n_\nu a_\nu)$ with $n \in \mathbb{Z}^\nu$ form a partition $\mathscr{P}_a$ of $\mathbb{Z}^\nu$. Let $n_\Lambda^+(a)$ denote the number of sets of this partition which have nonvoid intersection with Λ and let $\Gamma_\Lambda^+(a)$ be the union of these sets. Similarly let $n_\Lambda^-(a)$ denote the number of sets of $\mathscr{P}_a$ which are contained in Λ, and $\Gamma_\Lambda^-(a)$ the union of these latter sets. The finite subsets $\Lambda \subset \mathbb{Z}^\nu$ are defined to tend to infinity in the sense of van Hove if

$$\lim \frac{n_\Lambda^+(a)}{n_\Lambda^-(a)} = 1$$

for every partition $\mathscr{P}_a$ and in this case we write $\Lambda \rightsquigarrow \infty$.

Note that if $\Lambda(a)$ denotes the set of points which are contained in Λ and are a distance greater than $|a|_\infty = \sup_{1 \le i \le \nu} a_i$ from the boundary of Λ, then

$$|\Lambda| \ge |\Lambda(a)| \ge (n_\Lambda^-(a) - (n_\Lambda^+(a) - n_\Lambda^-(a))2^\nu)|\Lambda_a|\ .$$

Therefore

$$1 \ge \frac{|\Lambda(a)|}{|\Lambda|} \ge 1 - \left(1 - \frac{n_\Lambda^-(a)}{n_\Lambda^+(a)}\right)(2^\nu + 1)\ .$$

Thus as $\Lambda \rightsquigarrow \infty$ one has $|\Lambda(a)|/|\Lambda| \to 1$. A slight elaboration of this argument shows that the notion of van Hove convergence is equivalent to $|\Lambda| \to \infty$ and $|\Lambda(a)|/|\Lambda| \to 1$.

Proposition 6.2.38. *Let* $\Lambda \subset \mathbb{Z}^\nu \mapsto S_\Lambda(\omega) \in [0,\ |\Lambda|\log(N+1)]$ *denote the entropy of the* $\mathbb{Z}^\nu$*-invariant state* ω.

It follows that the limit

$$S(\omega) = \lim_{\Lambda \rightsquigarrow \infty} \frac{S_\Lambda(\omega)}{|\Lambda|}$$

exists and

$$S(\omega) = \inf_{a \in \mathbb{Z}^\nu_+} \frac{S_{\Lambda_a}(\omega)}{|\Lambda_a|} \ .$$

The functional $\omega \in E^{\mathbb{Z}^\nu}_{\mathfrak{A}} \to S(\omega) \in [0, \log(N+1)]$ *is affine and upper semi-continuous when* $E^{\mathbb{Z}^\nu}_{\mathfrak{A}}$ *is equipped with the weak* topology.*

Proof. The proof relies heavily on the subadditivity and strong subadditivity of $\Lambda \mapsto S_\Lambda(\omega)$ established in Proposition 6.2.24.

First, define S by

$$S(\omega) = \inf_{a \in \mathbb{Z}^\nu_+} \frac{S_{\Lambda_a}(\omega)}{|\Lambda_a|} \ .$$

Next let $\Lambda^-_a = \Lambda \backslash \Gamma^-_\Lambda(a)$, then

$$|\Lambda^-_a| \leq |\Gamma^+_\Lambda(a) - \Gamma^-_\Lambda(a)| = (n^+_\Lambda(a) - n^-_\Lambda(a))|\Lambda_a| \ .$$

Consequently,

$$S_{\Lambda^-_a}(\omega) \leq (n^+_\Lambda(a) - n^-_\Lambda(a))|\Lambda_a| \log(N+1) \ .$$

But as $\Lambda \mapsto S_\Lambda(\omega)$ is subadditive and $\mathbb{Z}^\nu$-invariant one also has

$$\begin{aligned} S_\Lambda(\omega) &\leq S_{\Gamma^-_\Lambda(a)}(\omega) + S_{\Lambda^-_a}(\omega) \\ &\leq n^-_\Lambda(a) S_{\Lambda_a}(\omega) + (n^+_\Lambda(a) - n^-_\Lambda(a))|\Lambda_a| \log(N+1) \ . \end{aligned}$$

Therefore,

$$\frac{S_\Lambda(\omega)}{|\Lambda|} \leq \frac{S_{\Lambda_a}(\omega)}{|\Lambda_a|} + \left(\frac{n^+_\Lambda(a)}{n^-_\Lambda(a)} - 1\right) \log(N+1) \ .$$

Similarly, if $\Lambda^+_a = \Gamma^+_\Lambda(a) \backslash \Lambda$, subadditivity gives

$$S_\Lambda(\omega) \geq S_{\Gamma^+_\Lambda(a)}(\omega) - S_{\Lambda^+_a}(\omega) \ .$$

Hence

$$\frac{S_\Lambda(\omega)}{|\Lambda|} \geq \frac{S_{\Gamma^+_\Lambda(a)}(\omega)}{|\Gamma^+_\Lambda(a)|} - \left(1 - \frac{n^-_\Lambda(a)}{n^+_\Lambda(a)}\right) \log(N+1) \ .$$

Thus for each $\varepsilon > 0$ one may choose a such that

$$\frac{S_{\Lambda_a}(\omega)}{|\Lambda_a|} < S(\omega) + \varepsilon$$

and it follows that

$$S(\omega) + \varepsilon \geq \frac{S_\Lambda(\omega)}{|\Lambda|} \geq \left(\frac{S_{\Gamma^+_\Lambda(a)}(\omega)}{|\Gamma^+_\Lambda(a)|} - \varepsilon\right)$$

for sufficiently large Λ. Next we bound the right-hand side.

Let us construct $\Gamma_\Lambda^+(a)$ by successively adding translates of Λ_a in the lexicographic ordering[4] of the vectors $n = (n_1, \ldots, n_\nu)$ which define these translates. Let Γ_n denote the union of the first n translates. Similarly, if $b = (m_1 a_1, \ldots, m_\nu a_\nu)$ with $m_i > 0$, then Λ_b can be constructed by successive addition, in lexicographic order, of translates of Λ_a. Let Δ_n denote the union of the first n of these translates.

Now assume that

$$S_{\Gamma_{n+1}}(\omega) - S_{\Gamma_n}(\omega) < (S(\omega) - \varepsilon)|\Lambda_a|$$

for some n. The strong subadditivity of S_Λ immediately implies that

$$S_{\Delta_{m+1}}(\omega) - S_{\Delta_m}(\omega) < (S(\omega) - \varepsilon)|\Lambda_a|$$

for all m such that there exists a translation of Γ_{n+1} into Δ_{m+1} with the property that the last translate of Λ_a in Γ_{n+1} is mapped onto the last translate of Λ_a in Δ_{m+1}. This is the case if the last translate in Δ_{m+1} is not "too near" the surface of Λ_b. For the remaining m subadditivity gives

$$S_{\Delta_{m+1}}(\omega) - S_{\Delta_m}(\omega) \leq |\Lambda_a| \log(N+1) \ .$$

Therefore, if b is large enough, we obtain

$$S_{\Lambda_b}(\omega) = \sum_m (S_{\Delta_{m+1}}(\omega) - S_{\Delta_m}(\omega)) < (S(\omega) - \varepsilon/2)|\Lambda_b|$$

which contradicts the definition of $S(\omega)$. Thus,

$$S_{\Gamma_{n+1}}(\omega) - S_{\Gamma_n}(\omega) \geq S(\omega)|\Lambda_a|$$

for all n. Hence

$$S_{\Gamma_\Lambda^+(a)}(\omega) = \sum_n (S_{\Gamma_{n+1}}(\omega) - S_{\Gamma_n}(\omega)) \geq S(\omega)|\Gamma_\Lambda^+(a)| \ .$$

Combining this with the previous estimates we have

$$S(\omega) + \varepsilon \geq \frac{S_\Lambda(\omega)}{|\Lambda|} \geq S(\omega) - \varepsilon$$

for sufficiently large Λ. This establishes the first two statements of the proposition.

The affinity of $\omega \mapsto S(\omega)$ follows directly from the concavity and convexity relations given in Proposition 6.2.25.

The upper semi-continuity follows because S is the infimum of the functions $S_{\Lambda_a}(\omega)/|\Lambda_a|$ which are continuous by Proposition 6.2.25.

Remark. Proposition 6.2.28 establishes that $-\tilde{S}_\Lambda(\omega)$ is strongly subadditive and has concavity and convexity properties similar to $S_\Lambda(\omega)$. Thus, by an identical argument one deduces that

$$\tilde{S}(\omega) = \lim_{\Lambda \rightsquigarrow \infty} \frac{\tilde{S}_\Lambda(\omega)}{|\Lambda|} = \sup_{a \in \mathbb{Z}_+^\nu} \frac{\tilde{S}_{\Lambda_a}(\omega)}{|\Lambda_a|}$$

defines an affine function over $E_{\mathfrak{A}}^{\mathbb{Z}^\nu}$ with values in $[-S(\omega), S(\omega)]$. Moreover, if ω is a Gibbs state with respect to some interaction Φ for which the surface

[4] This ordering is defined by setting $n < m$ if $n_j < m_j$ where $j = \min\{i;\ n_i \neq m_i\}$.

energies $W_\Phi(\Lambda)$, $\Lambda \subset L$, are well defined and satisfy $\|W_\Phi(\Lambda)\|/|\Lambda| \to 0$ as $|\Lambda| \to \infty$ then $\tilde{S}(\omega) = S(\omega)$. This is a corollary of Proposition 6.2.35. One has

$$\tilde{S}_\Lambda(\omega) - \beta\omega(\tilde{H}_\Phi(\Lambda)) \geq S_\Lambda(\omega') - \beta\omega'(\tilde{H}_\Phi(\Lambda))$$

for $\omega' = \omega|_{\mathfrak{A}_\Lambda} \otimes \omega|_{\mathfrak{A}_{\Lambda^c}}$. But $\tilde{S}_\Lambda(\omega') = S_\Lambda(\omega)$ and hence

$$S_\Lambda(\omega) - 2\|W_\Phi(\Lambda)\| \leq \tilde{S}_\Lambda(\omega) \leq S_\Lambda(\omega) \ .$$

Therefore $\tilde{S}(\omega) = S(\omega)$. Despite this identity on the Gibbs states the mean entropy and the mean conditional entropy do not coincide on the invariant states $E_{\mathfrak{A}}^{\mathbb{Z}^\nu}$ (see Notes and Remarks).

The new and somewhat surprising feature of the *mean entropy* $\omega \in E_{\mathfrak{A}}^{\mathbb{Z}^\nu} \mapsto S(\omega)$ is the affine property. This reflects an empirical physical phenomenon. The entropy of a mixed phase is obtained by superposition of the entropies of the pure phases in the appropriate proportions. In the sequel we will give a more detailed account of this interpretation.

The affine property also has an interesting corollary for periodic states.

Let $\tilde{\omega}$ be a state which is invariant under the subgroup

$$\mathbb{Z}_b^\nu = \{ba = (b_1a_1, \ldots, b_\nu a_\nu); a \in \mathbb{Z}^\nu\} \ ,$$

where $b \in \mathbb{Z}_+^\nu$. The states $\{\tau_a^*\tilde{\omega}; a \in \Lambda_b\}$ are periodic under the same subgroup and one verifies that

$$S_\Lambda(\tau_a^*\tilde{\omega}) = S_{\Lambda+a}(\tilde{\omega}) \ .$$

Hence the mean entropies are equal,

$$S(\tau_a^*\tilde{\omega}) = S(\tilde{\omega}) \ .$$

Thus if ω is the $\mathbb{Z}^\nu$-invariant state obtained by averaging $\tilde{\omega}$ over Λ_b, i.e.,

$$\omega(A) = |\Lambda_b|^{-1} \sum_{a \in \Lambda_b} \tilde{\omega}(\tau_{-a}(A)) \ ,$$

the affinity of S gives

$$S(\omega) = S\left(|\Lambda_b|^{-1} \sum_{a \in \Lambda_b} \tau_a^*\tilde{\omega}\right) = |\Lambda_b|^{-1} \sum_{a \in \Lambda_b} S(\tau_a^*\tilde{\omega}) = S(\tilde{\omega}) \ .$$

This equality will be of subsequent utility.

Next we examine the mean energy of an invariant interaction in an invariant state. This is basically a closed system problem and can be handled under weaker conditions on the interaction than those used to construct even the infinitesimal dynamics (see Proposition 6.2.3.).

Proposition 6.2.39. *Let Φ be a $\mathbb{Z}^\nu$-invariant interaction of a quantum spin system and suppose that*

$$\|\Phi\| = \sum_{X \ni 0} \frac{\|\Phi(X)\|}{|X|} < +\infty \ .$$

Further let ω be a $\mathbb{Z}^\nu$-invariant state over $\mathfrak{A}$.

It follows that the limit

$$H_\Phi(\omega) = \lim_{\Lambda \rightsquigarrow \infty} \frac{\omega(H_\Phi(\Lambda))}{|\Lambda|}$$

exists and

$$H_\Phi(\omega) = \omega(E_\Phi) \ ,$$

where $E_\Phi \in \mathfrak{A}$ is defined by

$$E_\Phi = \sum_{x \ni 0} \frac{\Phi(X)}{|X|} \ .$$

Thus $\omega \in E_{\mathfrak{A}}^{\mathbb{Z}^\nu} \mapsto H_\Phi(\omega)$ is an affine, weak-continuous, function satisfying*

$$|H_\Phi(\omega)| \leq \|\Phi\| \ .$$

PROOF. One has

$$\begin{aligned} \frac{\omega(H_\Phi(\Lambda))}{|\Lambda|} - \omega(E_\Phi) &= |\Lambda|^{-1} \omega\left(\sum_{X \subset \Lambda} \Phi(X) - \sum_{x \in \Lambda} \tau_x E_\Phi \right) \\ &= -|\Lambda|^{-1} \sum_{x \in \Lambda} \sum_{\substack{X \ni x \\ X \cap \Lambda^c \neq \varnothing}} \frac{\omega(\Phi(X))}{|X|} \ . \end{aligned}$$

But given $\varepsilon > 0$ one may choose a such that

$$\sum_{\substack{X \ni 0 \\ D(X) > a}} \frac{\|\Phi(X)\|}{|X|} < \varepsilon \ ,$$

where $D(X)$ is the diameter of X. Hence

$$\left| \frac{\omega(H_\Phi(\Lambda))}{|\Lambda|} - \omega(E_\Phi) \right| < \varepsilon + \left(\frac{|\Lambda(a)|}{|\Lambda|} \right) \|\Phi\| \ ,$$

where $\Lambda(a)$ now indicates the set of points in Λ which are at a distance less than a from the boundary. But we have already remarked that if $\Lambda \rightsquigarrow \infty$, then $|\Lambda(a)|/|\Lambda| \to 0$. Hence $H_\Phi(\omega)$ exists and is equal to $\omega(E_\Phi)$. It is evident that H_Φ is affine, weak*-continuous, and the bound follows because $\|E_\Phi\| \leq \|\Phi\|$.

Remark. If one replaces $H_\Phi(\Lambda)$ by the energy of the open subsystem, $\tilde{H}_\Phi(\Lambda) = H_\Phi(\Lambda) + W_\Phi(\Lambda)$, in the above discussion then it appears necessary to place stronger conditions on Φ. If, for example,

$$\sum_{X \ni 0} \|\Phi(X)\| < +\infty \ ,$$

then one easily deduces that

$$\lim_{\Lambda \rightsquigarrow \infty} \frac{\|W_\Phi(\Lambda)\|}{|\Lambda|} = 0$$

and hence

$$\lim_{\Lambda \rightsquigarrow \infty} \omega(\tilde{H}_\Phi(\Lambda)) = \lim_{\Lambda \rightsquigarrow \infty} \omega(H_\Phi(\Lambda)) = H_\Phi(\omega)$$

for each $\omega \in E_{\mathfrak{A}}^{\mathbb{Z}^\nu}$

Propositions 6.2.38 and 6.2.39 establish the existence of the *mean "free-energy" functional*

$$\omega \in E_{\mathfrak{A}}^{\mathbb{Z}^\nu} \mapsto F_{\beta\Phi}(\omega) = S(\omega) - \beta H_\Phi(\omega)$$

for a large class of invariant interactions Φ. But in the previous paragraph of this section the finite-volume equilibrium states were characterized as the states which maximize the corresponding finite-volume function $F_{\beta\Phi,\Lambda}(\omega) = S_\Lambda(\omega) - \beta\omega(H_\Phi(\Lambda))$. Moreover, the maximum value of the function was directly related to the equilibrium free energy, $F_\Lambda(\beta\Phi)$,

$$F_\Lambda(\beta\Phi) = -\beta^{-1} \log \mathrm{Tr}_{\mathfrak{H}_\Lambda}(e^{-\beta H_\Phi(\Lambda)}) = -\beta^{-1} \sup_{\omega \in E_{\mathfrak{A}_\Lambda}} F_{\beta\Phi,\Lambda}(\omega) \ .$$

Thus formally one expects the states which maximize $F_\Phi(\omega)$ to correspond to invariant thermodynamic equilibrium states and the maximum value $F(\Phi)$, of $F_\Phi(\omega)$, to be proportional to the equilibrium free energy per unit volume. The remainder of this paragraph is devoted to the examination of this tentative interpretation.

First we examine properties of the "free energy".

Theorem 6.2.40. *Let $\mathfrak{B}$ denote the Banach space of $\mathbb{Z}^\nu$-invariant interactions Φ with norm*

$$\|\Phi\| = \sum_{X \ni 0} \frac{\|\Phi(X)\|}{|X|} < +\infty \ .$$

The thermodynamic free energy

$$F(\Phi) = \lim_{\Lambda \rightsquigarrow \infty} |\Lambda|^{-1} \log \mathrm{Tr}_{\mathfrak{H}_\Lambda}(e^{-H_\Phi(\Lambda)})$$

exists for all $\Phi \in \mathfrak{B}$ and has the following properties:

(1) $$F(\Phi) = \sup_{\omega \in E_{\mathfrak{A}}^{\mathbb{Z}^\nu}} \{S(\omega) - H_\Phi(\omega)\}$$

where S and H_Φ denote the mean entropy and mean energy

(2) $\Phi \in \mathfrak{B} \mapsto F(\Phi)$ *is convex.*

(3) $\Phi \in \mathfrak{B} \mapsto F(\Phi)$ *is continuous and*

$$|F(\Phi) - F(\Psi)| \leq \|\Phi - \Psi\|$$

for all $\Phi, \Psi \in \mathfrak{B}$.

PROOF. For simplicity we only establish that the limit exists for parallelepipeds Λ_a whose edge lengths $a_i, i = 1, 2, \ldots, \nu$, all tend to infinity. The general convergence is subsequently obtained by comparison arguments using the matrix inequality

$$|\log \mathrm{Tr}(e^A) - \log \mathrm{Tr}(e^B)| \leq \|A - B\| \ .$$

First, it follows from the last statement of Proposition 6.2.22 that

$$|\Lambda|^{-1} \log \mathrm{Tr}_{\mathfrak{H}_\Lambda}(e^{-H_\Phi(\Lambda)}) \geq |\Lambda|^{-1}(S_\Lambda(\omega) - \omega(H_\Phi(\Lambda))) \ .$$

Thus, if

$$\underline{F}(\Phi) = \lim_{a \to \infty} \inf |\Lambda_a|^{-1} \log \mathrm{Tr}_{\mathfrak{H}_{\Lambda_a}}(e^{-H_\Phi(\Lambda_a)}) \ ,$$

then

$$\underline{F}(\Phi) \geq S(\omega) - H_\Phi(\omega)$$

for all $\omega \in E_{\mathfrak{A}}^{\mathbb{Z}^\nu}$. Consequently,

$$\underline{F}(\Phi) \geq \sup_{\omega \in E_{\mathfrak{A}}^{\mathbb{Z}^\nu}} \{S(\omega) - H_\Phi(\omega)\} \ .$$

Next consider a partition of $\mathbb{Z}^\nu$ formed by translates $\Lambda_n = \Lambda_a + na$ of the parallelepiped Λ_a. If

$$\Lambda = \bigcup_{i=1}^{N} \Lambda_{n_i} \ ,$$

we define a density matrix ρ_Λ on $\mathfrak{H}_\Lambda$ by

$$\frac{\rho_\Lambda = (\bigotimes_{i=1}^{N} e^{-H_\Phi(\Lambda_{n_i})})}{(\mathrm{Tr}_{\mathfrak{H}_{\Lambda_a}}(e^{-H_\Phi(\Lambda_a)}))^N} \ .$$

These density matrices determine a periodic state $\tilde{\omega}_a$ over $\mathfrak{A}$, i.e., a state invariant under $\mathbb{Z}_a^\nu$. The state ω_a defined by

$$\omega_a(A) = |\Lambda_a|^{-1} \sum_{x \in \Lambda_a} \tilde{\omega}_a(\tau_x(A))$$

is then $\mathbb{Z}^\nu$-invariant. But

$$S(\omega_a) = S(\tilde{\omega}_a) = |\Lambda_a|^{-1}(\tilde{\omega}_a(H_\Phi(\Lambda_a)) + \log \mathrm{Tr}_{\mathfrak{H}_{\Lambda_a}}(e^{-H_\Phi(\Lambda_a)}) \ ,$$

where the first equality follows from the discussion preceding Proposition 6.2.39 and the second by explicit computation. Now it is readily established that

$$\lim_{a \to \infty} \lim_{b \to \infty} \left| \frac{\omega_a(H_\Phi(\Lambda_b))}{|\Lambda_b|} - \frac{\tilde{\omega}_a(H_\Phi(\Lambda_a))}{|\Lambda_a|} \right| = 0$$

and therefore given $\varepsilon > 0$ one may choose a_0 such that

$$S(\omega_a) - H_\Phi(\omega_a) \geq |\Lambda_a|^{-1} \log \mathrm{Tr}_{\mathfrak{H}_{\Lambda_a}}(e^{-H_\Phi(\Lambda_a)}) - \varepsilon$$

for all $a > a_0$. Thus

$$\limsup_{a\to\infty}|\Lambda_a|^{-1}\log \mathrm{Tr}_{\mathfrak{H}_{\Lambda_a}}(e^{-H_\Phi(\Lambda_a)}) \le \varepsilon + \sup_{\omega\in E_{\mathfrak{A}}^{\mathbb{Z}^\nu}}\{S(\omega)-H_\Phi(\omega)\} \ .$$

Combination of this estimate with the previously obtained lower bound gives the existence of $F(\Phi)$ and the identification of statement (1).

(2) The convexity of $F(\Phi)$ follows from the affinity of $\Phi \to H_\Phi(\omega)$. Thus

$$\begin{aligned} F(\lambda\Phi+(1-\lambda)\Psi) &= \sup_{\omega\in E_{\mathfrak{A}}^{\mathbb{Z}^\nu}}\{S(\omega)-\lambda H_\Phi(\omega)-(1-\lambda)H_\Psi(\omega)\} \\ &\le \lambda \sup_{\omega\in E_{\mathfrak{A}}^{\mathbb{Z}^\nu}}\{S(\omega)-H_\Phi(\omega)\} \\ &\quad + (1-\lambda)\sup_{\omega\in E_{\mathfrak{A}}^{\mathbb{Z}^\nu}}\{S(\omega)-H_\Psi(\omega)\} \\ &= \lambda F(\Phi)+(1-\lambda)F(\Psi) \ . \end{aligned}$$

(3) The Bauer maximum principle, Lemma 4.1.12, establishes that each convex upper semi-continuous function over a convex compact set K attains its maximum at an extreme point of K. Thus, for each $\Phi \in \mathfrak{B}$ there must exist an ω_Φ such that

$$F(\Phi) = S(\omega_\Phi) - H_\Phi(\omega_\Phi) \ .$$

Therefore

$$\begin{aligned} F(\Phi) &= S(\omega_\Phi) - H_\Psi(\omega_\Phi) + H_{\Psi-\Phi}(\omega_\Phi) \\ &\le F(\Psi) + H_{\Psi-\Phi}(\omega_\Phi) \le F(\Psi) + \|\Psi-\Phi\| \ . \end{aligned}$$

Interchanging Φ and Ψ gives

$$F(\Psi) \le F(\Phi) + \|\Psi-\Phi\|$$

and this establishes the continuity relation.

Remark. The continuity relation can be used to bound F, e.g., if $\Psi = 0$, then $F(\Psi) = \log(N+1)$ and therefore

$$|F(\Phi) - \log(N+1)| \le \|\Phi\| \ .$$

Next we examine properties of the states which maximize $S - H_\Phi$. In the above proof of continuity of F we already remarked that for each $\Phi \in \mathfrak{B}$ the set of maximizing states

$$\Delta_\Phi = \{\omega; F(\Phi) = S(\omega) - H_\Phi(\omega)\}$$

is nonempty. Moreover, the discussion of the maximum entropy principle for open and closed systems given in the previous paragraph strongly indicates that these states correspond to $\mathbb{Z}^\nu$-invariant thermodynamic equilibrium states. Thus, it is natural to ask whether these states statisfy the various equilibrium criteria which we previously examined, e.g., the Gibbs condition, or the KMS condition. The first and most general result in this direction is the following.

Proposition 6.2.41. *Let Φ be a $\mathbb{Z}^\nu$-invariant interaction of a quantum spin system satisfying*

(1) $$\|\Phi\| = \sum_{X\ni 0}\frac{\|\Phi(X)\|}{|X|} < +\infty \ .$$

(2) *The surface energies* $\{W_\Phi(\Lambda); \Lambda \subset \mathbb{Z}^\nu\}$ *exist.*

(3) $$\liminf_{\Lambda \rightsquigarrow \infty} \frac{\|W_\Phi(\Lambda)\|}{|\Lambda|} = 0 \ .$$

It follows that each $\mathbb{Z}^\nu$ *-invariant state which satisfies the Gibbs condition with respect to* Φ *maximizes* $S - H_\Phi$.

Remarks

(1) Assumption (1) assures that $\omega \in E_{\mathfrak{A}}^{\mathbb{Z}^\nu} \mapsto H_\Phi(\omega) \in \mathbb{R}$ is defined and similarly assumption (2) is necessary for the Gibbs condition to be defined. Thus, the essential new condition is the third. All three assumptions are easily verified if

$$\sum_{X \ni 0} \|\Phi(X)\| < +\infty$$

and hence this condition could be taken as the sole hypothesis.

(2) The proposition does not establish the existence of invariant states satisfying the Gibbs condition. The existence problem will be solved subsequently under more stringent assumptions on Φ (see Theorem 6.2.42 and the discussion preceding it).

PROOF. Let ω denote the $\mathbb{Z}^\nu$-invariant state which satisfies the Gibbs condition and $\{\rho_\Lambda\}_{\Lambda \subset \mathbb{Z}^\nu}$ the associated density matrices. Moreover, let ω_Λ denote the local Gibbs state, i.e.,

$$\omega_\Lambda(A) = \mathrm{Tr}_{\mathfrak{H}_\Lambda}(\sigma_\Lambda A), \qquad \sigma_\Lambda = \frac{e^{-H_\Phi(\Lambda)}}{\mathrm{Tr}_{\mathfrak{H}_\Lambda}(e^{-H_\Phi(\Lambda)})} \ .$$

Thus, the conditional entropy of $\omega|_{\mathfrak{A}_\Lambda}$ with respect to ω_Λ is given by

$$\begin{aligned} S(\omega|_{\mathfrak{A}_\Lambda} | \omega_\Lambda) &= -\mathrm{Tr}_{\mathfrak{H}_\Lambda}(\rho_\Lambda \log \rho_\Lambda - \rho_\Lambda \log \sigma_\Lambda) \\ &= S_\Lambda(\omega) - \omega(H_\Phi(\Lambda)) - \log \mathrm{Tr}_{\mathfrak{H}_\Lambda}(e^{-H_\Phi(\Lambda)}) \ . \end{aligned}$$

But the Gibbs condition gives

$$\omega_\Lambda = \omega^{W_\Phi(\Lambda)}|_{\mathfrak{A}_\Lambda}$$

and hence it follows from the monotonicity of the conditional entropy, Proposition 6.2.33, that

$$0 \geq S(\omega|_{\mathfrak{A}_\Lambda}|\omega_\Lambda) \geq S(\omega|\omega^{W_\Phi(\Lambda)}) \ .$$

Moreover

$$S(\omega|\omega^{W_\Phi(\Lambda)}) \geq -2\|W_\Phi(\Lambda)\|$$

by the discussion preceding Example 6.2.30. Combination of these observations leads to the bounds

$$0 \geq S_\Lambda(\omega) - \omega(H_\Phi(\Lambda)) - \log \mathrm{Tr}_{\mathfrak{H}_\Lambda}(e^{-H_\Phi(\Lambda)}) \geq -2\|W_\Phi(\Lambda)\| \ .$$

Up to this point $\mathbb{Z}^\nu$-invariance was irrelevant but now if one divides by $|\Lambda|$ and takes the limit $\Lambda \rightsquigarrow \infty$, then assumption (3) and the existence of the mean entropy $S(\omega)$, mean energy $H_\Phi(\omega)$, and free energy $F(\Phi)$, lead to the relation

$$S(\omega) - H_\Phi(\omega) - F(\Phi) = 0 \ ,$$

i.e., ω maximizes $S - H_\Phi$.

Next we examine the relationship between invariant KMS states and the states that maximize $S - H_\Phi$.

The KMS condition has an advantage over the Gibbs condition insofar as one can deduce the existence of $\mathbb{Z}^\nu$-invariant KMS states. If the interaction Φ is such that τ^Φ exists, i.e.,

$$\lim_{\Lambda \to \infty} \|\tau_t^\Phi(A) - e^{itH_\Phi(\Lambda)} A e^{-itH_\Phi(\Lambda)}\| = 0$$

for all $A \in \mathfrak{A}, t \in \mathbb{R}$, then (τ^Φ, β)-KMS states exist by Proposition 6.2.15. Now let ω be such a state and define $\bar{\omega}$ by

$$\bar{\omega}(A) = M(\omega(\tau(A))) \ ,$$

where M is an invariant mean over $\mathbb{Z}^\nu$. It follows immediately that $\bar{\omega}$ is $\mathbb{Z}^\nu$-invariant. But it also satisfies the (τ^Φ, β)-KMS condition whenever Φ is $\mathbb{Z}^\nu$-invariant. This follows by observing that τ_x and τ_t^Φ commute and hence

$$\begin{aligned} \bar{\omega}(A\tau_{i\beta}^\Phi(B)) &= M(\omega(\tau(A)\tau_{i\beta}^\Phi(\tau(B)))) \\ &= M(\omega(\tau(B)\tau(A))) = \bar{\omega}(BA) \ . \end{aligned}$$

Thus $\bar{\omega}$ is a $\mathbb{Z}^\nu$-invariant (τ^Φ, β)-KMS state.

Every τ^Φ-KMS sate ω satisfies the Gibbs condition by Proposition 6.2.17. Hence, if Φ satisfies the supplementary hypotheses of Proposition 6.2.41, then ω will maximize $S - H_\Phi$. We now aim to derive a converse of this statement. The proof of the converse depends upon a number of approximation, continuity, and density arguments. Instead of trying to isolate a minimum number of implicit properties of Φ which ensure the validity of these arguments we specify an explicit space of interactions, the Banach space of Theorem 6.2.4.

Theorem 6.2.42. *Let Φ be a $\mathbb{Z}^\nu$-invariant interaction of a quantum spin system such that*

$$\|\Phi\|_\lambda = \sum_{X \ni 0} \|\Phi(X)\| e^{\lambda|X|} < +\infty$$

for some $\lambda > 0$, and let τ^Φ denote the associated dynamical group of *-automorphisms of the spin algebra $\mathfrak{A}$.

If ω is a $\mathbb{Z}^\nu$-invariant state and $\beta \in \mathbb{R}$, then the following conditions are equivalent

(1) ω is a (τ^{Φ}, β)-*KMS state.*
(2) ω *satisfies the Gibbs condition with respect to* $\beta\Phi$.
(3) ω *maximizes* $S - \beta H_{\Phi}$.

PROOF. First note that τ^{Φ} exists and $\bigcup_{\Lambda \subset \mathbb{Z}^{\nu}} \mathfrak{A}_{\Lambda}$ is a core for its generator by Theorem 6.2.4. Moreover,

$$\|\Phi\|_0 = \sum_{X \ni 0} \|\Phi(X)\| < +\infty \ .$$

Hence, $W_{\Phi}(\Lambda)$ exists and

$$|\Lambda|^{-1} \|W_{\Phi}(\Lambda)\| \leq |\Lambda|^{-1} \sum_{x \in \Lambda} \sum_{\substack{X \ni x \\ X \cap \Lambda^c \neq \emptyset}} \|\Phi(X)\| \underset{\Lambda = \infty}{\longrightarrow} 0 \ .$$

Therefore, the combined hypotheses of Corollary 6.2.19 and Proposition 6.2.41 are satisfied. Consequently, (1) $\Leftrightarrow$ (2) $\Rightarrow$ (3).

It remains to prove (3) $\Rightarrow$ (1). This will be achieved by use of various convexity properties.

Let B_{λ} denote the Banach space of $\mathbb{Z}^{\nu}$-invariant interactions for which $\|\Phi\|_{\lambda} < +\infty$. It follows from Theorem 6.2.40 that the free energy

$$F(\Phi) = \lim_{\Lambda \rightsquigarrow \infty} |\Lambda|^{-1} \log \mathrm{Tr}_{\mathfrak{H}_{\Lambda}}(e^{-H_{\Phi}(\Lambda)})$$

exists for each $\Phi \in B_{\lambda}$ and defines a convex continuous function over B_{λ}. The key observation is that each state ω_{Φ} which maximizes $S - H_{\Phi}$ defines a tangent functional to the graph of F at Φ. Convex analysis can then be fruitfully used in the examination of the maximizing states.

Recall that if F is a convex, continuous, function over a Banach space X, then an element $f_x \in X^*$ is said to be a tangent functional to the graph of F at x if

$$F(x + \xi) \geq F(x) + f_x(\xi)$$

for all $\xi \in X$. Moreover, there is a unique tangent functional to the graph of F at x if, and only if F is differentiable at x and in this case the tangent functional is the derivative ∂F_x of F at x. For example, if F is differentiable at x and $0 < h < 1$, convexity gives

$$F(x + \xi) - F(x) \geq h^{-1}(F(x + h\xi) - F(x)) \underset{h=0}{\longrightarrow} \partial F_x(\xi)$$

and ∂F_x is a tangent functional at x. But if

$$f_x(\xi) \leq F(x + \xi) - F(x) \ ,$$

then

$$f_x(\xi) = h^{-1} f_x(h\xi) \leq h^{-1} F((x + h\xi) - F(x)) \underset{h=0}{\longrightarrow} \partial F_x(\xi) \ .$$

Replacing ξ by $-\xi$ in this bound one finds the opposite bound and hence $f_x = \partial F_x$. Thus, differentiability implies that ∂F_x is the unique tangent functional. The converse is easily deduced by arguing that nondifferentiability leads to nonuniqueness.

Let us now reexamine the relationship between the free energy $F(\Phi)$ and the maximizing state ω_{Φ}. One has

$$\begin{aligned} F(\Phi+\Psi) &\geq S(\omega_\Phi) - H_{\Phi+\Psi}(\omega_\Phi) \\ &= S(\omega_\Phi) - H_\Phi(\omega_\Phi) - H_\Psi(\omega_\Phi) = F(\Phi) - \omega_\Phi(E_\Psi) \ , \end{aligned}$$

where E_Ψ is the interaction energy at the origin,

$$E_\Psi = \sum_{X \ni 0} \frac{\Psi(X)}{|X|} \ ,$$

and we have used the maximum entropy principle together with Proposition 6.2.39. Thus, ω_Φ defines a tangent functional f_Φ to the graph of F at Φ through the relation

$$f_\Phi(\Psi) = -\omega_\Phi(E_\Psi) \ .$$

Now we begin the derivation of the $(\tau^\Phi, 1)$-KMS condition for ω_Φ by examination of those Φ for which ω_Φ is unique, i.e., those Φ for which the graph of F at Φ is differentiable. (The (τ^Φ, β)-KMS condition for $\omega_{\beta\Phi}$ and $\beta \in \mathbb{R}\backslash\{0\}$ follows by rescaling.)

The free energy F is defined by the thermodynamic limit $\Lambda \rightsquigarrow \infty$ of the mean free energies

$$F_\Lambda(\Phi) = |\Lambda|^{-1} \log \mathrm{Tr}_{\mathfrak{H}_\Lambda}(e^{-H_\Phi(\Lambda)})$$

and each of the functionals $\Phi \in B_\lambda \mapsto F_\Lambda(\Phi)$ is convex and continuous by the arguments used to derive similar properties of F. The F_Λ are, however, simply defined in terms of finite-dimensional matrices and it follows that they are everywhere differentiable. Therefore, there is a unique tangent functional $f_{\Lambda,\Phi}$ to F_Λ at Φ, the derivative of F_Λ at Φ, and this is given by

$$f_{\Lambda,\Phi}(\Psi) = -|\Lambda|^{-1} \frac{\mathrm{Tr}_{\mathfrak{H}_\Lambda}(e^{-H_\Phi(\Lambda)} H_\Psi(\Lambda))}{\mathrm{Tr}_{\mathfrak{H}_\Lambda}(e^{-H_\Phi(\Lambda)})} \ .$$

Next for $\Lambda_0 \subset \Lambda$ and $A = A^* \in \mathfrak{A}_{\Lambda_0}$ one can define a $\mathbb{Z}^\nu$-invariant interaction Ψ_A by setting $\Psi_A(\Lambda_0 + x) = \tau_x(A)$ for all $x \in \mathbb{Z}^\nu$, and $\Psi_A(\Lambda') = 0$ if Λ' is not a translate of Λ_0. Adopting this definition one sees that the linear functional

$$\begin{aligned} A \in \mathfrak{A}_{\Lambda 0} \mapsto \omega_{\Lambda,\Phi}(A) &= -f_{\Lambda,\Phi}(\Psi_{(A+A^*)/2}) - i f_{\Lambda,\Phi}(\Psi_{(A-A^*)/2i}) \\ &= |\Lambda|^{-1} \sum_{\substack{x \in \mathbb{Z}^\nu \\ \Lambda_0 + x \subseteq \Lambda}} \frac{\mathrm{Tr}_{\mathfrak{H}_\Lambda}(e^{-H_\Phi(\Lambda)} \tau_x(A))}{\mathrm{Tr}_{\mathfrak{H}_\Lambda}(e^{-H_\Phi(\Lambda)})} \end{aligned}$$

is both positive and normalized. Hence $\omega_{\Lambda,\Phi}$ is a state over $\mathfrak{A}_{\Lambda_0}$ which we identify with any extension to the complete spin algebra $\mathfrak{A}$. It then follows from weak* compactness of $E_{\mathfrak{A}}$ that $\Lambda \subset \mathbb{Z}^\nu \mapsto \omega_{\Lambda,\Phi}$ has weak*-limit points. Therefore, there exist nets $\Lambda_\alpha \mapsto f_{\Lambda_\alpha,\Phi}(\Psi_A)$ which converge for all $\{\Psi_A; A = A^* \in \mathfrak{A}_{\Lambda_0}, \Lambda_0 \subset \mathbb{Z}^\nu\}$. But the linear span of the latter set is norm dense in B_λ and hence $\Lambda_\alpha \mapsto f_{\Lambda_\alpha,\Phi}$ is weak* convergent. Each limit point f_Φ is, however, a tangent functional to the graph of F at Φ because

$$\begin{aligned} f_\Phi(\Psi) &= \lim_\alpha f_{\Lambda_\alpha,\Phi}(\Psi) \\ &\leq \lim_\alpha (F_{\Lambda_\alpha}(\Phi+\Psi) - F_{\Lambda_\alpha}(\Phi)) = F(\Phi+\Psi) - F(\Phi) \ . \end{aligned}$$

Since we are assuming F to have a unique tangent at Φ, it follows that all the nets $\Lambda_\alpha \mapsto f_{\Lambda_\alpha,\Phi}$ have the same limit and hence $\Lambda \subset \mathbb{Z}^\nu \mapsto f_{\Lambda,\Phi}$ converges in the weak* topology. Moreover, combining the identifications of f_Φ and $f_{\Lambda,\Phi}$, one concludes that

$$\begin{aligned}\omega_\Phi(A) &= \omega_\Phi(E_{\Psi(A+A^*)/2}) + i\omega_\Phi(E_{\Psi(A-A^*)/2i})\\ &= -f_\Phi(\Psi_{(A+A^*)/2}) - if_\Phi(\Psi_{(A-A^*)/2i})\\ &= -\lim_{\Lambda\to\infty}(f_{\Lambda,\Phi}(\Psi_{(A+A^*)/2}) + if_{\Lambda,\Phi}(\Psi_{(A-A^*)/2i}))\\ &= \lim_{\Lambda\to\infty}|\Lambda|^{-1}\sum_{\substack{x\in\mathbb{Z}^\nu\\ \Lambda_0+x\subseteq\Lambda}}\frac{\mathrm{Tr}_{\mathfrak{H}_\Lambda}(e^{-H_\Phi(\Lambda)}\tau_x(A))}{\mathrm{Tr}_{\mathfrak{H}_\Lambda}(e^{-H_\Phi(\Lambda)})}\end{aligned}$$

for $A \in \mathfrak{A}_{\Lambda_0}$ and all $\Lambda_0 \subset \mathbb{Z}^\nu$. Thus, the unique state ω_Φ which maximizes $S - H_\Phi$ is the thermodynamic limit of space averages of the local Gibbs states ω_Λ^Φ. It is this identification which allows the deduction of the $(\tau^\Phi, 1)$-KMS condition.

Let Λ_a denote a cubic array

$$\Lambda_a = \{x;\, x \in \mathbb{Z}^\nu, -a \le x_i \le a, i = 1, \ldots, \nu\}\ .$$

It follows from Theorem 6.2.4 that for each $\varepsilon > 0, b \in \mathbb{Z}_+$, one may choose a_0 such that

$$\|e^{itH_\Phi(\Lambda_a)}\tau_x(A)e^{-itH_\Phi(\Lambda_a)} - \tau_t^\Phi\tau_x(A)\| < \varepsilon$$

for all $x \in \Lambda_b$ and all $a > a_0$. Next remark that for $A, B \in \mathfrak{A}_{\Lambda_0}$ the analytic function $t \mapsto F_{\Lambda,\Phi}^{A,B}(t)$ defined by

$$F_{\Lambda,\Phi}^{A,B}(t) = |\Lambda|^{-1}\sum_{\substack{x\in\Lambda\\ \Lambda_0+x\subset\Lambda}}\frac{\mathrm{Tr}_{\mathfrak{H}_\Lambda}(e^{-H_\Phi(\Lambda)}\tau_x(A)e^{itH_\Phi(\Lambda)}\tau_x(B)e^{-itH_\Phi(\Lambda)})}{\mathrm{Tr}_{\mathfrak{H}_\Lambda}(e^{-H_\Phi(\Lambda)})}$$

satisfies the KMS identity

$$F_{\Lambda,\Phi}^{A,B}(t+i) = F_{\Lambda,\Phi}^{B,A}(-t)\ .$$

But from the previous estimate and the convergence of $\omega_{\Lambda,\Phi}$ to ω_Φ one concludes that

$$\lim_{a\to\infty} F_{\Lambda_a,\Phi}^{A,B}(t) = \omega_\Phi(A\tau_t^\Phi(B))\ .$$

Therefore, ω_Φ satisfies the $(\tau^\Phi, 1)$-KMS condition as a corollary of Proposition 5.3.12 (see the discussion following the proof of this proposition).

It remains to handle the $\Phi \in B_\lambda$ for which the tangent functional to F at Φ is not unique. This is achieved by an approximation technique based upon the fact that convex continuous functions are automatically differentiable at a "large" set of points, and at the exceptional points a general tangent functional can be constructed by convex combinations of limits of unique functionals. For example, if F is a convex function of one real variable it is automatically continuous, differentiable at all but a countable set of points, and at these points each tangent functional is a convex combination of the left derivative and the right derivative. The generalization that we need is contained in the following lemma.

Lemma 6.2.43. *Let F be a convex, continuous function over a separable Banach space X and let $f \in X^*$ be a tangent functional to the graph of F at zero.*

It follows that f is contained in the weak-closed convex hull of the set of tangent functionals $\mathscr{T}$ defined by*

$$\mathscr{T} = \{g \in X^*; \textit{there exist } x_\alpha \to 0 \textit{ (in norm) such that } F \textit{ is differentiable at each } x_\alpha \textit{ and } \lim_\alpha \partial F(x_\alpha)(x) = g(x),\ x \in X\}.$$

We omit the proof of this result (see Notes and Remarks).

End Of Proof Of Theorem 6.2.42. It follows from Lemma 6.2.43, and the weak* compactness of KMS states, that it suffices to prove that ω_Φ satisfies the $(\tau^\Phi, 1)$-KMS condition in the special case

$$\omega_\Phi = \lim_\alpha \omega_{\Phi_\alpha}$$

where $\Phi_\alpha \in B_\lambda$ and $\omega_{\Phi_\alpha} \in \boldsymbol{E}_{\mathfrak{A}}^{\mathbb{Z}^\nu}$ have the properties

(1) $$\|\Phi_\alpha - \Phi\|_\lambda \to 0\ ,$$

(2) $S - H_{\Phi_\alpha}$ is maximized by a unique state ω_{Φ_α}.

But it follows from this second property and the foregoing analysis that ω_{Φ_α} must satisfy the$(\tau^{\Phi_\alpha}, 1)$-KMS condition. Moreover, it follows from the first property and the discussion following Example 6.2.5 that

$$\lim_\alpha \|\tau_t^\Phi(A) - \tau_t^{\Phi_\alpha}(A)\| = 0$$

uniformly for t in any bounded interval. Therefore, ω_Φ satisfies the $(\tau^\Phi, 1)$-KMS condition by Proposition 5.3.25.

Finally it remains to prove (3) $\Rightarrow$ (1) when $\beta = 0$, i.e., we must prove that if ω maximizes S, then ω is a trace-state. We argue by negation. If ω is not a trace, $\omega|_{\mathfrak{A}_\Lambda}$ cannot be a trace for sufficiently large Λ and hence $\omega|_{\mathfrak{A}_\Lambda}$cannot maximize S_Λ, i.e.,

$$S_\Lambda(\omega) < |\Lambda| \log(N+1)$$

for Λ sufficiently large. But this implies

$$S(\omega) < \log(N+1)$$

and hence ω does not maximize S.

Remark. We have chosen to prove the equivalences of Theorem 6.2.42 under the assumption $\Phi \in B_\lambda$.This can, however, be replaced by the hypotheses of Theorem 6.2.6 and this is of interest for one- and two-dimensional systems.

The identifications provided by Theorem 6.2.42 give a new criterion for invariant equilibrium states, maximum mean entropy at fixed mean energy. The theorem is slightly unsatisfactory insofar as the proof of equivalence of the three criteria is only established under relatively strong assumptions on Φ, i.e., $\Phi \in B_\lambda$ for some $\lambda > 0$. The Gibbs condition, and the maximum entropy property, can of course be defined under much weaker hypotheses, e.g., $\Phi \in B_0$, and it would be of interest to derive equivalence of these two conditions under

weaker assumptions on Φ. This would demand a converse to Proposition 6.2.41 and in particular a proof of existence of $\mathbb{Z}^\nu$-invariant states satisfying the Gibbs condition which is independent of the existence of dynamical group τ^Φ. Despite these shortcomings the theorem motivates the study of the set of states which maximize $S - H_\Phi$ as candidates for $\mathbb{Z}^\nu$-invariant equilibrium states corresponding to the interaction Φ.

Theorem 6.2.44. *Let $\mathfrak{B}$ denote the Banach space of $\mathbb{Z}^\nu$-invariant spin interactions Φ with norm given by*

$$\|\Phi\| = \sum_{X \ni 0} \frac{\|\Phi(X)\|}{|X|} < +\infty$$

and define $\Delta_\Phi \subset E_{\mathfrak{A}}^{\mathbb{Z}^\nu}$ by

$$\Delta_\Phi = \left\{\omega; \omega \in E_{\mathfrak{A}}^{\mathbb{Z}^\nu}, S(\omega) - H_\Phi(\omega) = \sup_{\omega' \in E_{\mathfrak{A}}^{\mathbb{Z}^\nu}} \{S(\omega') - H_\Phi(\omega')\}\right\} ,$$

where S and H_Φ denote the mean entropy and mean energy.

It follows that:

(1) *Δ_Φ is a nonempty, weak*-compact face of $E_{\mathfrak{A}}^{\mathbb{Z}^\nu}$.*

(2) *Δ_Φ is a simplex with $\mathscr{E}(\Delta_\Phi) \subset \mathscr{E}(E_{\mathfrak{A}}^{\mathbb{Z}^\nu})$ and the unique barycentric decomposition of each $\omega \in \Delta_\Phi$ coincides with the unique decomposition of ω into extremal $\mathbb{Z}^\nu$-invariant states.*

PROOF

(1) It follows once again from the Bauer maximum principle, Lemma 4.1.12, and the upper semi-continuity of $S - H_\Phi$ that Δ_Φ is nonempty and in fact Δ_Φ must contain an extremal $\mathbb{Z}^\nu$-invariant state, i.e., an $\omega \in \mathscr{E}(E_{\mathfrak{A}}^{\mathbb{Z}^\nu})$. Weak* compactness follows by noting that if $\omega_\alpha \in \Delta_\Phi$ and $\omega_\alpha \to \omega$, then

$$\lim_\alpha \{S(\omega_\alpha) - H_\Phi(\omega_\alpha)\} \leq \{S(\omega) - H_\Phi(\omega)\}$$

by upper semi-continuity of $S - H_\Phi$. Consequently, $\omega \in \Delta_\Phi$.

Similarly if we assume that $\omega_\Phi \in \Delta_\Phi$ and

$$\omega_\Phi = \lambda\omega_1 + (1 - \lambda)\omega_2$$

with $\omega_1, \omega_2 \in E_{\mathfrak{A}}^{\mathbb{Z}^\nu}$ but $\omega_1 \notin \Delta_\Phi$, then the affinity of $S - H_\Phi$ implies the contradiction

$$\begin{aligned}\sup_{\omega \in E_{\mathfrak{A}}^{\mathbb{Z}^\nu}} \{S(\omega) - H_\Phi(\omega)\} &> \lambda\{S(\omega_1) - H_\Phi(\omega_1)\} + (1 - \lambda)\{S(\omega_2) - H_\Phi(\omega_2)\} \\ &= S(\omega_\Phi) - H_\Phi(\omega_\Phi) = \sup_{\omega \in E_{\mathfrak{A}}^{\mathbb{Z}^\nu}} \{S(\omega) - H_\Phi(\omega)\} .\end{aligned}$$

Thus Δ_Φ is a face.

(2) The spin algebra is $\mathbb{Z}^\nu$-asymptotically abelian in the norm sense. Thus $E_{\mathfrak{A}}^{\mathbb{Z}^\nu}$ is a simplex by Corollary 4.3.11. The remaining statements follow because Δ_Φ is a stable face of $E_{\mathfrak{A}}^{\mathbb{Z}^\nu}$.

Note that if Δ_Φ is composed of one point ω, then ω is automatically an extremal $\mathbb{Z}^\nu$-invariant state and it has the cluster properties in mean discussed in Section 4.3.2. Interpreting the elements of Δ_Φ to be invariant equilibrium states, this indicates that if there exists a unique $\mathbb{Z}^\nu$-invariant equilibrium state, i.e., a unique $\mathbb{Z}^\nu$-invariant thermodynamic phase, this state, or phase, is automatically $\mathbb{Z}^\nu$-ergodic. Therefore if Δ_Φ consists of more than one state, the unique decomposition of each element $\omega \in \Delta_\Phi$ into extremal elements corresponds to the separation of the mixed thermodynamic phases into pure phases, i.e., $\mathbb{Z}^\nu$-ergodic states. But the mean entropy S is affine and upper semicontinuous and therefore it respects the barycentric decomposition of ω, by Corollary 4.1.18, e.g. if $\mu_\omega \in M_\omega(E_{\mathfrak{A}}^{\mathbb{Z}^\nu})$,

$$\omega(A) = \int d\mu_\omega(\omega')\, \omega'(A), \quad A \in \mathfrak{A}$$

and

$$S(\omega) = \int d\mu_\omega(\omega')\, S(\omega') \ .$$

Thus, accepting the foregoing interpretation of mixed phases and pure phases, one concludes that the mean entropy of a mixture is the mixture of the mean entropies. A similar conclusion is valid for the mean energy.

We conclude with various observations concerning the set of states Δ_Φ which follow by elaboration of the convexity arguments used to prove Theorem 6.2.42. Throughout these observations we take $\mathfrak{B}_1$ to be a Banach space of invariant interactions which contains the space $\mathfrak{B}_0$ of invariant finite range interactions as a norm dense subspace and moreover we assume that $\mathfrak{B}_1 \subset \mathfrak{B}$ where $\mathfrak{B}$ is the space of Theorem 6.2.44.

Observation 1. *There is a one-to-one correspondence between tangent functionals f_Φ to the graph of the free energy, $\Phi \in \mathfrak{B}_1 \mapsto F(\Phi)$, at Φ and states ω_Φ which maximize $S - H_\Phi$. This correspondence is such that*

$$f_\Phi(\Psi) = -\omega_\Phi(E_\Psi),\ \Psi \in \mathfrak{B}_1 \ .$$

This was almost established in the proof of Theorem 6.2.42. In particular we showed that each state ω_Φ which maximizes $S - H_\Phi$ defines a tangent functional f_Φ through the above relation. Moreover, as $\mathfrak{B}_0 \subset \mathfrak{B}_1$ each state is determined by its values on $\{E_\Psi; \Psi \in \mathfrak{B}_1\}$. Therefore, distinct maximizing states lead to distinct tangent functionals and if there is a unique tangent functional f_Φ, there is a unique maximizing state ω_Φ. But if f_Φ is not unique, then by Lemma 6.2.43 there exist $\Phi_\alpha \in \mathfrak{B}_1$ such that f_{Φ_α} is unique, $\|\Phi_\alpha - \Phi\| \to 0$, and

$$f_\Phi(\Psi) = \lim_\alpha f_{\Phi_\alpha}(\Psi) = -\lim_\alpha \omega_{\Phi_\alpha}(E_\Psi) \ .$$

But this implies that ω_{Φ_α} converges in the weak* topology to a state ω_Φ which has the required correspondence with f_Φ.

Observation 2. *The set $\Phi \in \mathfrak{B}_1$ for which Δ_Φ consists of a single point is norm dense.*

This follows immediately from Observation 1 and Lemma 6.2.43.

By an extension of the latter lemma one can even show that this set contains a countable intersection of dense open subsets. The implication of this last observation is that the Φ for which Λ_Φ is a singleton forms a "large" set and in the physical interpretation this implies that the spin system tends to have a pure thermodynamic phase "almost always". Nevertheless, it may happen for a fixed Φ that $\Delta_{\beta\Phi}$ consists of more than one point for all β in an interval of the form $\langle \beta_c, \infty \rangle$ (see Section 6.2.6). It is, however, possible to prove the existence of a dense subset $D \subset \mathfrak{B}_1$, such that for $\Phi \in D$ and Lebesgue-almost every $\beta \in \mathbb{R}$ the set $\Delta_{\beta\Phi}$ is a singleton.

Observation 3

$$E_{\mathfrak{A}}^{\mathbb{Z}^\nu} = \overline{\bigcup_{\Phi \in \mathfrak{B}_1} \Delta_\Phi}$$

where the bar denotes the uniform closure.

If F is a convex continuous function over a Banach space X, then $f \in X^*$ is called F-bounded if there is a $c \in \mathbb{R}$ such that

$$F(x) \geq f(x) + c$$

for all $x \in X$. One can prove that the tangent functionals to F are norm dense in the F-bounded functionals.

Now suppose $\omega \in E_{\mathfrak{A}}^{\mathbb{Z}^\nu}$, then

$$F(\Phi) \geq S(\omega) - H_\Phi(\omega) \geq -\omega(E_\Phi)$$

because $S \geq 0$ and $H_\Phi(\omega) = \omega(E_\Phi)$. Thus the function $f \in \mathfrak{B}_1^*$ defined by

$$f(\Phi) = -\omega(E_\Phi)$$

is F-bounded (with bound zero). Therefore, by the general result just cited there must exist $\Phi_\alpha \in \mathfrak{B}_1$ and tangent functionals f_{Φ_α} to the graph of F at Φ_α such that

$$\sup_{\Psi \in \mathfrak{B}_1} \frac{|f_{\Phi_\alpha}(\Psi) - f(\Psi)|}{\|\Psi\|} \underset{\alpha \to \infty}{\longrightarrow} 0 \ .$$

But by Observation 1 the tangent functionals f_{Φ_α} determine states $\omega_{\Phi_\alpha} \in \Delta_{\Phi_\alpha}$. Moreover, if $A = A^* \in \mathfrak{A}_X$ and Ψ_A is defined by $\Psi_A(X + x) = \tau_x(A)$, and $\Psi_A(Y) = 0$ if Y is not a translate of X, then the $\mathfrak{B}$-norm of Ψ_A satisfies $\|\Psi_A\| = \|A\|$. Thus,

$$\frac{|\omega_{\Phi_\alpha}(A) - \omega(A)|}{\|A\|} = \frac{|f_{\Phi_\alpha}(\Psi_A) - f(\Psi_A)|}{\|\Psi_A\|}$$

and consequently the ω_{Φ_α} converge uniformly to ω.

The foregoing observation implies that each invariant state is close to an equilibrium state of some $\Phi \in \mathfrak{B}$. The norm approximation gives a strong control which one can exploit to obtain a stronger statement of this form.

Observation 4. *If* $\omega_1, \ldots, \omega_n \in \mathscr{E}(E_{\mathfrak{A}}^{\mathbb{Z}^\nu})$, *then there is a* $\Phi \in \mathfrak{B}$ *such that*

$$\omega_1, \ldots, \omega_n \in \Delta_\Phi \ .$$

First note that $E_{\mathfrak{A}}^{\mathbb{Z}^\nu}$ is a simplex by Corollary 4.3.11. We next argue that the isomorphism between $\omega \in E_{\mathfrak{A}}^{\mathbb{Z}^\nu}$ and maximal probability measures $\mu_\omega \in M_\omega(E_{\mathfrak{A}}^{\mathbb{Z}^\nu})$ is isometric from the norm topology to the norm topology, i.e., $\|\omega - \omega'\| = \|\mu_\omega - \mu_{\omega'}\|$. To establish this let $\omega - \omega' = \omega_+ - \omega_-$ denote the Jordan decomposition of $\omega - \omega'$ given by Proposition 3.2.7. By uniqueness the $\omega_\pm$ must be $\mathbb{Z}^\nu$-invariant and hence there exist unique maximal probability measures $\mu_\pm$ with barycenters $\omega_\pm/\|\omega_\pm\|$. But $\omega + \omega_- = \omega' + \omega_+$ and hence by uniqueness $\mu_\omega + \|\omega_-\|\mu_- = \mu_{\omega'} + \|\omega_+\|\mu_+$. Therefore,

$$\begin{aligned}\|\omega - \omega'\| &= \|\omega_+\| + \|\omega_-\| \\ &\geq \|\|\omega_-\|\mu_- - \|\omega_+\|\mu_+\| \\ &= \|\mu_\omega - \mu_{\omega'}\| \geq \|\omega - \omega'\| \ .\end{aligned}$$

Now let $\omega' = n^{-1}(\omega_1 + \omega_2 + \cdots + \omega_n)$ and take $\varepsilon < n^{-1}$. By Observation 3 one can find $\Phi \in \mathfrak{B}$ and $\omega \in \Delta_\Phi$ such that $\|\omega - \omega'\| < \varepsilon$ and hence $\|\mu_\omega - \mu_{\omega'}\| < \varepsilon$. But this implies that $\mu_{\omega'}(\{\omega_i\}) > 0$ for each $i = 1, 2, \ldots, n$, and hence $\omega_i \in \mathscr{E}(\Delta_\Phi)$ for each $i = 1, 2, \ldots, n$.

Thus although Observation 2 indicates that Δ_Φ "often" consists of a single point Observation 4 proves the existence of interactions Φ for which Δ_Φ contains many different $\mathbb{Z}^\nu$-ergodic states. Despite the interest of these general observations they shed little light on the structure of $\{\Delta_{\beta\Phi}; \beta \in \mathbb{R}\}$ for Φ fixed. The convexity arguments are inherently too weak to obtain details of the phase structure for a fixed interaction as the inverse temperature β varies. For this it is necessary to develop more analytic methods.

The foregoing results give a reasonably satisfactory description of spatially invariant equilibrium states. In particular Theorem 6.2.42 establishes under quite general conditions that the Gibbs and KMS conditions are equivalent to the principle of maximal mean entropy at fixed mean energy. Equilibrium is a balance between the disorder characteristic of large entropy and the order associated with low energy. The main disadvantage of the theory is, however, the strong invariance assumption. Although many physical systems exhibit pronounced features of spatial homogeneity the assumption of strict spatial invariance appears to be a somewhat unrealistic idealization. It would be of interest to understand the entropy principle in a broader setting of 'homogeneous' systems. There are several classes of physical models which lack in-

variance but retain strong spatial uniformity. For example models of magnetic impurities or models of spin glasses.

A typical impurity model has a translationally invariant interaction Φ together with an additional one-body interaction Ψ which only contributes at a subset of randomly chosen points $x_n \in \mathbb{Z}^\nu$ and which represents the presence of magnetic impurities. The points x_n could be distributed in a homogenous fashion and Ψ could be invariant, i.e., $\Psi(\{x_n\}) = \tau_{x_n}(\Psi(\{0\}))$, but if the x_n are not the points of a regular sublattice there is no underlying symmetry. One can introduce an evolution τ and the corresponding KMS states and also define the mean free energy by exploiting subadditivity, homogeneity and boundedness properties. The problems arise with the states and in particular the mean entropy and energy as functions over the states.

General spin glass models can also be defined in terms of two translationally invariant interactions Φ and Ψ. One assumes that the interaction energy arises from Φ for one class L_Φ of subsets $X \subset \mathbb{Z}^\nu$ and from Ψ for the complementary set L_Ψ, i.e., the energy is given by

$$H(\Lambda) = \sum_{\substack{X \in L_\Phi \\ X \subseteq \Lambda}} \Phi(X) + \sum_{\substack{X \in L_\Psi \\ X \subseteq \Lambda}} \Psi(X) \ .$$

For example, Φ and Ψ could be nearest-neighbor interactions and L_Φ a randomly chosen subset of the nearest-neighbors. If Φ is an 'attractive' interaction which tends to align neighboring spins and Ψ a 'repulsive' interaction which energetically favors anti-parallel spins then there are competing forces which ensure non-translationally invariant equilibrium states. Nevertheless if the set L_Φ has a regular pattern of distribution the states should be relatively homogeneous. Again one can introduce an evolution τ and the corresponding KMS states and define the mean free energy. Difficulties arise, however, in defining the mean entropy and energy as functions over the states. The principal problem in characterizing the KMS states in terms of entropy and energy considerations consists of finding a suitable replacement for the invariant states. Any concept of homogeneous interaction requires a corresponding concept of homogeneous state in order to be useful. But there appear to be no viable alternatives to the invariant theory.

A different class of models which lack invariance arises from theories built on lattices without periodicity. Although this appears initially to be a more radical departure from homogeneous theories on $\mathbb{Z}^\nu$ it is not necessarily the case. Quasicrystals seem to have strong regularity properties which are, however, not consistent with a strictly periodic structure. Therefore it is appealing to model these phenomena with aperiodic lattices, for example, lattices associated with aperiodic tilings of the underlying configuration space. But the most common lattices of this type do have repetitive symmetry patterns even if they lack complete periodicity. Therefore one can build the theory to take these symmetries into account and consider interactions with the corresponding invariances. Again the difficulty in fully developing the theory is the identification of a suitable set of states whose structure adequately reflects the symmetries

and invariances. This can to a certain extent be achieved (see Notes and Remarks) but there is no really adequate counterpart for the compact set of translationally invariant states.

6.2.5. Uniqueness of KMS States

Spin systems were originally introduced as models of paramagnetism and ferromagnetism. A material is paramagnetic if it assumes a magnetic moment in the presence of an external magnetic field and ferromagnetic if it is capable of possessing a magnetic moment in the absence of a field. Ferromagnetism is a relatively rare quality and the majority of ferromagnets are alloys, or compounds, of iron, nickel, or cobalt. If a ferromagnet is heated, it loses its spontaneous magnetization at a certain critical temperature T_c, but above T_c it remains paramagnetic. Thus, ferromagnets exhibit a type of phase transition; above T_c there is a unique state of equilibrium whose magnetization is completely determined by the external field but below T_c and in the absence of a field there are various possible states distinguished by the orientation of the spontaneous magnetization.

In this and the next subsection we demonstrate that quantum spin systems exhibit this type of phase structure. This subsection is devoted to the discussion of high temperatures and in the next we examine the more interesting, and more complex, low-temperature phenomena. We only consider interactions Φ for which the dynamics is given by a strongly continuous one-parameter group τ^Φ of *-automorphisms of the spin algebra $\mathfrak{A}$ and we accept the (τ^Φ, β)-KMS condition as a criterion for equilibrium at inverse temperature β. In Section 6.2.2 we established the existence of (τ^Φ, β)-KMS states for all $\beta \in \mathbb{R}$ and our immediate aim is to prove uniqueness for small β, i.e., for large temperatures.

If $\beta = 0$, the KMS condition reduces to the trace condition,

$$\omega(AB) = \omega(BA)$$

for all $A, B \in \mathfrak{A}$, and ω is the unique trace state on $\mathfrak{A}$. The uniqueness of the trace can be deduced by an explicit calculation which is a model for the subsequent perturbation argument. Let $e(i_x, j_x), i_x, j_x = 0, 1, \ldots, N$ be a set of matrix units for $\mathfrak{A}_{\{x\}}$ and choose $B \in \mathfrak{A}_\Lambda$ where $x \notin \Lambda$. The trace condition, local commutativity, and the identity

$$e(i_x, j_x) = (N+1)^{-1} \sum_{k_x = 0}^{N} e(i_x, k_x) e(k_x, j_x)$$

give

$$\begin{aligned}
\omega(e(i_x, j_x)B) &= (N+1)^{-1} \sum_{k_x = 0}^{N} \omega(e(k_x, j_x) B e(i_x, k_x)) \\
&= (N+1)^{-1} \sum_{k_x = 0}^{N} \delta_{i_x, j_x} \omega(e(k_x, k_x) B) \\
&= (N+1)^{-1} \delta_{i_x, j_x} \omega(B) \ .
\end{aligned}$$

Iteration of this argument yields

$$\omega\left(\prod_{l=1}^{n} e(i_{x_l}, j_{x_l})\right) = (N+1)^{-n} \prod_{l=1}^{n} \delta_{i_{x_l}, j_{x_l}}$$

and ω is uniquely determined.

If $\beta \neq 0$, the trace property is replaced by the (τ^{Φ}, β)-KMS condition and one finds

$$\begin{aligned}\omega(e(i_x, j_x)B) &= (N+1)^{-1} \sum_{k_x=0}^{n} \{\omega(e(k_x, j_x)Be(i_x, k_x)) \\ &\quad + \omega(e(k_x, j_x)B(\tau_t^{\Phi} - \imath)e(i_x, k_x))\}\Big|_{t=i\beta} \\ &= (N+1)^{-1}\delta_{i_x, j_x}\omega(B) \\ &\quad + (N+1)^{-1} \sum_{k_x=0}^{N} \omega(e(k_x, j_x)B(\tau_t^{\Phi} - \imath)e(i_x, k_x))\Big|_{t=i\beta} .\end{aligned}$$

Now assume the strictly local elements of $\mathfrak{A}$ are analytic for τ^{Φ}. The second term on the right-hand side of the last equation can then be expressed as a power series in β, without constant term, and iteration of the resulting equation allows one to deduce that ω is uniquely determined for β sufficiently small and for a large class of Φ. The details are as follows.

Each $B \in \mathfrak{A}_X$ can be expressed as a linear combination of matrix units

$$e(I_X, J_X) = \prod_{l=1}^{n} e(i_{x_l}, j_{x_l})$$

where $X = \{x_1, \ldots, x_n\}, I_X = \{i_{x_1}, \ldots, i_{x_n}\}$, and $J_X = \{j_{x_1}, \cdots j_{x_n}\}$. Thus it suffices to consider the special choices $B = e(I_X, J_X), I_X, J_X \in \{0, 1, \cdots, N\}^X$, $X \subset L$. Now adopting the assumptions of Theorem 6.2.4 one has

$$(\tau_{i\beta}^{\Phi} - \imath)(e(i_x, k_x)) = \sum_{n \geq 1} \frac{(-\beta)^n}{n!} \sum_{\substack{X_1, \ldots, X_n \\ X_j \cap S_{j-1} \neq \varnothing}} C_n^{\Phi}(\{X_i\}; i_x, k_x) ,$$

where

$$C_n^{\Phi}(\{X_i\}; i_x, k_x) = [\Phi(X_n), [\cdots [\Phi(X_1), e(i_x, k_x)]]] ,$$

$S_0 = \{x\}$, and $S_j = X_j \cup X_{j-1} \cup \cdots \cup X_1 \cup \{x\}$. But if

$$A = \sum_{I_X, J_X} A(I_X, J_X) e(I_X, J_X)$$

is the decomposition of $A \in \mathfrak{A}_X$, the complex coefficients $A(I_X, J_X)$ satisfy

$$|A(I_X, J_X)| \leq \|A\| .$$

Therefore

$$C_n^{\Phi}(\{X_i\};\, i_x, k_x) = \sum_{I_{S_n}, J_{S_n}} C_n^{\Phi}(\{X_i\}; i_x, k_x; I_{S_n}, J_{S_n}) e(I_{S_n}, J_{S_n}) \ ,$$

where

$$|\, C_n^{\Phi}(\{X_i\}; i_x, k_x; I_{S_n}, J_{S_n})\, | \leq 2^n \prod_{i=1}^{n} \|\Phi(X_i)\| \ .$$

Moreover,

$$e(k_x, j_x) e(I_X, J_X) C_n^{\Phi}(\{X_i\}; i_x, k_x) = \sum_{i_{S_n^x}, J_{S_n^x}} \alpha^{\Phi}(I_{S_n^x}, J_{S_n^x}) e(I_{S_n^x}, J_{S_n^x})$$

where $S_n^x = \{x\} \cup X \cup S_n$, and there are at most $(N+1)^{2|S_n|}$ nonzero coefficients α^{Φ} which satisfy

$$|\alpha^{\Phi}(I_{S_n^x}, J_{S_n^x})| \leq 2^n \prod_{i=1}^{n} \|\Phi(X_i)\| \ .$$

This perturbation expansion can now be combined with the previous identity for ω, evaluated with $B = e(I_X, J_X)$, to obtain a linear equation for the family $\{\omega(e(I_Y, J_Y)); Y \subset L\}$. This equation will be interpreted as an integral equation on a suitable Banach space.

Let $\mathfrak{X}$ be the Banach space of bounded complex functions f on the pairs $\{I_X, J_X\}$ where $I_X, J_X \subset \{0, 1, \ldots, N\}^X, X \subset L$, and $f(I_\varnothing, J_\varnothing) \in \mathbb{C}$. The space $\mathfrak{X}$ is equipped with the natural operations of addition and scalar multiplication together with the supremum norm. If $\underline{\omega}$ denotes the family $\{\omega(e(I_X, J_X)); X \subset L\}$, where we take $e(I_\varnothing, J_\varnothing) = \mathbb{1}$, it follows that $\underline{\omega} \in \mathfrak{X}$ and $\|\underline{\omega}\| = 1$. The foregoing identity and perturbation expansion yield the equation

$$\underline{\omega} = \underline{\delta} + K\underline{\omega} + L_{\beta\Phi}\underline{\omega}$$

for $\underline{\omega}$ where $\underline{\delta}, K$, and $L_{\beta\Phi}$ are defined as follows: $\underline{\delta} \in \mathfrak{X}$ and

$$\underline{\delta}(I_X, J_X) = \begin{cases} 1 & \text{if } X = \varnothing \\ (N+1)^{-1}\delta_{i_x, j_x} & \text{if } X = \{x\} \\ 0 & \text{otherwise} \ , \end{cases}$$

K is a linear operator with action

$$(Kf)(I_X, J_X) = (N+1)^{-1}\delta_{i_{x_1}, j_{x_1}} f(I_{X'}, J_{X'})$$

if $X = \{x_1, \ldots, x_n\}, X' = \{x_2, \ldots, x_n\}, n \geq 2$, and

$$(Kf)(I_X, J_X) = 0$$

if $|X| < 2, L_{\beta\Phi}$ is a linear operator such that

$$(L_{\beta\Phi}f)(I_X, J_X) = (N+1)^{-1} \sum_{k_x=0}^{N} \sum_{n\geq 1} \frac{(-\beta)^n}{n!} \sum_{\substack{X_1,\ldots,X_n \\ X_j \cap S_{j-1} \neq \varnothing}} \sum_{I_{S_n^x}, J_{S_n^x}}$$
$$\times\, \alpha_n^{\Phi}(I_{S_n^x}, J_{S_n^x}) f(I_{S_n^x}, J_{S_n^x}) \ ,$$

where the coefficients α_n^{Φ} arising from the perturbation expansion are associated with a fixed splitting $X = \{x\} \cup X'$ with $X' = X \backslash \{x\}$.

The above integral equation has the form

$$(\imath - K - L_{\beta\Phi})\underline{\omega} = \underline{\delta} \ .$$

Hence $\underline{\omega}$ is uniquely determined, and

$$\underline{\omega} = \sum_{n\geq 0} (K + L_{\beta\Phi})^n \underline{\delta}$$

whenever $\|K + L_{\beta\Phi}\| < 1$. But $\|K\| = (N+1)^{-1}$ and so uniqueness is ensured if $\|L_{\beta\Phi}\| < (1 - \|K\|) = N(N+1)^{-1}$. The norm of $L_{\beta\Phi}$ can, however, be bounded by use of the estimates on C_n^{Φ} and the procedure used in the proof of Theorem 6.2.4.

Proposition 6.2.45. *Let Φ be an interaction such that*

$$\|\Phi\|_\lambda = \sum_{n\geq 0} e^{\lambda n}(N+1)^{2n} \left(\sup_{x\in L} \sum_{\substack{X \ni x \\ |X| = n+1}} \|\Phi(X)\| \right) < +\infty$$

for some $\lambda > 0$.

It follows that there exists a unique (τ^{Φ}, β)-KMS state whenever

$$|\beta|\ \|\Phi\|_\lambda < \left(\frac{\lambda}{2}\right) \left(1 + \frac{e^{\lambda}(N+1)^3}{N}\right)^{-1} \ .$$

Proof. The estimation procedure used to prove Theorem 6.2.4 together with the definition of $L_{\beta\Phi}$ gives

$$\|L_{\beta\Phi}\| \leq \sum_{n\geq 1} 2^n \frac{|\beta|^n}{n!} \sum_{n_1,\ldots,n_n} \left(\prod_{i=1}^{n} (n_1 + \cdots + n_{i-1} + 1) \|\Phi\|_{n_i} (N+1)^{2n_i} \right) (N+1)^2 \ ,$$

where

$$\|\Phi\|_n = \sup_{x\in L} \sum_{\substack{X \ni x \\ |X| = n+1}} \|\Phi(X)\| \ .$$

But

$$\prod_{i=1}^{n} (n_1 + n_2 + \cdots + n_{i-1} + 1) \leq (n_1 + n_2 + \cdots + n_n + 1)^n \leq \lambda^{-n} n! e^{\lambda} \prod_{i=1}^{n} e^{\lambda n_i} \ .$$

Therefore

$$\|L_{\beta\Phi}\| \leq (N+1)^2 e^{\lambda}\left(\frac{2|\beta|}{\lambda}\right)\|\Phi\|_{\lambda}\left(1-\left(\frac{2|\beta|}{\lambda}\right)\|\Phi\|_{\lambda}\right)^{-1}$$

whenever $(2|\beta|/\lambda)\|\Phi\|_{\lambda} < 1$. The stated result follows from the discussion preceding the theorem after a simple rearrangement.

Proposition 6.2.45 establishes uniqueness of the equilibrium state whenever $|\beta|\,\|\Phi\|_{\lambda}$ is sufficiently small. We have made no attempt to optimize the estimate on $|\beta|$ and this can certainly be improved in numerous ways. First, if $\Phi(X) = 0$ for $|X| > m$ more efficient norms can be introduced. Second, for any given interaction the bounds on the important lowest-order terms in the perturbation series for $L_{\beta\Phi}$ can be individually calculated and this may significantly improve the total bound. Third, it is possible to exploit other matrix parametrizations, i.e., if $N = 1$, each 2×2 matrix is a linear combination of Pauli matrices and this parametrization can lead to better bounds. Thus Proposition 6.2.45 should only be taken as a general qualitative statement.

For physical applications to magnetic systems this proposition is delinquent in one important respect. It does not establish uniqueness for small β and all external field strengths. To obtain this result it is necessary to use two additional techniques. First, one handles the one-body interaction corresponding to the external field in a separate manner and, second, one must separate out the lowest eigenstate of this field. To introduce the first of these techniques we must reexamine the integral equation for ω.

Let $\Phi = \Phi^{(1)} + \Phi'$ where $\Phi^{(1)}$ is the one-body part of Φ, i.e., $\Phi^{(1)}(\{x\}) = \Phi(\{x\}), \Phi^{(1)}(X) = 0$ if $|X| \neq 1$, and Φ' is the multiparticle interaction. We again assume that Φ determines a one-parameter dynamical group τ^{Φ} for which the strictly local elements of $\mathfrak{A}$ are analytic. The one-particle interaction $\Phi^{(1)}$ automatically determines a second group $\tau^{\Phi^{(1)}}$ with the property that $\tau^{\Phi^{(1)}}(\mathfrak{A}_{\{x\}}) = \mathfrak{A}_{\{x\}}$ for all $x \in L$, and we further assume that τ^{Φ} and $\tau^{\Phi^{(1)}}$ commute. Therefore, $t \in \mathbb{R} \mapsto \tau_t = \tau_t^{\Phi}\tau_{-t}^{\Phi^{(1)}}$ is a one-parameter group and for $A \in \mathfrak{A}_{\Lambda}, \Lambda \subset L$,

$$\frac{d\tau_t(A)}{dt} = i\tau_t\left(\sum_{X \cap \Lambda \neq \varnothing}[\Phi'(X), A]\right) .$$

It follows readily that Φ' generates a dynamical group $\tau^{\Phi'}$ and $\tau^{\Phi'} = \tau_t^{\Phi}\tau_{-t}^{\Phi^{(1)}}$.

Next consider the identity

$$\begin{aligned}\omega(e(i_x, j_x)B) =& \omega(e(k_x, j_x)B\tau_{i\beta}^{\Phi^{(1)}}(e(i_x, k_x))) \\ &+ \omega(e(k_x, j_x)B(\tau_{i\beta}^{\Phi}\tau_{-i\beta}^{\Phi^{(1)}} - \imath)\tau_{i\beta}^{\Phi^{(1)}}(e(i_x, k_x))) .\end{aligned}$$

Now suppose that the matrix units correspond to an eigenfunction basis of $\Phi^{(1)}(\{x\})$ and let $\varphi_x(i), i = 0, 1, 2, \ldots, N$ denote the eigenvalues of $\Phi^{(1)}(\{x\})$ arranged in increasing order repeated according to multiplicity. Then one has

$$\tau_{i\beta}^{\Phi^{(1)}}(e(i_x,k_x)) = e^{-\beta(\varphi_x(i_x)-\varphi_x(k_x))}e(i_x,k_x) \ .$$

Therefore

$$e^{\beta(\varphi_x(i_x)-\varphi_x(k_x))}\omega(e(i_x,j_x)B) = \delta_{i_x,j_x}\omega(e(k_x,k_x)B) + \omega(e(k_x,j_x)B(\tau_{i\beta}^{\Phi'} - \imath)e(i_x,k_x))$$

for all $B \in \mathfrak{A}_\Lambda$ with $x \notin \Lambda$. Summing over k_x yields the identity

$$\omega(e(i_x,j_x)B) = \left(\sum_{k_x=0}^{N} e^{\beta(\varphi_x(i_x)-\varphi_x(k_x))}\right)^{-1} \times \left\{\delta_{i_x,j_x}\omega(B) + \sum_{k_x=0}^{N} \omega(e(k_x,j_x)B(\tau_{i\beta}^{\Phi'} - \imath)e(i_x,k_x))\right\} \ .$$

This family of identities can again be translated into an integral equation for $\underline{\omega}$ on the Banach space $\mathfrak{X}$. The major new feature is the separation of the $\Phi^{(1)}$-dependence into the extra factor

$$\left(\sum_{k_x=0}^{N} e^{\beta(\varphi_x(i_x)-\varphi_x(k_x))}\right)^{-1} .$$

A moment of reflection establishes that if this factor is "small," the kernels of the integral equation are small in norm and the equation has a unique solution. But if $\beta > 0$,

$$\left(\sum_{k_x=0}^{N} e^{\beta(\varphi_x(i_x)-\varphi_x(k_x))}\right)^{-1} < \frac{1}{2}$$

except if $i_x = 0$ and $\varphi_x(0) < \varphi_x(1)$. Similarly if $\beta < 0$, the factor is less than 1/2 except if $i_x = N$ and $\varphi_x(N) > \varphi_x(N-1)$. In both the exceptional cases, however, the factor can take values arbitrarily close to one. Thus the factor remains small, i.e., less than 1/2, in all but two situations.

We now concentrate on the case $\beta > 0$ and describe a method of circumventing the "large" behavior for $i_x = 0$. The case $\beta < 0$ is handled similarly.

The new idea is to parametrize each $A \in \mathfrak{A}_X$ in terms of the identity $\mathbb{1}_x \in \mathfrak{A}_{\{x\}}$ and matrix units $e(I_X, J_X)$ in which $e(i_x, j_x)$ with $i_x = 0 = j_x$ is excluded. This is possible because

$$e(0,0) = \mathbb{1} - \sum_{i=1}^{N} e(i,i) \ .$$

Thus one can find a decomposition

$$A = \sum_{I_X, J_X}{}' A(I_X, J_X)e(I_X, J_X) \ ,$$

where the prime denotes the exclusion of the $i_x = 0 = j_x$ units, and it is readily checked that

$$|A(I_X, J_X)| \leq 2^{|X|}\|A\| \ .$$

Note also that the number of terms in this decomposition is $(N+1)^{2|X|}$.

Now introduce the Banach space $\mathfrak{X}'$ of bounded complex functions on the pairs of indices $\{I_X, J_X\}$ with the $i_x = 0 = j_x, x \in X$, possibilities excluded. The state ω defines an element $\underline{\omega} = \{\omega(e(I_X, J_X)); X \subset L\}$ of this space and the state is determined by $\underline{\omega}$ and the normalization condition $\omega(\mathbb{1}) = 1$. Moreover, if one takes the perturbation expansion for $\tau_{i\beta}^{\Phi'} - \imath$ in the new identity for ω, the resulting relation is interpretable as an integral equation on $\mathfrak{X}'$. This equation has the form

$$\underline{\omega} = \underline{\delta} + K_{\beta\Phi^{(1)}}\underline{\omega} + L_{\beta\Phi}\underline{\omega}$$

where $\underline{\delta} \in \mathfrak{X}'$,

$$\underline{\delta}(I_X, J_X) = \begin{cases} 1 & \text{if } X = \varnothing \\ \left(\sum_{k_x=0}^{N} e^{\beta(\varphi_x(i_x)-\varphi_x(k_x))}\right)^{-1} \delta_{i_x, j_x} & \text{if } X = \{x\} \\ 0 & \text{otherwise} \end{cases} ,$$

and $K_{\beta\Phi^{(1)}}$ is a linear operator with action

$$(K_{\beta\Phi^{(1)}} f)(I_X, J_X) = \left(\sum_{k_{x_1}=0}^{N} e^{\beta(\varphi_{x_1}(i_{x_1})-\varphi_{x_1}(k_{x_1}))}\right)^{-1} \delta_{i_{x_1}, j_{x_1}} f(I_{X'}, J_{X'})$$

if $X = \{x_1, \ldots, x_n\}, X' = \{x_2, \ldots, x_n\}, n \geq 2$ and

$$(K_{\beta\Phi^{(1)}} f)(I_x, J_X) = 0$$

if $|X| < 2$. Therefore, if $\beta > 0$, $\exp\{\beta(\varphi_x(1) - \varphi_x(0))\} \geq 1$ and

$$\begin{aligned} \|K_{\beta\Phi^{(1)}}\| &= \sup_{x \in L}\left(e^{\beta(\varphi_x(1)-\varphi_x(0))} + 1 + \sum_{k_x=2}^{N} e^{-\beta(\varphi_x(k_x)-\varphi_x(1))}\right)^{-1} \\ &\leq \frac{1}{2} \ . \end{aligned}$$

Thus

$$\|K_{\beta\Phi^{(1)}} + L_{\beta\Phi}\| \leq \frac{1}{2} + \|L_{\beta\Phi}\|$$

and there is a unique solution to the integral equation whenever

$$\|L_{\beta\Phi}\| < \frac{1}{2} \ .$$

Now the operator $L_{\beta\Phi}$ is similar to the operator occurring in the previous equations and its norm can be estimated by a slight modification of the earlier

estimates. The new $L_{\beta\Phi}$ differs from the old one in four respects. First Φ is replaced by Φ'. Second, an additional factor

$$(N+1)\left(\sum_{k_x=0}^{N} e^{\beta(\varphi_x(i_x)-\varphi_x(k_x))}\right)^{-1}$$

occurs. Third, the action of $L_{\beta\Phi}$ is slightly modified by the omission of the $i_x = 0 = j_x$ terms. In particular the perturbation expansion of

$$e(I_X, J_X)(\tau_{i\beta}^{\Phi'} - \imath)(e(i_x, k_x))$$

contains terms proportional to $e(I_X, J_X)e(I_{S_n}, J_{S_n})$ and $e(0,0)$ terms may occur through products $e(0,j)e(j,0)$ if $X \cap S_n \neq \varnothing$. To eliminate the $e(0,0)$ we must use the identity

$$e(0,0) = \mathbb{1} - \sum_{k=1}^{N} e(k,k)$$

and hence one term may expand into $(N+1)^{|S_n|}$ terms. Fourth, the coefficients in the expansion are possibly larger by a factor $2^{|S_n|}$ and these last two effects introduce a combined factor $(2(N+1))^{|S_n|}$ in the term-by-term perturbation estimate $\|L_{\beta\Phi}\|$. Thus one obtains

$$\|L_{\beta\Phi}\| \leq \frac{(N+1)}{2} \cdot 2 \cdot (N+1)^3 e^{\lambda}\left(\frac{2\beta}{\lambda}\right)\|\Phi'\|_\lambda\left(1 - \left(\frac{2\beta}{\lambda}\right)\|\Phi'\|_\lambda\right)^{-1}$$

where we have assumed that

$$\|\Phi'\|_\lambda = \sum_{n \geq 1} 2^n e^{\lambda n}(N+1)^{3n} \sup_{x \in L} \sum_{\substack{X \ni x \\ |X| = n+1}} \|\Phi(X)\| < \frac{\lambda}{2\beta}$$

for some $\lambda > 0$. Therefore, if

$$\beta\|\Phi'\|_\lambda < \left(\frac{\lambda}{2}\right)(1 + 2(N+1)^4 e^{\lambda})^{-1}$$

one has $\|L_{\beta\Phi}\| < \frac{1}{2}$ and hence $\underline{\omega}$ is unique.

If $\beta < 0$, this argument may be repeated with the $i_x = N = j_x$ terms omitted. The final result is summarized by the following:

Theorem 6.2.46. *Let Φ be an interaction with one-body part $\Phi^{(1)}$, i.e., $\Phi^{(1)}(\{x\}) = \Phi(\{x\})$ and $\Phi^{(1)}(X) = 0$ if $|X| \neq 1$. Define $\Phi' = \Phi - \Phi^{(1)}$ and assume*

$$\|\Phi'\|_\lambda = \sum_{n \geq 1} 2^n e^{\lambda n}(N+1)^{3n} \sup_{x \in L} \sum_{\substack{X \ni x \\ |X| = n+1}} \|\Phi(X)\| < +\infty$$

for some $\lambda > 0$. Further assume that $\tau^{\Phi^{(1)}}$ and τ^{Φ} commute.

It follows that there exists a unique (τ^{Φ}, β)*-KMS state whenever*

$$\beta\|\Phi'\|_{\lambda} < \left(\frac{\lambda}{2}\right)(1 + 2(N+1)^4 e^{\lambda})^{-1} \ .$$

Note that no uniform bound on $\|\Phi^{(1)}(\{x\})\|$ is needed. Thus, uniqueness occurs for all strengths and all inhomogeneities of the external field.

The integral equation method establishes more than we have actually stated. Both integral equations have the form

$$\underline{\omega} = \underline{\delta} + M_{\beta\Phi}\underline{\omega}$$

and for the interactions described by Proposition 6.2.45 and Theorem 6.2.46 the unique (τ^{Φ}, β)-KMS state $\omega^{\beta\Phi}$ is determined by

$$\begin{aligned}\omega^{\beta\Phi}(e(I_X, J_X)) &= ((\imath - M_{\beta\Phi})^{-1}\underline{\delta})(I_X, J_X) \\ &= \sum_{n \geq 0}(M^n_{\beta\Phi}\underline{\delta})(I_X, J_X) \ .\end{aligned}$$

But if $\beta\Phi$ varies within the appropriate domain of uniqueness, one may deduce that $\beta\Phi \mapsto \omega^{\beta\Phi}(e(I_X, J_X))$ is continuous, and hence $\beta\Phi \mapsto \omega^{\beta\Phi}(A)$ is continuous for each $A \in \mathfrak{A}_{\Lambda}$ and $\Lambda \subset L$. A similar argument for continuity of τ^{Φ} was outlined after Example 6.2.5. In fact, this estimation procedure establishes that if $\beta(\Phi + x_1\Phi_1 + \cdots + x_n\Phi_n)$ is in the region of uniqueness for some Φ, Φ_1, $\Phi_2, \cdots, \Phi_n$ and all $(x_1, x_2, \ldots, x_n)$ in an open subset of $\mathbb{R}^n$, then

$$(x_1, \ldots, x_n) \mapsto \omega^{\beta(\Phi + x_1\Phi_1 + \cdots + x_n\Phi_n)}(A)$$

extends to a holomorphic function of n variables, for each strictly local A.

Next one may deduce some basic characteristics of paramagnetism. In applications to magnetic systems the one-body interaction is usually of the form

$$\Phi^{(1)}(\{x\}) = -h_x L_3^x$$

where $h_x \in \mathbb{R}$ is the external field strength at x and L_3^x is the third component of the atomic angular momentum. This interaction corresponds to the coupling of the atomic magnetic moment and an electromagnetic field in the direction of the third coordinate axis. With this interpretation the mean magnetization of the atom at the point x is given by

$$M(\beta, h_x) = \omega^{\beta\Phi}(L_3^x)$$

and the considerations of the previous paragraph, coupled with Theorem 6.2.46, establish that $h_x \in \mathbb{R} \mapsto M(\beta, h_x)$ extends to an entire analytic function. Now L_3^x has $N+1$ distinct eigenvalues $i - N/2, i = 0, 1, \ldots, N$, in suitable units. If $e(i_x, j_x)$ are matrix units defined by a corresponding eigenfunction basis, the identity for $\omega^{\beta\Phi}$ used in the proof of Theorem 6.2.46 implies

$$|\omega^{\beta\Phi}(e(i_x, i_x))| \leq C_{\beta,\Phi'}\left(\sum_{k=0}^{N} e^{-\beta h_x(i_x - k)}\right)^{-1},$$

where $C_{\beta,\Phi'}$ is a positive constant independent of the external field strength. Thus if $\beta > 0$, i.e., the temperature is positive,

$$\lim_{h_x \to +\infty} \omega^{\beta\Phi}(e(i_x, i_x)) = 0 \quad \text{if } i_x \neq N$$

and

$$\lim_{h_x \to -\infty} \omega^{\beta\Phi}(e(i_x, i_x)) = 0 \quad \text{if } i_x \neq 0 \ .$$

Consequently, as $h_x \to +\infty$ the atom at site x is in the eigenstate of L_3^x with eigenvalue $N/2$ with probability one and as $h_x \to -\infty$ the eigenstate with eigenvalue $-N/2$ plays the predominant role. Explicitly one has

$$\lim_{h_x \to \pm\infty} M(\beta, h_x) = \pm \frac{N}{2}$$

and this demonstrates that for large external field the atoms align themselves with the field, i.e., the system is paramagnetic. Therefore, one concludes that in the high-temperature regime spin systems are paramagnetic but not ferromagnetic.

There are several notable corollaries of uniqueness of the (τ^Φ, β)-KMS state $\omega^{\beta\Phi}$. First, $\omega^{\beta\Phi}$ is automatically an extremal (τ^Φ, β)-KMS state, and hence a factor state by Theorem 5.3.30. But if $L = \mathbb{Z}^\nu$, the spin algebra is norm asymptotically abelian with respect to the group $\mathbb{Z}^\nu$ of space translations. Thus $\omega^{\beta\Phi}$ is strongly clustering (strongly mixing) in space by Example 4.3.24. Next if Φ is $\mathbb{Z}^\nu$-invariant uniqueness implies that $\omega^{\beta\Phi}$ is $\mathbb{Z}^\nu$-invariant and hence strongly clustering (strongly mixing) to all orders by another application of Example 4.3.24. Next assume that the finite-volume dynamical groups $\tau^{\Lambda,\Phi}$ converge strongly to τ^Φ. Uniqueness of $\omega^{\beta\Phi}$ then implies that the finite-volume Gibbs states $\omega_\Lambda^{\beta\Phi}$ must converge in the weak* topology to $\omega^{\beta\Phi}$ as $\Lambda \to \infty$. This follows because each weak*-limit point of $\omega_\Lambda^{\beta\Phi}$ is a (τ^Φ, β)-KMS state by Proposition 6.2.15. Therefore, all weak*-limit points must be equal to $\omega^{\beta\Phi}$ and hence the limit must exist.

There is another general class of models for which uniqueness of the equilibrium state is usual, one-dimensional models with uniformly bounded surface energies. For these systems, however, the uniqueness is independent of the temperature and hence no form of phase transitions can occur. Thus one-dimensional models with bounded surface energy do not exhibit ferromagnetism.

Theorem 6.2.47. *Let Φ be an interaction satisfying*

$$\sum_{X \ni x} \|\Phi(X)\| < +\infty$$

and assume there exists an increasing sequence $\Lambda_n \subset L$ such that $\Lambda_n \to \infty$.

$$\left\| \sum_{\substack{X \cap \Lambda_n \neq \varnothing \\ X \cap \Lambda_n^c \neq \varnothing}} \Phi(X) \right\| \leq M$$

for some $M < +\infty$. Further, let τ^Φ denote the corresponding automorphism group (constructed in Theorem 6.2.6).

It follows that there is a unique (τ^Φ, β)-KMS state for all $\beta \in \mathbb{R}$.

PROOF. As this result is not central to any subsequent results we content ourselves with an outline of the proof which uses the W^*-version of the theory of perturbed states described in Section 5.4.1.

First, let $\omega_{\Lambda_{n'}} (= \omega^{\beta\Phi}_{\Lambda_{n'}})$ be a weak*-convergent subsequence of the local Gibbs states with limit ω'. Next, let ω be an arbitrary extremal (τ^Φ, β)-KMS state. The idea is to prove that $\omega = \omega'$ and hence deduce that ω is unique. To accomplish this we introduce the perturbed states $\omega^{\beta P_{n'}}$, defined in Theorem 5.4.4 but rescaled to β, with the perturbations $P_{n'}$ given by

$$P_{n'} = W_\Phi(\Lambda_{n'}) = \sum_{\substack{X \cap \Lambda_{n'} \neq \varnothing \\ X \cap \Lambda^c_{n'} \neq \varnothing}} \Phi(X) \ .$$

It follows from Theorems 6.2.6 and 6.2.18 that ω satisfies the Gibbs condition and hence the restriction of $\omega^{\beta P_{n'}}$ to $\mathfrak{A}_{\Lambda_{n'}}$ is equal to $\omega_{\Lambda_{n'}}$ Therefore, ω' is the weak*-limit of $\omega^{\beta P_{n'}}$ as $n' \to \infty$. Next, we must prove that $\omega^{\beta P_{n'}}$ converges to ω. Basically this happens because ω and $\omega^{\beta P_{n'}}$ differ only by a perturbation across the boundary of $\Lambda_{n'}$ and hence as $\Lambda_{n'} \to \infty$ this difference becomes negligible. Unfortunately the proof of convergence is rather intricate.

The key to the proof is the introduction of the family of functions

$$F_n(z; A) = (e^{-iz(H-\pi_\omega(P_n))}\Omega_\omega, \pi_\omega(A)e^{iz(H-\pi_\omega(P_n))}\Omega_\omega) \ ,$$

where $(\mathfrak{H}_\omega, \pi_\omega, U_\omega, \Omega_\omega)$ denotes the representation associated with the τ^Φ-invariant state ω. It follows from Theorem 5.4.4, and its proof, that each F_n is holomorphic in the strip $\mathfrak{D}_{\beta/2}$; $\operatorname{Im} z \in \langle 0, \beta/2\rangle$ and is strongly continuous and bounded on the closure $\overline{\mathfrak{D}}_{\beta/2}$ of the strip. The functions F_n interpolate between ω and its perturbations $\omega^{\beta P_{n'}}$. For example, one has

$$F_n(t\,; A) = (\Gamma^{-P_n}_{-t}\Omega_\omega, \pi_\omega(A)\Gamma^{-P_n}_t\Omega_\omega) \ ,$$

and

$$F_n(t + i\beta/2\,; A) = (\Omega^{\beta\tau^\Phi_t(P_n)}_\omega, \ \Gamma^{-P_{n^*}}_t \pi_\omega(A)\Gamma^{-P_n}\Omega^{\beta\tau^\Phi_t(P_n)}_\omega)$$

when $t \in \mathbb{R}$ and

$$\Gamma^{-P_n}_t = e^{it(H-\pi_\omega(P_n))}e^{-itH}$$

is the unitary co-cycle associated with the perturbation of $U_\omega(t) = \exp\{itH\}$. Thus

$$F_n(0\,; A) = \omega(A) \ .$$

Moreover,

$$F_n(i\beta/2\,; A) = \omega^{\beta P_n}(A)\|\Omega^{\beta P_n}_\omega\|^2 = \omega^{\beta P_n}(A)F_n(i\beta/2\,; \mathbb{1}) \ .$$

Next one argues that the functions $t \in \mathbb{R} \mapsto F_n(t + i\beta/2\,; A)$ and $t \in \mathbb{R} \mapsto F_n(t\,; A)$ are uniformly bounded and equi-continuous, i.e., continuous uniformly in n. The uniform boundedness hypothesis of the theorem, $\|P_n\| \leq M$, is essential for both these properties. Consequently, one may choose a subsequence n'' of the sequence n' such that the limits

$$F(z\,;A) = \lim_{n''\to\infty} F_{n''}(z\,;A)\ ,$$

$$F(z\,;\mathbb{1}) = \lim_{n''\to\infty} F_{n''}(z\,;\mathbb{1})\ ,$$

exist for all $z \in \overline{\mathfrak{D}}_{\beta/2}$ and $A \in \mathfrak{A}$. In fact, the convergence is uniform for z in compact subsets of $\overline{\mathfrak{D}}_{\beta/2}$ and $z \mapsto F(z\,;A)$ and $z \mapsto F(z\,;\mathbb{1})$ are holomorphic in $\mathfrak{D}_{\beta/2}$ and strongly continuous and bounded on $\overline{\mathfrak{D}}_{\beta/2}$.

Next one reinterprets this convergence in operator form. One argues that $\|[P'_n, A]\| \to 0$ for all $A \in \mathfrak{A}$ and hence

$$\lim_{n'\to\infty} \|[\Gamma_t^{-P_n'}, \pi_\omega(A)]\| = 0\ .$$

But the convergence of $F_{n''}$ to F on $\mathbb{R}$ then implies that $(\Gamma_{-t}^{-P_{n''}})^*\Gamma_t^{-P_{n''}}$ converges weakly and the limit is automatically an element of the center of $\pi_\omega(\mathfrak{A})''$. Since ω is an extremal (τ^Φ, β)-KMS state this center is, however, trivial by Theorem 5.3.30. Thus $(\Gamma_{-t}^{-P_{n''}})^*\Gamma_t^{-P_{n''}}$ converges weakly to $F(t\,;\mathbb{1})\mathbb{1}(=\mathbb{1})$. Hence

$$F(t\,;A) = \omega(A)F(t\,;\mathbb{1})$$

and

$$F(i\beta/2\,;A) = \omega(A)F(i\beta/2\,;\mathbb{1})$$

by analytic continuation. But from the identification of F_n and the Gibbs condition one has

$$\begin{aligned} F(i\beta/2\,;A) &= \lim_{n''\to\infty} F_{n''}(i\beta/2\,;A) \\ &= \lim_{n''\to\infty} \omega^{\beta P_{n''}}(A)F_{n''}(i\beta/2\,;\mathbb{1}) = \omega'(A)F(i\beta/2\,;\mathbb{1})\ . \end{aligned}$$

Thus

$$(\omega(A) - \omega'(A))F(i\beta/2\,;\mathbb{1}) = 0\ ,$$

and to conclude that $\omega = \omega'$ it suffices to prove that $F(i\beta/2\,;\mathbb{1}) \neq 0$. But if we apply the Peiels–Bogoliubov inequality

$$F_n(i\beta/2\,;\mathbb{1}) = \|\Omega_\omega^{\beta P_n}\|^2 \geq \exp\{-\beta\omega(P_n)\}$$

established prior to Example 6.2.30, the desired conclusion follows from the uniform boundedness hypothesis.

6.2.6. Nonuniqueness of KMS States

Our next topic, the nonuniqueness of KMS states at sufficiently low temperature, is of paramount importance for the explanation of phase transitions in magnetic materials. Physically, the nonuniqueness implies the existence of several distinct thermodynamic phases. But at high temperature there is usually a unique phase, by the results of the previous section, and hence the phase structure varies with temperature and transitions can occur.

There are at least two phenomena which lead to phase transitions in paramagnetic materials, ferromagnetism and anti-ferromagnetism. The first of these has already been mentioned. It is the ability of a material to retain a

residual magnetism in the absence of an external field. The second is physically less apparent and is detectable from the behavior of the *magnetic susceptibility*. This is given by $\chi = M/H$, where M is the overall magnetization and H is the external field strength. The susceptibility tends to increase as the temperature decreases and ferromagnetism is signaled by a divergence of χ for small H at a critical temperature T_c. In contrast the susceptibility of an anti-ferromagnet increases to a finite maximum at some T_c and then decreases as the temperature is lowered, i.e., χ has a cusp at T_c . Thus, below the critical temperature, anti-ferromagnets tend to resist external magnetic forces.

The simplest phenomenological explanation of the spontaneous magnetization of ferromagnets is given by postulating that the interaction favors the alignment of neighboring atoms. The alignment of the magnetic moments of a sufficiently large proportion of the individual atoms gives rise to an overall magnetic moment. Similarly anti-ferromagnetism can be explained by supposing that neighboring atoms prefer to be anti-parallel. Unfortunately, these explanations are insufficient. For example, we have already deduced that one-dimensional systems with uniformly bounded surface energy cannot have multiple phases. Therefore the cooperative effects of alignment or misalignment of the magnetic moments is not explainable by purely energetic considerations.

One way of understanding this difficulty is through the principle of maximum entropy. This principle characterizes equilibrium by maximum entropy S at fixed energy H_Φ, i.e., by maximization of the function $S - \beta H_\Phi$. Thus, for positive temperature, $\beta > 0$, two competing effects occur, maximization of the entropy versus minimization of the energy. Large entropy is associated with large disorder but low energy is favored by the orderly alignment, or misalignment, of neighboring atoms with the particular choice dictated by the sign of the interatomic forces. Thus, the existence of ferromagnetism and anti-ferromagnetism, and the details of the phase structure, depend upon a delicate interplay of these two effects.

Detailed theoretical understanding of ferromagnetism and anti-ferromagnetism is based upon the study of specific models within the class of general spin systems and it is now necessary to specialize considerably. The simplest quantum system is the spin-$\frac{1}{2}$ Heisenberg model introduced in Example 6.2.2. We examine the anisotropic version of this model and establish that for sufficiently low temperatures and suitable values of the anisotropy there are at least two distinct extremal KMS states. The idea behind this analysis is to view the Heisenberg model as a 'perturbation' of its classical limit, the Ising model. The anisotropy plays the role of perturbation parameter.

We emphasize that a great deal of work has been done on particular models and we make no attempt to survey the subject. We merely try to describe the two most common phenomena which lead to multiple phases and some methods used to elucidate them. The classical Ising model provides the basic insight into these phenomena and plays a key role in understanding the more complex quantum mechanical models.

Let $L = \mathbb{Z}^\nu$. The spin-$\frac{1}{2}$ quantum algebra $\mathfrak{A}_{\{x\}}$ consists of linear combinations of the Pauli matrices $\sigma_0^x(=\mathbb{1}), \sigma_1^x, \sigma_2^x, \sigma_3^x$ defined in Example 4.2.7 and the corresponding classical algebra $\mathfrak{C}_{\{x\}}$ consists of linear combinations of σ_0^x and σ_3^x. More generally the spin-$\frac{1}{2}$ quantum algebra $\mathfrak{A}_\Lambda$ is generated by polynomials in the Pauli matrices $\{\sigma_i^x; i = 0, 1, 2, 3, x \in \Lambda\}$ and the classical algebra $\mathfrak{C}_\Lambda$ by polynomials in $\{\sigma_i^x; i = 0, 3,\ x \in \Lambda\}$. The anisotropic Heisenberg model with nearest neighbor interaction and zero external field is given by the interaction Φ where

$$\begin{aligned}
\Phi(X) &= 0 && \text{if} \quad |X| \neq 2 \\
\Phi(\{x, y\}) &= 0 && \text{if} \quad |x - y| \neq 1 \\
\Phi(\{x, y\}) &= -j(x, y)\{\delta(\sigma_1^x\sigma_1^y + \sigma_2^x\sigma_2^y) + \sigma_3^x\sigma_3^y\} \\
& && \text{if} \quad |x - y| = 1
\end{aligned}$$

where $|x| = |x_1| + \cdots + |x_\nu|$ and $j(x, y), \delta \in \mathbb{R}$. An external field can be introduced by the addition of a one-body interaction, e.g.,

$$\Phi^{(1)}(\{x\}) = -h(x)\sigma_3^x \ .$$

The parameter δ measures the anisotropy. The value $\delta = 1$ corresponds to isotropy and $\delta = 0$ corresponds to the classical Ising interaction $\Phi(\{x, y\}) = -j(x, y)\sigma_3^x\sigma_3^y \in \mathfrak{C}_{\{x, y\}}$. Note that $-j(x, y)\sigma_3^x\sigma_3^y$ viewed as an element of $\mathfrak{A}_{\{x,y\}} \simeq M_4$ has two doubly degenerate eigenvalues $\pm j(x, y)$. The value $-j(x, y)$ occurs if σ_3^x and σ_3^y have the same eigenvalue, i.e., the atoms at x and y are aligned. Thus the model is defined to be ferromagnetic if $j(x, y) > 0$ since the aligned state is then the state of lower energy. Similarly the model is defined to be anti-ferromagnetic if $j(x, y) < 0$ since the non-aligned state is then energetically favored.

We assume that the real functions j and h are uniformly bounded and then the Heisenberg interaction Φ defines a dynamical group of *-automorphisms τ^Φ of the spin algebra $\mathfrak{A}$ by the theory of Section 6.2.1, for example by Theorem 6.2.4. Our aim is to establish the nonuniqueness of (τ^Φ, β)-KMS states for sufficiently large β and small anisotropy. First we discuss criteria for nonuniqueness.

The first criterion is the existence of a non-zero *spontaneous magnetization*. If $h = 0$ and there exists a (τ^Φ, β)-KMS state ω with $\omega(\sigma_3^x) \neq 0$ for some $x \in \mathbb{Z}^\nu$ then there is more than one (τ^Φ, β)-KMS state. For example, a second such state is given by $\alpha^*\omega$ where α^* is the adjoint of the *-automorphism α of $\mathfrak{A}$ with the action

$$\alpha(\sigma_1^x) = \sigma_1^x, \qquad \alpha(\sigma_2^x) = -\sigma_2^x, \qquad \alpha(\sigma_3^x) = -\sigma_3^x$$

for all $x \in \mathbb{Z}^\nu$. This follows because $\alpha\tau^\Phi = \tau^\Phi\alpha$. We refer to α as the spin reflection symmetry. Note that if there is a (τ^Φ, β)-KMS state ω with $\omega(\sigma_1^x) \neq 0$, or $\omega(\sigma_2^x) \neq 0$, then a similar argument establishes that there is more than one (τ^Φ, β)-KMS state even if $h \neq 0$.

The second criterion for nonuniqueness is the existence of *long range order*. This gives an inconsistency between α-invariance and extremality. Assume that

ω is an α-invariant extremal (τ^Φ, β)-KMS state. In particular $\omega(\sigma_3^x) = 0$ for all $x \in \mathbb{Z}^\nu$. But $\pi_\omega(\mathfrak{A})''$ is a factor by Theorem 5.3.30. Moreover $\mathfrak{A}$ is asymptotically abelian with respect to the group $x \in \mathbb{Z}^\nu \mapsto \tau_x$ of space translations. Hence ω is strongly clustering in space by Example 4.3.24. In particular

$$\lim_{|y| \to \infty} \omega(\sigma_3^x \sigma_3^y) = \lim_{|y| \to \infty} \{\omega(\sigma_3^x \sigma_3^y) - \omega(\sigma_3^x)\omega(\sigma_3^y)\} = 0 \ .$$

Thus, if for a given α-invariant (τ^Φ, β)-KMS state one can deduce

$$\inf_{x, y \in \mathbb{Z}^\nu} \omega(\sigma_3^x \sigma_3^y) > 0$$

then ω cannot be an extremal (τ^Φ, β)-KMS state. Hence there must exist at least two distinct extremal KMS states. We will verify this criterion in the Heisenberg model for suitable values of β and δ. It corresponds to long range order in the system.

Theorem 6.2.48. *Let Φ denote the ferromagnetic Heisenberg interaction with nearest-neighbor coupling $j(x,y) > 0$, anisotropy $\delta \in \langle -1, 1 \rangle$ and zero external field. Assume $\nu \geq 2$ and*

$$j = \inf_{(x,y)} j(x, y) > 0 \ .$$

It follows that there is a $\beta_c > 0$ such that there exist at least two extremal (τ^Φ, β)-KMS states for all $\beta > \beta_c$.

Note that this result does not establish nonuniqueness of the KMS states for the isotropic model, i.e., for the case $\delta = 1$. In fact if $\nu = 2$ the criterion of nonzero spontaneous magnetization, $\omega(\sigma_3^x) \neq 0$, fails by symmetry arguments. This will be discussed in detail later in the section.

We will not give a complete proof of Theorem 6.2.48 except for the special case $\delta = 0$, the Ising model. We explain, however, how the $\delta = 0$ result can be extended to small δ by a routine perturbation argument which does not depend upon the detailed form $(\sigma_1^x \sigma_1^y + \sigma_2^x \sigma_2^y)$ of the transverse interaction. Finally we give a brief discussion of the more sophisticated argument used for values of δ close to one. The starting point is the following observation.

Observation 1. *Let Φ be any interaction such that τ^Φ commutes with the spin reflection symmetry α. If there exists an α invariant (τ^Φ, β)-KMS state ω with*

$$\sup_{x,y \in \mathbb{Z}^\nu} \omega(P_+^x P_-^y) < 1/4 \ ,$$

where $P_\pm^x = (\mathbb{1} \pm \sigma_3^x)/2$, then there exist at least two distinct extremal (τ^Φ, β)-KMS states.

This is just a rephrasing of the criterion of long range order established before the statement of the theorem since

$$\omega(P_+^x P_-^y) = 1/4 - \omega(\sigma_3^x \sigma_3^y)$$

by reflection symmetry.

Next let ω_Λ denote a state on the local algebra $\mathfrak{A}_\Lambda$. Because $P_+^z + P_-^z = \mathbb{1}$ for all $z \in \mathbb{Z}^\nu$ one may write

$$\omega_\Lambda(P_+^x P_-^y) = \omega_\Lambda\Big(P_+^x P_-^y \prod_{z \in \Lambda\setminus\{x,y\}} (P_+^z + P_-^z)\Big) \ .$$

We will expand the product on the right-hand side and obtain an identity which is useful for calculating an upper bound. We must first introduce some terminology and notation.

Let $\mathrm{NN}(\Lambda)$ denote the set of *nearest neighbors* in Λ, i.e., the set of ordered pairs (x, y) with $x, y \in \Lambda$ such that $|x - y| = 1$. If $U \subseteq \mathrm{NN}(\Lambda)$ is a subset of $\mathrm{NN}(\Lambda)$, we say that a set $X \subseteq \Lambda$ is U-connected if for any two points $x, y \in X$ there exists a chain $\{x_1 = x, x_2, \ldots, x_{n+1} = y\}$ in Λ such that $(x_i, x_{i+1}) \in U$ and $(x_{i+1}, x_i) \in U$ for $i = 1, 2, \ldots$. A *contour* γ is a subset of $\mathrm{NN}(\Lambda)$ with the following properties:

(1) Λ is not $\mathrm{NN}(\Lambda)\setminus\gamma$-connected.
(2) There exists two nonempty subsets $\Lambda_1(\gamma)$ and $\Lambda_2(\gamma)$ such that $\Lambda_1(\gamma)$ and $\Lambda_2(\gamma)$ are $\mathrm{NN}(\Lambda)\setminus\gamma$-connected, $\Lambda_1(\gamma) \cap \Lambda_2(\gamma) = \varnothing$, and $\Lambda_1(\gamma) \cup \Lambda_2(\gamma) = \Lambda$.
(3) If $(x, y) \in \gamma$, then $x \in \Lambda_1(\gamma)$ and $y \in \Lambda_2(\gamma)$.

Hence, if Λ is $\mathrm{NN}(\Lambda)$-connected, there is a one-to-one correspondence between ordered partitions (Λ_1, Λ_2) of Λ into $\mathrm{NN}(\Lambda)$-connected subsets Λ_1 and Λ_2, and contours $\gamma \subseteq \mathrm{NN}(\Lambda)$ given by

$$\gamma = \{(x, y) \in \mathrm{NN}(\Lambda);\ x \in \Lambda_1, y \in \Lambda_2\} \ .$$

We will always assume Λ to be $\mathrm{NN}(\Lambda)$-connected.

A *configuration* c is a function on Λ with values in $\{+, -\}$. Fix a configuration c and two points $x, y \in \Lambda$ such that $c(x) = +, c(y) = -$. Let $\Gamma(c)$ denote the class of all contours $\gamma = \{(x_1, y_1), \ldots, (x_n, y_n)\}$ with $c(x_i) = +, c(y_i) = -, i = 1, 2, \ldots, n$. Let Λ_c be the largest $\mathrm{NN}(\Lambda)$-connected subset of Λ such that $x \in \Lambda_c$ and $c(z) = +$ for all $z \in \Lambda_c$. Then there exists a unique contour $\gamma(c) = \{(x_1, y_1), \ldots, (x_n, y_n)\} \in \Gamma(c)$ such that $x_1, \ldots, x_n \in \Lambda_c$ and $x \in \Lambda_1(\gamma(c))$ and $y \in \Lambda_2(\gamma(c))$. Even though $\Lambda_c \subseteq \Lambda_1(\gamma(c))$ it can happen that the two sets are unequal. This is illustrated by the second of the following two figures, which give examples of how $\gamma(c)$ is defined for two different configurations c on a two-dimensional lattice.

$$\begin{array}{cccccc}
- & - & + & - & - & + \\
+ & - & + & - & + & + \\
+ & \underset{y}{-} & - & + & - & - \\
+ & - & + & \underset{x}{+} & - & - \\
- & + & + & + & - & - \\
+ & - & - & - & - & +
\end{array}
\qquad\qquad
\begin{array}{cccccc}
+ & - & - & - & - & + \\
- & + & + & + & + & - \\
+ & \underset{y}{-} & - & + & + & - \\
+ & - & + & \underset{x}{+} & + & - \\
+ & + & + & + & - & + \\
- & - & - & - & + & +
\end{array}$$

In these examples, the contour $\gamma(c)$ is the set of nearest neighbors separated by the indicated curve and ordered such that the point in the x-connected component occurs first.

Using these definitions we now have

$$P_+^x \; P_-^y = \sum_c \prod_{z \in \Lambda} P_{c(z)}^z = \sum_\gamma \sum_{\{c\,;\,\gamma(c)=\gamma\}} \prod_{z \in \Lambda} P_{c(z)}^z \;,$$

where the sum is over all configurations c with $c(x) = +$ and $c(y) = -$. But the $P_\pm^z$ are mutually commuting projections and hence

$$0 \leq \prod_{z \in X} P_{c(z)}^z \leq \prod_{z \in Y} P_{c(z)}^z \leq \mathbb{1}$$

for all c whenever $Y \subseteq X \subseteq \Lambda$. Therefore,

$$\begin{aligned} \sum_{\{c\,;\,\gamma(c)=\gamma\}} \prod_{z \in \Lambda} P_{c(z)}^z &\leq \sum_{\{c\,;\,\Gamma(c) \ni \gamma\}} \prod_{z \in \Lambda} P_{c(z)}^z \\ &= P_+^x P_-^y \prod_{(s,t) \in \gamma} P_+^s P_-^t \quad \leq \prod_{(s,t) \in \gamma} P_+^s P_-^t \end{aligned}$$

and we deduce the following bound.

Observation 2. *For any region Λ one has*

$$P_+^x P_-^y \leq \sum_\gamma P_\gamma$$

where

$$P_\gamma = \prod_{(s,t) \in \gamma} P_+^s P_-^t$$

and the sum is over all contours γ with $x \in \Lambda_1(\gamma)$ and $y \in \Lambda_2(\gamma)$.

Next we use a contour counting argument, commonly called the Peierls argument, which is fundamental to most of the current proofs of phase transitions in spin systems. It gives a quantitative assessment of entropy loss versus energy gain introduced by an ordering of the system.

Let $|\gamma|$ denote the number of nearest-neighbor pairs in γ. In order to bound the above sum in the state ω_Λ we must estimate the number of γ with a fixed value of $|\gamma|$, at least for large Λ. For this we use a geometric argument in which we implicitly assume $\nu \geq 2$. This argument is partially illustrated by the preceding figures.

To each nearest-neighbor pair $(s,t) \in \gamma$ we associate the $(\nu - 1)$-dimensional hypercube centered at the midpoint of (s,t) and oriented perpendicular to $s - t$. These hypercubes form a hypersurface which separates x and y in Λ. Now one can construct this surface by successive addition of hypercubes. If one hypercube is fixed and a face specified for the positioning of an adjacent hypercube, there are at most three possible orientations. Given a hypercube on the hypersurface and a face on it there are two possibilities, either it is possible to attach another hypercube to it lying between a nearest-neighbor pair in Λ, or not, according to whether the face lies in the interior of Λ or on the boundary. In the first case it follows from the definition of a contour that another hypercube in the hyperplane is actually attached to the face, but not in the second

case. Thus, by an exhaustion of possibilities argument, there are at most $3^{|\gamma|-1}$ ways of building up the remainder of the surface once the first hypercube is given.

Now assume that the linear dimension of Λ is large compared to the distance between x and y, and let $\{(x,x_1),(x_1,x_2),\ldots,(x_n,y)\}$ be a set of nearest neighbors connecting x and y of minimal cardinality. If γ is a contour separating x and y, it follows that one of the pairs (x_i, x_{i+1}) is contained in γ, and if $|\gamma|$ is given we must either have $i<|\gamma|/2$ or $n-i<|\gamma|/2$, i.e., the hypersurface corresponding to γ must be built up from one of the hypercubes between x_i and x_{i+1}, where i satisfies the stated conditions. It follows that there are at most

$$|\gamma|\,3^{|\gamma|-1}$$

admissible contours of length $|\gamma|$. As the minimal length of a contour is 2ν one obtains the following.

Observation 3. *If ω_Λ is any state such that*

$$\omega_\Lambda(P_\gamma)\le e^{-K|\gamma|}$$

for large Λ and for some $K>\log 3$, then

$$\omega_\Lambda(P_+^x P_-^y)\le\sum_{l=2\nu}^{\infty} l\,3^{l-1}e^{-lK}\ .$$

Up to this point the state ω_Λ on $\mathfrak{A}_\Lambda$ has been arbitrary. Now, however, we assume that ω_Λ is a (τ^Λ,β)-KMS state for a group τ^Λ of *-automorphisms of $\mathfrak{A}_\Lambda$. Then if Λ contains γ and U_γ is any unitary element of $\mathfrak{A}_\Lambda$ one has

$$\begin{aligned}\omega_\Lambda(P_\gamma) &= \omega_\Lambda(P_\gamma U_\gamma U_\gamma^* P_\gamma)\\ &\le \omega_\Lambda(U_\gamma^* P_\gamma \tau_{i\beta}^\Lambda(P_\gamma U_\gamma))\le\|\tau_{i\beta}^\Lambda(P_\gamma U_\gamma)\|\end{aligned}$$

by the (τ^Λ,β)-KMS condition. Next suppose the norm limit τ of the τ^Λ commutes with α and ω is an α-invariant weak* limit point of the ω_Λ, in the limit $\Lambda\to\infty$. Then ω is a (τ,β)-KMS state and

$$\omega(P_\gamma)\le\sup_\Lambda\|\tau_{i\beta}^\Lambda(P_\gamma U_\gamma)\|\ .$$

Hence if one can establish suitable bounds,

$$\sup_\Lambda\|\tau_{i\beta}^\Lambda(P_\gamma U_\gamma)\|\le e^{-\beta K_\beta|\gamma|}\ ,$$

for the local evolutions τ^Λ arising from a given interaction Φ then non-uniqueness of the (τ^Φ,β)-KMS state follows by combination of Observations 1 and 3. This outlines the general tactic and the problem is to make a choice of U_γ appropriate for the interaction.

Let $\tau^{\Phi,\Lambda}$ denote the local evolution associated with the Heisenberg interaction and choose

$$U_\gamma=\prod_{x\in\Lambda_1(\gamma)}\sigma_1^x=U_\gamma^*\ .$$

This choice is such that the U_γ implement the spin reflection symmetry α for $\mathfrak{A}_{\Lambda_1(\gamma)}$, i.e.,

$$\alpha(A) = U_\gamma A U_\gamma^*$$

for all $A \in \mathfrak{A}_{\Lambda_1(\gamma)}$.Then

$$\tau_{i\beta}^{\Phi,\Lambda}(P_\gamma U_\gamma) = e^{-\beta H_\Phi(\Lambda)} P_\gamma e^{\beta U_\gamma H_\Phi(\Lambda) U_\gamma} U_\gamma \ .$$

But $U_\gamma H_\Phi(\Lambda) U_\gamma$ differs from $H_\Phi(\Lambda)$ only in the interaction between the nearest neighbor pairs $(s,t) \in \gamma$. Specifically

$$U_\gamma H_\Phi(\Lambda) U_\gamma = H_\Phi(\Lambda) + H_\gamma - C_\gamma$$

where

$$H_\gamma = 2 \sum_{(s,t) \in \gamma} \Phi_\delta(s,t), \quad C_\gamma = 2 \sum_{(s,t) \in \gamma} j(s,t)$$

and

$$\Phi_\delta(s,t) = j(s,t)\Big\{(\mathbb{1} + \sigma_3^s \sigma_3^t) + \delta \sigma_2^s \sigma_2^t\Big\} \ .$$

Therefore

$$\tau_{i\beta}^{\Phi,\Lambda}(P_\gamma U_\gamma) = e^{-\beta H_\Phi(\Lambda)} P_\gamma e^{\beta(H_\Phi(\Lambda) + H_\gamma)} U_\gamma e^{-\beta C_\gamma} \ .$$

Thus one has bounds

$$\|\tau_{i\beta}^{\Phi,\Lambda}(P_\gamma U_\gamma)\| \le e^{-\beta C_\gamma} \|e^{-\beta H_\Phi(\Lambda)} P_\gamma e^{\beta H_\Phi(\Lambda) + \beta H_\gamma}\| \ .$$

This last expression is the key to obtaining bounds on $\|\tau_{i\beta}^{\Phi,\Lambda}(P_\gamma U_\gamma)\|$ uniform in Λ. It is particularly easy to handle in the case $\delta = 0$, i.e., for the Ising model.

One has decompositions

$$H_\Phi(\Lambda) = V_\Lambda + \delta T_\Lambda \ , \qquad H_\gamma = V_\gamma + \delta T_\gamma$$

where V_Λ and V_γ are the Ising contributions to the energies and T_Λ and T_γ arise from the transverse X–Y part of the interaction. Therefore V_Λ and V_γ are functions of the commuting variables σ_3^x. But P_γ is the projection onto the eigenspace with $\sigma_3^s \sigma_3^t = -1$ for all $(s,t) \in \gamma$. Hence $V_\gamma P_\gamma = 0$ and

$$\tau_{i\beta}^{\Phi,\Lambda}(P_\gamma U_\gamma)|_{\delta=0} = e^{-\beta V_\Lambda} P_\gamma e^{\beta V_\Lambda + \beta V_\gamma} U_\gamma e^{-\beta C_\gamma} = P_\gamma U_\gamma e^{-\beta C_\gamma}$$

and one has bounds

$$\|\tau_{i\beta}^{\Phi,\Lambda}(P_\gamma U_\gamma)\|_{\delta=0} \le e^{-\beta C_\gamma} \le e^{-2\beta j|\gamma|} \ .$$

Combination of these estimates with Observation 3 establishes that for $\delta = 0$ the α-invariant Gibbs states ω_Λ satisfy the bounds

$$\sup_{x,y \in \mathbf{Z}^\nu} \omega_\Lambda(P_+^x P_-^y) \le 3 \sum_{l \ge 2} l \exp\{-l(2\beta j - \log 3)\}$$

uniformly in Λ. Then Observation 1 implies the existence of at least two distinct extremal (τ,β)-KMS states for the Ising interaction and all large $\beta, \beta > \beta_c$.

The Ising estimates provide the starting point for a perturbation calculation of bounds for the Heisenberg interaction. Now one has

$$\|\tau_{i\beta}^{\Phi,\Lambda}(P_\gamma U_\gamma)\| \leq e^{-\beta C_\gamma}\|X_\gamma^\Lambda(\delta)\|$$

with

$$X_\gamma^\Lambda(\delta) = e^{-\beta(V_\Lambda+\delta T_\Lambda)}P_\gamma e^{\beta(V_\Lambda+\delta T_\Lambda+V_\gamma+\delta T_\gamma)} \ .$$

In order to bound X_γ^Λ we introduce the function F by

$$F(t) = e^{-\beta(1-t)V_\Lambda}e^{-\beta t(V_\Lambda+\delta T_\Lambda)}P_\gamma e^{\beta t((V_\Lambda+V_\gamma)+\delta(T_\Lambda+T_\gamma))}e^{\beta(1-t)(V_\Lambda+V_\gamma)}$$

and note that $F(1) = X_\gamma^\Lambda(\delta)$ and $F(0) = P_\gamma$ where the latter identification again uses $V_\gamma P_\gamma = 0$. Moreover,

$$\frac{dF}{dt}(t) = -\delta\beta\,\tau_{i\beta(1-t)}^\Lambda(T_\Lambda)\,F(t) + \delta\beta F(t)\,\tau_{i\beta(1-t)}^{\Lambda,\gamma}(T_\Lambda + T_\gamma)$$

where τ^Λ denotes the local Ising interaction, $\tau_t^\Lambda(A) = e^{iV_\Lambda t}Ae^{-iV_\Lambda t}$, and $\tau^{\Lambda,\gamma}$ is the evolution perturbed by V_γ, i.e.,

$$\tau_t^{\Lambda,\gamma}(A) = e^{i(V_\Lambda+V_\gamma)t}Ae^{-i(V_\Lambda+V_\gamma)t} \ .$$

But then $\tau^{\Lambda,\gamma} = \tau^\Lambda\tau^\gamma$ where $\tau_t^\gamma(A) = e^{iV_\gamma t}Ae^{-iV_\gamma t}$. In particular, if $A \in \mathfrak{A}_{\{x,y\}}$ then $\tau_t^\gamma(A) = A$ unless x, or y, is in $\Lambda_1(\gamma)$, or $\Lambda_2(\gamma)$. Thus $\tau_{i\beta t}^{\Lambda,\gamma}(T_\Lambda + T_\gamma) = \tau_{i\beta t}^\Lambda(T_\Lambda) + T_{\beta t,\gamma}$ where the $T_{\beta t,\gamma}$ are localized around the contour γ and satisfy bounds $\|T_{\beta t,\gamma}\| \leq aj\,|\gamma|e^{2\beta jt}$. Then

$$F(t) = F(0) - \delta\beta\int_0^t ds\Big\{\big[\tau_{i\beta(1-s)}^\Lambda(T_\Lambda), F(s)\big] - F(s)T_{\beta(1-s),\gamma}\Big\} \ .$$

This integral equation can be iterated to give a perturbation expansion of $X_\gamma^\Lambda(\delta) = F(1)$ in terms of $P_\gamma = F(0)$. Convergence of the series can then be established through term by term estimates following the arguments used to prove Theorem 6.2.4. The estimates are uniform in Λ because of the localization properties of the Ising evolution and because the evolutes $\tau_{i\beta t}^\Lambda(T_\Lambda)$ only occur in commutators with elements localized on or around the contour γ. The calculation is outlined as follows.

The n-th iterate of the integral equation for $F(t)$ is an n-fold integral, over a set $0 \leq t_1 \leq t_2 \leq \ldots \leq t_n \leq 1$, multiplied by a factor $(\delta\beta)^n$. The integrand contains 2^n terms each of which is formed by a mixture of commutators of $\tau_{i\beta(1-t_i)}^\Lambda(T_\Lambda)$ with $F(0) = P_\gamma$ and products with $T_{\beta(1-t_i),\gamma}$. Now $T_{\beta t,\gamma}$ is localized around γ in a set with at most $(2^\nu + 1)|\gamma|$ points, the points in γ and their nearest neighbors. Moreover, $\tau_{i\beta}^\Lambda(T_\Lambda)$ is a sum of two-body interactions translated under the Ising evolution and hence a sum of $(2^{\nu+1} + 1)$-body interactions. Therefore the commutators of $\tau_{i\beta}^\Lambda(T_\Lambda)$ with P_γ has at most $(2^{\nu+1} + 1)|\gamma|$ terms localized in a set with at most $|\gamma| + 2^{\nu+1} + 1$ points. The number of terms in a commutator with $T_{\beta t,\gamma}$ has the same bound but is localized in a set with a possible $(2^{\nu+1} + 1)|\gamma|$ points. Now one estimates the total number of terms in the nth-integrand by the counting argument used to prove Theorem 6.2.4.

Effectively one has a $(2^{\nu+1}+1)$-body interaction and a local element with support in a set of $(2^{\nu+1}+1)|\gamma|$ points. Therefore the number of terms is majorized by $(2^{\nu+2}(|\gamma|+n))^n \leq n!\exp\{2^{\nu+2}(|\gamma|+n)\}$. But each term will have a norm bounded by $a^n j^n e^{2\beta(t_1+\ldots+t_n)}$. Therefore one obtains norm bounds

$$\begin{aligned}\|X_\gamma^\Lambda(\delta)\| &\leq 1+\sum_{n\geq 1}(|\delta|\beta)^n\int_0^1 dt_1\ldots\int_0^{t_{n-1}} dt_n\, 2^n(2^{\nu+2}(|\gamma|+n))^n a^n j^n e^{2\beta(t_1+\ldots+t_n)}\\ &\leq 1+\sum_{n\geq 1}(b|\delta|e^{\beta j})^n e^{2^{\nu+2}|\gamma|} \;\leq\; e^{2^{\nu+2}|\gamma|}(1-b|\delta|e^{2\beta j})^{-1}\end{aligned}$$

for a suitable $b>0$ independent of δ, j and β. The last estimate is valid for $|\delta|<b^{-1}e^{-2\beta j}$. Consequently,

$$\sup_{x,y\in\mathbf{Z}^\nu}\omega_\Lambda(P_+^x P_-^y) \;\leq\; 3(1-b|\delta|e^{2\beta j})^{-1}\sum_{l\geq 2} l\exp\{-l(2\beta j-2^{\nu+2}-\log 3)\} < 1/4$$

uniformly in Λ, for all sufficiently large $\beta, \beta>\beta_c$, and δ satisfying $|\delta|<b^{-1}e^{-2\beta j}$. Hence under these conditions the anisotropic Heisenberg ferromagnet has at least two distinct extremal (τ^Φ,β)-KMS states.

Therefore we have proved Theorem 6.2.48 for all δ in a β-dependent interval, $\delta\in\langle-\delta_\beta,\delta_\beta\rangle$, and all large β. This calculation, which is extremely, crude, has the unfortunate feature that $\delta_\beta\to 0$ as $\beta\to\infty$. On the other hand it does have the fortunate feature that it does not depend on the details of the transverse part of the interaction. In the foregoing calculation T_Λ could be replaced by any Hamiltonian $H_\Psi(\Lambda)$ coming from an interaction Ψ satisfying the assumptions of Theorem 6.2.4. The estimates only depend on the local structure of the interaction and not its detailed form. In order to prove the full statement of Theorem 6.2.48 one needs much more refined combinatorial arguments which take into account the details of the action of the X–Y part T_Λ of the Heisenberg Hamiltonian.

One method of improving the Peierls argument in the quantum framework is to adapt ideas of functional integration and to reformulate the ν-dimensional quantum problem as a $(\nu+1)$-dimensional classical problem. First we introduce an orthonormal basis of the local vector space $\mathfrak{H}_\Lambda$ which is in one-to-one correspondence with the set of configurations on Λ. It is convenient to label the vectors by subsets $X\subseteq\Lambda$ and use Dirac notation $|X\rangle$. Specifically $|X\rangle$ is a simultaneous eigenfunction of the matrices $\{\sigma_3^x;\, x\in\Lambda\}$ with eigenvalue $+1$ for the matrices $\{\sigma_3^x;\, x\in X\}$ and -1 for the matrices $\{\sigma_3^x;\, x\in\Lambda\backslash X\}$; the scalar product is denoted by $\langle X|Y\rangle(=\delta_{X,Y})$ and the matrix elements of $A\in\mathfrak{A}_\Lambda$ by $\langle X|A|Y\rangle$. Second, we reintroduce the spin raising and lowering operators $\sigma_\pm^x=(\sigma_1^x\pm i\sigma_2^x)/2$ of Example 6.2.13. One has $(\sigma_\pm^x)^2=0$ and

$$[\sigma_\pm^x,\sigma_3^x]=\mp 2\sigma_\pm^x\,,\quad [\sigma_+^x,\,\sigma_-^x]=\sigma_3^x\ ,$$

with the σ corresponding to different $x,y\in\Lambda$ mutually commuting. It then follows that $\sigma_-^x|\varnothing\rangle=0$ for all $x\in\Lambda$ and

$$|X\rangle=\Big(\prod_{x\in X}\sigma_+^x\Big)|\varnothing\rangle\ .$$

Third, remark that the X–Y contribution to the Hamiltonian $H_\Phi(\Lambda)$ of the anisotropic Heisenberg model is given by δT_Λ where

$$T_\Lambda = -\sum_{x,y\in\Lambda} j(x,y)(\sigma_1^x\sigma_1^y + \sigma_2^x\sigma_2^y) = -2\sum_{x,y\in\Lambda} j(x,y)(\sigma_+^x\sigma_-^y + \sigma_-^x\sigma_+^y) \ .$$

It follows immediately that

$$\langle X|T_\Lambda|Y\rangle = 0$$

unless X and Y differ by one point x being replaced by a nearest neighbor x', in which case the matrix element takes the value $-2j(x,x')$. Fourth, recall the Trotter product formula

$$e^{-\beta H_\Phi(\Lambda)} = \lim_{n\to\infty}\left(e^{-\beta V_\Lambda/n}(I-\beta\delta T_\lambda/n)\right)^n \ .$$

This expression can then be used with the aid of the orthonormal basis to evaluate matrix elements or traces. For example,

$$\mathrm{Tr}_{\mathfrak{H}_\Lambda}(e^{-\beta H_\Phi(\Lambda)}A) = \lim_{n\to\infty}\sum_{X_1,\ldots,X_n\subseteq\Lambda}\langle X_1|A|X_2\rangle\langle X_2|e^{-\beta V_\Lambda/n}|X_2\rangle\langle X_2|(I-\beta\delta T_\Lambda/n)|X_3\rangle$$
$$\ldots\langle X_n|e^{-\beta V_\Lambda/n}|X_n\rangle\langle X_n|(I-\beta\delta T_\Lambda/n)|X_1\rangle$$

for each $A \in \mathfrak{A}_\Lambda$. But if $A = \sigma_3(X) = \prod_{x\in X}\sigma_3^x$ then $|X\rangle$ is an eigenfunction of both A and V_Λ. Let $E_\Lambda(X)$ denote the eigenvalue corresponding to V_Λ. Then

$$\mathrm{Tr}_{\mathfrak{H}_\Lambda}(e^{-\beta H_\Phi(\Lambda)}\sigma_3(X)) = \lim_{n\to\infty}\sum_{X_t}\langle X_1|\sigma_3(X)|X_1\rangle e^{-(\beta/n)\sum_{t=1}^n E_\Lambda(X_t)}$$
$$\times\prod_{t=1}^n\langle X_t|(I-\beta\delta T_\Lambda/n)|X_{t+1}\rangle$$

where we identify $X_{n+1} = X_1$. In this representation the integer $t \in [1,n]$ is interpreted as the time and X_t the classical configuration at time t. Thus the quantum configurations are viewed as a subset of the classical configurations in a subset $\Lambda\times[1,n+1]$ on a $(\nu+1)$-dimensional lattice. Each quantum configuration is a sequence $\Gamma = \{X_t;\ t = 1,2,\ldots,n+1\}$ of classical configurations with $X_{n+1} = X_1$. As the discrete time variable t changes the classical configuration X_t evolves with the evolution governed by the value of the product in the representation. But there are a limited number of possibilities. Either $X_t = X_{t+1}$ and the factor in the product is one, or X_t and X_{t+1} differ by one point x being replaced by a nearest neighbor x' and then the factor in the product is $2\beta\delta j(x,x')/n$. Thus the configurations of spins can be thought of as evolving in time with the possibility at each step of a spin and one of its nearest neighbors flipping over. Alternatively, if one adopts the particle picture, with the configuration X corresponding to particles occupying the sites $x \in X$, then at each instant the configuration either remains unchanged or evolves by a particle jumping to a nearest neighbor site. Since we are examining the ferromagnetic model the weighting factor $2\beta\delta j(x,x')/n$ associated with the jump from x to x' is positive whenever $\delta \geq 0$. In this case the quantum Gibbs state

defines a sequence of probability measures P_n over the $(\nu+1)$-dimensional classical configurations Γ. If $n(\Gamma)$ denotes the number of jumps in the path associated with Γ and $j(\Gamma)$ the product of the $j(x,x')$ along the path then the probability of the configuration Γ is given by

$$P_n(\Gamma) = e^{-\beta E_\Lambda(\Gamma)/n}(2\beta\delta)^{n(\Gamma)}j(\Gamma)\Big/\Big(\sum_\Gamma e^{-\beta E_\Lambda(\Gamma)/n}\,(2\beta\delta/n)^{n(\Gamma)}j(\Gamma)\Big)$$

where

$$E_\Lambda(\Gamma) = \sum_{X_t \in \Gamma} E_\Lambda(X_t) \ .$$

Note that the probability of a path of length n, i.e., a path with n quantum jumps has a weighting factor δ^n. So small values of δ mean long paths are unlikely. This is the perturbation characteristic of the calculation.

The probabilities for the Heisenberg model can now be estimated by combining the earlier considerations for the Ising model with an analysis of paths followed by the classical configurations. We will not give any further details of this analysis (see Notes and Remarks) which involves a variety of combinatorial counting arguments following the well-trodden path of random walks.

Finally, however, we note that the conclusions for $\delta \geq 0$ can be extended to $\delta \leq 0$ by symmetry. Let L_0 and L_1 denote the sublattices defined by

$$L_0 = \{x;\, x \in \mathbb{Z}^\nu,\ |x| = 0 \bmod 2\}$$

$$L_1 = \{x;\, x \in \mathbb{Z}^\nu,\ |x| = 1 \bmod 2\}$$

and α_0' the *-automorphism of $\mathfrak{A}$ such that $\alpha_0'(\sigma_1^x) = -\sigma_1^x$, $\alpha_0'(\sigma_2^x) = -\sigma_2^x$ and $\alpha_0'(\sigma_3^x) = \sigma_3^x$ for $x \in L_0$ and $\alpha_0'(\sigma_i^x) = \sigma_i^x$ for $x \in L_1$ and $i = 1,2,3$. Then if ω is a KMS state for the Heisenberg interaction with $\delta \geq 0$ then $\omega \circ \alpha_0'$ is a KMS state for the interaction with $-\delta$ and vice versa.

One can also use analogous symmetry arguments to deduce a nonuniqueness statement for the anti-ferromagnet from the ferromagnetic result. Let α_0 and α_1 be the *-automorphisms of $\mathfrak{A}$ which correspond to spin reversal of atoms at points of L_0 and L_1, respectively. The assumption of nearest-neighbor interaction Φ in the ferromagnetic Ising model immediately gives

$$\alpha_0(\Phi(\{x,y\})) = -\Phi(\{x,y\}) = \alpha_1(\Phi(\{x,y\})) \ ,$$

i.e., α_0 and α_1 map the ferromagnetic interaction into the anti-ferromagnetic interaction. Consequently, in the absence of an external field there is an isomorphism between the sets of KMS states for the two models. This conclusion must be modified, however, in the presence of an external magnetic field because $\alpha_0(h(x)\sigma_3^x) = \pm h(x)\sigma_3^x$ with the plus sign if $x \in L_1$ and the minus sign if $x \in L_0$, i.e., the sublattice spin reversal transforms a uniform external field into a staggered field. Indeed, one can show that the Ising anti-ferromagnet has at least two phases for low temperatures and a uniform, but weak, *nonzero external* field. This is not to be expected for the ferromagnet. Then the introduction of a uniform external field should remove the spontaneous magnetization and the long range order.

The nonuniqueness result for the anti-ferromagnet with a translationally invariant nearest-neighbor interaction and a uniform external field can be proved by a chain of arguments similar to those used for Theorem 6.2.48. The previous proof was based upon the observation that extremality of the (τ^Φ, β)-KMS state and invariance under the spin reversal symmetry are contradictory. The anti-ferromagnetic result is deduced from an inconsistency between extremality and translation invariance.

Observation 1 is replaced by the following.

Observation 1′. *If Φ is a translationally invariant interaction and ω a translationally invariant (τ^Φ, β)-KMS state which satisfies*

$$\sup_{x \in L_0,\, y \in L_1} \omega(P_+^x P_+^y) < \tfrac{1}{4} \ , \qquad \sup_{x \in L_0,\, y \in L_1} \omega(P_-^x P_-^y) < \tfrac{1}{4} \ ,$$

then there are two distinct extremal (τ^Φ, β)-KMS states.

Proof. It suffices to prove that ω is not an extremal (τ^Φ, β)-KMS state. Assume the contrary, then ω is strongly clustering in space and hence

$$1 > \lim_{\substack{|x-y| \to \infty \\ x \in L_0,\, y \in L_1}} 4\omega(P_+^x P_+^y) = \lim_{\substack{|x-y| \to \infty \\ x \in L_0,\, y \in L_1}} \omega\Big((\mathbb{1} + \sigma_3^x)(\mathbb{1} + \sigma_3^y)\Big) = (M+1)^2$$

where $M = \omega(\sigma_3^x)$. Using P_-^x and P_-^y in place of P_+^x and P_+^y one also finds

$$1 > (M-1)^2 \ .$$

But these two inequalities are inconsistent. Hence ω cannot be extremal.

Next we must adapt the definition of configurations and contours etc., to the anti-ferromagnetic case. Let $x \in \Lambda \cap L_0$ and $y \in \Lambda \cap L_1$. We now examine configurations c such that $c(x) = c(y) = +$ (or $c(x) = c(y) = -$). The definition of a contour remains unchanged but the class of contours $\Gamma(c)$ is taken as the set of $\gamma = \{(x_1, y_1), \ldots, (x_n, y_n)\}$ with $c(x_i) = c(y_i)$. Since $c(x) = c(y)$, and $x \in L_0$ and $y \in L_1$, we argue as before that there must exist a contour $\gamma(c)$ which separates x and y but the set $\Lambda_c \subset \Lambda_x(\gamma(c))$ is now the largest NN(Λ)-connected set such that $x \in \Lambda_c$, $c(z) = +$ for $z \in \Lambda_c \cap L_0$, $c(z) = -$ for $z \in \Lambda_c \cap L_1$. Thus one obtains:

Observation 2′. *For any region Λ one has*

$$P_\pm^x P_\pm^y \le \sum_\gamma P_\gamma \ ,$$

where

$$P_\gamma = \prod_{(s,t) \in \gamma} P_{c(s)}^s P_{c(t)}^t$$

(and $c(s) = c(t)$ by definition)

The enumeration of the contours γ remains the same and Observation 3 is replaced by the following:

Observation 3′. *If $x \in L_0, y \in L_1$ and ω_Λ is a state on $\mathfrak{A}_\Lambda$ such that*

$$\omega_\Lambda(P_\gamma) \leq e^{-K|\gamma|}$$

for large Λ and for some $K > \log 3$, then

$$\omega_\Lambda(P_\pm^x P_\pm^y) \leq \sum_{l=2\nu}^{\infty} l\, 3^{l-1} e^{-lK} < +\infty \ .$$

Finally, if ω_Λ is a (τ^Λ, β)-KMS state, one has the bound

$$\omega_\Lambda(P_\gamma) \leq \|\tau_{i\beta}^\Lambda(P_\gamma U_\gamma)\| \ .$$

It remains to make an appropriate choice of U_γ. To explain this choice let us reconsider the ferromagnetic case from a slightly different angle.

Let $|X\rangle$ denote the orthonormal basis of the local vector space $\mathfrak{H}_\Lambda$ used above. Then the X are in one-to-one correspondence with configurations c_X of spins and the effect of the ferromagnetic U_γ is such that

$$U_\gamma |X\rangle = |X^*\rangle \tag{$*$}$$

where c_X* is the unique configuration with $\Gamma(c_X*) = \Gamma(c_X)\backslash\gamma$, i.e., the spin reflection removes the contour γ. But the $|X\rangle$ are eigenfunctions of the Ising part V_Λ of the Hamiltonian and the calculation following Observation 3 can be rephrased as

$$\tau_{i\beta}^\Lambda(P_\gamma U_\gamma) = P_\gamma U_\gamma e^{-\beta(E_\Lambda(X) - E_\Lambda(X^*))} \tag{$**$}$$

where $E_\Lambda(X)$ is the eigenvalue of V_Λ.

This indicates how to proceed in the anti-ferromagnetic case. One chooses any unitary U_γ with the property $(*)$ but with the anti-ferromagnetic definition of $\Gamma(c)$. It then follows that $(**)$ remains valid and one argues almost as before.

The translation-invariant, nearest-neighbor anti-ferromagnetic Ising interaction with external field has

$$\Phi(\{x\}) = -h\sigma_3^x$$

for all $x \in \mathbb{Z}^\nu$,

$$\Phi(\{x, y\}) = j\sigma_3^x \sigma_3^y$$

with $j > 0$ if $|x - y| = 1$ and $\Phi(X) = 0$ in all other cases. Therefore,

$$E_\Lambda(X) - E_\Lambda(X^*) \geq 2(j - |h|)|\gamma|$$

and

$$\|\tau_{i\beta}^\Lambda(P_\gamma U_\gamma)\| \leq e^{-2\beta(j-|h|)|\gamma|}$$

for $\beta > 0$. Let ω be any limit point of the local Gibbs states ω_Λ for this interaction. Either ω is not $\mathbb{Z}^\nu$-invariant and there is automatically more than one KMS state or it is translationally invariant and by combination of the foregoing estimates the conditions of Observation 1′ are valid for β sufficiently

large. Therefore we can conclude that the Ising anti-ferromagnet has at least two distinct extremal KMS states for sufficiently large β if the external field satisfies $|h| < j$. But this conclusion can then be extended to the anisotropic Heisenberg model by the perturbation calculation outlined in the ferromagnetic case.

Theorem 6.2.49. *Let Φ denote the translationally invariant anti-ferromagnetic Heisenberg interaction with nearest-neighbor coupling j, anisotropy δ and uniform external field h. Assume $\nu \geq 2$.*

It follows that there is a $\beta_c > 0$ and for each $\beta > \beta_c$ a $\delta_\beta > 0$ such that there exist at least two extremal (τ^Φ, β)-KMS states for all $\beta > \beta_c$ and $\delta \in \langle -\delta_\beta, \delta_\beta \rangle$.

The value of δ_β obtained by the crude perturbation calculation tends to zero exponentially fast as $\beta \to \infty$. The refined calculation based on the path estimates is better. One can establish bounds with $\delta_\beta = O(\beta^{-1/2})$. It is not known whether the model exhibits anti-ferromagnetism for all $\delta \in \langle -1, 1 \rangle$ but there are several indications that this is the case, e.g., the classical Heisenberg model and numerical calculations.

The phase structure for the Heisenberg model appears to be somewhat different if $\delta = 1$, i.e., in the isotropic case. In two dimensions it is possible to rule out the possibility of spontaneous magnetization for the ferromagnetic model, or spontaneous magnetization of the sublattices in the anti-ferromagnetic model. Although this does not entirely exclude the possibility of non-uniqueness for the corresponding (τ^Φ, β)-KMS states it does rule out the most likely mechanism. Instead of establishing this result directly we derive a more general statement on the absence of spontaneous symmetry breaking based on the general criterion in Theorem 5.3.33A. The properties of the Heisenberg model will then follow as a corollary.

Theorem 6.2.50 (Fröhlich-Pfister). *Let G be a compact, connected Lie group, $g \mapsto V(g)$ a unitary representation of G on $\mathbb{C}^{N+1} \simeq \mathfrak{H}_{\{x\}}$ which determines an action $g \in G \mapsto \mathrm{Ad}(V(g)) = \gamma_x(g)$ on each $\mathfrak{A}_{\{x\}}$ and hence the action $\gamma(g) = \otimes_{x \in \mathbb{Z}^2} \gamma_x(g)$ on the spin algebra $\mathfrak{A}$ over $\mathbb{Z}^2$. Let Φ be a two-body interaction which is invariant under the action of G,*

$$\gamma(g)(\Phi(X)) = \Phi(X)$$

for all $g \in G$ and all two-point sets X. Further suppose that

$$\|\Phi(\{x, y\})\| \leq C(|x - y| + 1)^{-4}$$

for some $C > 0$.

If τ^Φ denotes the evolution associated with Φ and if ω is a (τ^Φ, β)-KMS state for some $\beta \in \mathbb{R}$ then

$$\omega \circ \gamma(g) = \omega$$

for all $g \in G$, i.e., there is no spontaneous breaking of symmetry.

Remark. One can demonstrate by example that the conditions in this theorem are in many senses optimal (see Notes and Remarks).

PROOF. Fix $g \in G$. By Theorem 5.3.33A it suffices to find a sequence $U_L \in \mathfrak{A}$, $L = 1, 2 \ldots$, such that

$$\gamma(g)(A) = \lim_{L \to \infty} U_L A U_L^*$$

for all $A \in \mathfrak{A}$ and, in addition,

$$\sup_{L \geq 1} \|\delta_\Phi(U_L)\| < \infty$$

where δ_Φ denotes the generator of τ^Φ. The first attempt to construct such a sequence would be

$$U_L = \otimes_{x \in \Lambda_L} V(g)$$

where $\Lambda_L = \{(x_1, x_2) \in \mathbb{Z}^2;\ |x_i| \leq L\}$. This fulfils the first requirement but not the second, since the lattice is two-dimensional (in one-dimension the second requirement would also be fulfilled). To overcome this problem we 'switch off' the action of g slowly across the boundary of Λ_L in the following manner.

Choose a one-parameter group $t \to g^t$ of G such that $g^1 = g$ and that the length of the path $t \to g^t$ over $0 \leq t \leq t_0$ is at most πt_0. This is possible since we may assume that $g \mapsto V(g)$ is faithful and then G is a closed connected subgroup of $U(N+1)$. Now define

$$U_L = \otimes_{x \in \Lambda_{2L}} V(g_x)$$

where $g_x = g$ for $x \in \Lambda_L$ and $g_x = g^{k/L}$ for $x = (x_1, x_2) \in \Lambda_{2L} \backslash \Lambda_L$ with $k = 2L - \max\{|x_1|, |x_2|\}$. Then

$$\|\delta_\Phi(U_L)\| \leq \sum_{X \subset \mathbb{Z}^2} \|\Phi(X)U_L - U_L\Phi(X)\| = \sum_{(x,y) \in \mathbb{Z}^2} \|U_L^*\Phi(\{x,y\})U_L - \Phi(\{x,y\})\| \ .$$

To estimate this sum it is convenient to use the metric

$$|x - y| = \max\{|x_1 - y_1|, |x_2 - y_2|\}$$

on $\mathbb{Z}^2$. Then, using the invariance of $\Phi(\{x,y\})$ under $\gamma(g)$, the terms with $|x| \leq L$ and $|y| \leq L$ vanish. Similarly the terms with $|x| \geq 2L$ and $|y| \geq 2L$ are zero. For the remaining terms we use

$$\begin{aligned}
\|U_L^*\Phi(\{x,y\})U_L - \Phi(\{x,y\})\| &= \|V^*(g_x) \otimes V^*(g_y)\Phi(\{x,y\})V(g_x) \otimes V(g_y) - \Phi(\{x,y\})\| \\
&= \|V^*(g_x) \otimes V^*(g_y)\Phi(\{x,y\})V(g_x) \otimes V(g_y) \\
&\qquad - V^*(g_y) \otimes V^*(g_y)\Phi(\{x,y\})V(g_y) \otimes V(g_y)\| \\
&\leq 2\|V(g_x) - V(g_y)\| \cdot \|\Phi(\{x,y\})\| \\
&\leq 2\pi\big||x| - |y|\big| \cdot \|\Phi(\{x,y\})\| \ .
\end{aligned}$$

Therefore

$$\|\delta_\Phi(U_L)\| \leq \sum_{\substack{L \leq |x| \leq 2L \\ \text{or } L \leq |y| \leq 2L}} 2\pi\big||x| - |y|\big| \cdot \|\Phi(\{x,y\})\| \ .$$

Hence

$$\|\delta_\Phi(U_L)\| \leq \sum_{(x,y)\in\mathbb{Z}^2} 2\pi\big||x|-|y|\big|\, C\,(|x-y|+1)^{-4} < \infty$$

since the sum is over two dimensions. Thus Theorem 6.2.50 follows from Theorem 5.3.33A.

This theorem has several implications for the Heisenberg model.

First, remark that the group $SO(3)$ of rotations acts as a continuous group of *-automorphisms of the spin-$\frac{1}{2}$ quantum algebra $\mathfrak{A}$ by rotation of the spin vectors σ^x. The action γ on a local algebra $\mathfrak{A}_\Lambda$ is determined by unitaries $\exp\{i\sum_{x\in\Lambda} a.\sigma^x\}$ with $a \in \mathbb{R}^3$. But the interaction of the two-body Heisenberg model, $\Phi(\{x,y\}) = -j(x,y)\sigma^x.\sigma^y$, is invariant under the simultaneous rotation of the spin vectors σ^x and σ^y, i.e., Φ is invariant under γ. Hence if there is no external field and no many-body interactions one deduces that each (τ^Φ,β)-KMS state ω of the one-, or two-, dimensional model is γ-invariant. In particular $\omega(\sigma_3^x) = 0$ for all x. But if ω_h is a (τ^Φ,β)-KMS state of the ferromagnetic model with external field $\Phi^{(1)}(\{x\}) = -h(x)\sigma_3^x$ then the energetically favored configurations are those with spins positively aligned parallel to the third axis. Thus one expects $\omega_h(\sigma_3^x) > 0$. Then at sufficiently low temperature any (τ^Φ,β)-KMS state obtained in the limit $\|h\|_\infty \to 0$ should exhibit a residual magnetism, i.e., one should have

$$\lim_{\|h\|_\infty\to 0}\ \lim_{L\to\infty} |\Lambda_L|^{-1} \sum_{x\in\Lambda_L} \omega_h(\sigma_3^x) > 0\ .$$

But any such limit state is a (τ^Φ,β)-KMS state for the limiting dynamics, i.e., the interaction with $h = 0$, by Theorem 5.3.25. Thus Theorem 6.2.50 demonstrates that spontaneous magnetization cannot occur for the isotropic Heisenberg model in one, or two, dimensions whenever

$$\sup_x \sum_y |x-y|^2 |j(x,y)| < \infty\ .$$

Alternatively, if one considers the anisotropic model $\Phi(\{x,y\}) = -j(x,y)\cdot\{\delta(\sigma_1^x\sigma_1^y + \sigma_2^x\sigma_2^y) + \sigma_3^x\sigma_3^y\}$ then the interaction is invariant under the subgroup of rotations of the spins around the third axis. Hence if ω_h now corresponds to a (τ^Φ,β)-KMS state with external field in the first direction

$$\lim_{\|h\|_\infty\to 0}\ \lim_{L\to\infty} |\Lambda_L|^{-1} \sum_{x\in\Lambda_L} \omega_h(\sigma_1^x) = 0$$

and there can be no residual magnetization in the first direction in either one or two space dimensions.

One can also prove the absence of spontaneous magnetization by use of the Bogoliubov inequality mentioned in the Notes and Remarks to Section 5.3.1 as an early form of a correlation inequality.

Lemma 6.2.51 (Bogoliubov Inequality). *Let ω be a (τ,β)-KMS state over the C^*-algebra $\mathfrak{A}$ and let δ denote the generator of τ.*

It follows that

$$-i\beta\omega(AA^* + A^*A)\omega([C, \delta(C^*)]) \geq 2|\omega([C, A^*])|^2$$

for all $A \in \mathfrak{A}$ *and* $C \in D(\delta)$.

PROOF. Let

$$(A, B)_\sim = \frac{1}{\beta}\int_0^\beta d\lambda\, \omega(A^*\tau_{i\lambda}(B))$$

denote the sesquilinear form on the analytic elements $\mathfrak{A}_\tau$ introduced prior to Theorem 5.3.17. The Cauchy–Schwarz inequality gives

$$|(A, B)_\sim|^2 \leq (A, A)_\sim (B, B)_\sim \ .$$

But if $B = \delta(C)$

$$\begin{aligned}(A, B)_\sim &= \frac{1}{\beta}\int_0^\beta d\lambda \frac{1}{i}\frac{d}{d\lambda}\omega(A^*\tau_{i\lambda}(C)) \\ &= (i\beta)^{-1}\{\omega(A^*\tau_{i\beta}(C)) - \omega(A^*C)\} \\ &= (i\beta)^{-1}\omega([C, A^*])\end{aligned}$$

by the (τ, β)-KMS condition.

Alternatively, if $U_\omega(t) = \exp\{itH_\omega\}$ is the unitary group which implements τ in the representation $(\mathfrak{H}_\omega, \pi_\omega, \Omega_\omega)$,

$$(A, B)_\sim = \left(\pi_\omega(A)\Omega_\omega, (\beta H_\omega)^{-1}(\mathbb{1} - e^{-\beta H_\omega})\pi_\omega(B)\Omega_\omega\right) \ .$$

Therefore, the inequality $(1 - e^{-x})/x \leq (1 + e^{-x})/2$ gives

$$\begin{aligned}(A, A)_\sim &\leq (\pi_\omega(A)\Omega_\omega, (\mathbb{1} + e^{\beta H_\omega})\pi_\omega(A)\Omega_\omega)/2 \\ &= \{\omega(A^*A) + \omega(A^*\tau_{i\beta}(A))\}/2 = \omega(\{A^*, A\})/2 \ .\end{aligned}$$

Combining this estimate with the previous evaluation and the Cauchy–Schwarz inequality for $(A, B)_\sim$, one finds

$$\begin{aligned}\beta^{-2}|\omega([C, A^*])|^2 &= |(A, B)_\sim|^2 \\ &\leq \omega(\{A^*, A\})(B, B)_\sim/2 \\ &= (i\beta)^{-1}\omega(\{A^*, A\})\omega([C, B^*])/2\end{aligned}$$

or

$$-i\beta\omega(\{A^*, A\})\omega([C, \delta(C^*)]) \geq 2|\omega([C, A^*])|^2$$

for τ-analytic A and C. The full result follows by continuity because $\mathfrak{A}_\tau$ is norm dense in $\mathfrak{A}$ and it is also a core for δ.

We next demonstrate how the Bogoliubov inequality can be used to reproduce the earlier conclusion on the absence of spontaneous magnetization for the two-dimensional anisotropic Heisenberg model.

Assume there is an external magnetic field $\Phi(\{x\}) = -h(x)\sigma_1^x$, in the direction of the first axis, and set $\|h\| = \sup_{x \in \mathbf{Z}^2} |h(x)|$. Further assume there is a two-body interaction.

$$\Phi(\{x, y\}) = -j(x, y)\left\{\delta(\sigma_1^x\sigma_1^y + \sigma_2^x\sigma_2^y) + \sigma_3^x\sigma_3^y\right\}$$

and set

$$\|j\| = \sup_{x \in \mathbb{Z}^2} \sum_{y \in \mathbb{Z}^2} |x-y|^2 |j(x,y)| \ .$$

We aim to show that there is no spontaneous magnetization whenever $\|j\| < \infty$.

Let Δ_a denote the lattice of pairs (p_1, p_2) where $p_i = 2\pi n_i/a_i$ and the n_i are integers such that $-a_i/2 < n_i \leq a_i/2$. Introduce the Fourier transforms, $\hat{\sigma}_i$, by

$$\hat{\sigma}_i^p = \sum_{x \in \Lambda_a} e^{-ipx} \sigma_i^x = (\hat{\sigma}_i^{-p})^* ,$$

where $px = p_1 x_1 + p_2 x_2$. Thus

$$\sigma_i^x = |\Lambda_a|^{-1} \sum_{p \in \Delta_a} e^{ipx} \hat{\sigma}_i^p \ .$$

Next define the mean magnetization $M_a(h)$ by

$$M_a(h) = |\Lambda_a|^{-1} \sum_{x \in \Lambda_a} \omega(\sigma_1^x) = |\Lambda_a|^{-1} \omega(\hat{\sigma}_1^0)$$

and introduce

$$\overline{M}(h) = \limsup_{a \to \infty} |M_a(h)| \ .$$

We will bound $\overline{M}(h)$ by choosing $A = \hat{\sigma}_2^p, C = \hat{\sigma}_3^p$ in the Bogoliubov inequality. This choice is motivated by the observation that

$$|\Lambda_a|^{-2} |\omega([\hat{\sigma}_3^p, \hat{\sigma}_2^{-p}])|^2 = 4 M_a(h)^2 \ .$$

Moreover, one has

$$|\Lambda_a|^{-2} \sum_{p \in \Delta_a} \omega(\hat{\sigma}_2^p \hat{\sigma}_2^{-p} + \hat{\sigma}_2^{-p} \hat{\sigma}_2^p)/2 = 1 \ .$$

The idea for determining the bound is to find a volume-independent positive continuous function E such that

$$-i\beta\omega([\hat{\sigma}_3^p, \delta(\hat{\sigma}_3^{-p})]) \leq |\Lambda_a| E(p) \ .$$

The Bogoliubov inequality then implies the bounds

$$\begin{aligned} 1 = & \ |\Lambda_a|^{-2} \sum_{p \in \Delta_a} \omega(\hat{\sigma}_2^p \hat{\sigma}_2^{-p} + \hat{\sigma}_2^{-p} \hat{\sigma}_2^p)/2 \\ \geq & \ |\Lambda_a|^{-2} \sum_{p \in \Delta_a} \left\{ \frac{i|\omega([\hat{\sigma}_3^p, \hat{\sigma}_2^{-p}])|^2}{\beta\omega([\hat{\sigma}_3^p, \delta(\hat{\sigma}_3^{-p})])} \right\} \\ \geq & \ 4 M_a(h)^2 |\Lambda_a|^{-1} \sum_{p \in \Delta_a} E(p)^{-1} . \end{aligned}$$

Thus, taking the limit $a \to \infty$ and rearranging gives

$$\overline{M}(h)^2 \leq \left[4(2\pi)^{-2} \int_{\substack{|p_1| \leq \pi \\ |p_2| \leq \pi}} d^2p \, E(p)^{-1} \right]^{-1} .$$

To find an appropriate E one has to calculate $\omega([\hat{\sigma}_3^p, \delta(\hat{\sigma}_3^{-p})])$ and this gives

$$-i\beta\omega([\hat{\sigma}_3^p, \delta(\hat{\sigma}_3^{-p})]) = 8\beta \sum_{x,y\in\Lambda_a} j(x,y)(1-\cos p(x-y))\omega(\sigma_1^x\sigma_1^y + \sigma_2^x\sigma_2^y)$$
$$+ 8\beta \sum_{x\in\Lambda_a}\sum_{y\in\Lambda_a^c} j(x,y)\omega(\sigma_1^x\sigma_1^y + \sigma_2^x\sigma_2^y) + 4\beta \sum_{x\in\Lambda_a} h(x)\omega(\sigma_1^x) \ .$$

Hence

$$\limsup_{a\to\infty} -i\beta|\Lambda_a|^{-1}\omega([\hat{\sigma}_3^p, \delta(\hat{\sigma}_3^{-p})]) \le 8|\beta|\|j\|p^2 + 4|\beta|\|h\| \ .$$

Combination of these results yields the bound

$$\overline{M}(h)^2 \le \left[4(2\pi)^{-2}\int_{\substack{|p_1|\le\pi\\|p_2|\le\pi}} d^2p(8|\beta|\|j\|p^2 + 4|\beta|\|h\|)^{-1}\right]^{-1} .$$

An alternative weaker bound can be obtained by integrating over the smaller region $|p_1|^2 + |p_2|^2 \le \pi^2$. This, however, allows the introduction of radial coordinates and hence one obtains

$$\overline{M}(h)^2 \le \left[4(2\pi)^{-1}\int_0^\pi dp\, p(8|\beta|\|j\|p^2 + 4|\beta|\|h\|)^{-1}\right]^{-1}$$
$$= \left[(8|\beta|\|j\|\pi)^{-1}\log(1 + 2\pi^2\|j\|)/\|h\|)\right]^{-1} .$$

Hence $\overline{M}(h) \to 0$ as $\|h\| \to 0$ and there is no residual magnetization in the direction of the first axis or, by symmetry, in the plane defined by the first two axes. A similar argument establishes that the X–Y model has no spontaneous magnetization in one or two dimensions.

A slight modification of the proof rules out the possibility of spontaneous magnetization of a sublattice for the general Heisenberg antiferromagnet. One replaces $A = \hat{\sigma}_2^p$ by $A = \hat{\sigma}_2^{p+P}$ and considers the generalized magnetization

$$M_a(h) = |\Lambda_a|^{-1}\sum_{x\in\Lambda_a}\omega(\sigma_1^x)e^{-iPx} \ .$$

Despite these results one should perhaps emphasize that the bound on $\overline{M}(h)$ is rather weak. One has $\overline{M}(h) \sim |\log\|h\||^{-1/2}$ as $\|h\| \to 0$ and all derivatives of this bound diverge at the origin. Thus, the argument does not rule out singular behavior of the derivatives of the magnetization.

The above argument can in certain cases be inverted and used to prove the existence of multiple phases. The estimate

$$-i\omega([\hat{\sigma}_3^p, \delta(\hat{\sigma}_3^{-p})]) \le ap^2 + b$$

corresponds physically to a bound on the energy of excitations around equilibrium. The behavior of this energy at zero momentum, i.e., at $p = 0$, was the critical feature that ruled out ferromagnetism. The basic idea for exploiting infrared bounds to obtain the opposite conclusion can be outlined as follows.

Suppose that ω is a $\mathbb{Z}^\nu$-invariant (τ^Φ, β)-KMS state for some interaction Φ and some $\beta \in \mathbb{R}$. Next, introduce the functions F_A by

$$F_A(x) = \omega(\hat{A}^* \tau_x(\hat{A})), \quad A \in \mathfrak{A} \ ,$$

where $\hat{A} = A - \omega(A)\mathbb{1}$. As F_A is a function of positive type of the lattice $\mathbb{Z}^\nu$ it is automatically the Fourier transform of a measure μ_A,

$$F_A(x) = \int_{|p| \leq \pi} d\mu_A(p)\, e^{ipx} \ .$$

If ω is not strongly clustering in space, F_A will have a nonzero asymptote, for some $A \in \mathfrak{A}$, and this will be reflected by the presence of a Dirac point measure δ at $p = 0$. Thus, to deduce that ω is not extremal (τ^Φ, β)-KMS it suffices to find an A for which this point measure occurs. Next, we remark that μ_A should be related to the dynamical propagator, or Green's function, of the Hamiltonian determining the excitations around the equilibrium state. The variable p corresponds to a lattice momentum and the energy of excitations should be given by a positive function E of p. For $p \neq 0$ general dynamical reasoning indicates that $\mu_A(p) \sim (\beta E(p))^{-1}$. The factor β enters because the inverse temperature determines the scale of energy. Thus, one expects

$$d\mu_A(p) = c_A\, \delta(p) + d_A(\beta E(p))^{-1} d^\nu p$$

for $c_A \geq 0$ and $d_A > 0$. But one has the simple identity

$$\begin{aligned} \omega(\hat{A}^* \hat{A}) &= F_A(0) \\ &= \int_{|p| \leq \pi} d\mu_A(p) = c_A + \frac{d_A}{\beta} \int_{|p| \leq \pi} d^\nu p\, E(p)^{-1} \ . \end{aligned}$$

Now suppose

$$\int_{|p| \leq \pi} d^\nu p\, E(p)^{-1} < +\infty \ .$$

In this case one must have $c_A > 0$ for sufficiently large β because the second term in this identity for $\omega(\hat{A}^* \hat{A})$ tends to zero as $\beta \to \infty$. Thus, the crux of this argument is an estimate of the form

$$\mu_A(p) \leq \beta E(p)^{-1}$$

for some $A \in \mathfrak{A}$ and an E such that E^{-1} is integrable.

Let us examine the application of this technique to the anisotropic Heisenberg model with translationally invariant ferromagnetic interaction. One expects a spontaneous magnetization at low temperature. Hence, any spin reversal symmetric KMS state ω should not be extremal and the above argument should apply to

$$F_{\sigma_3}(x) = \omega(\sigma_3^0 \sigma_3^x) \ .$$

But the Heisenberg model is a lattice analogue of a continuous system with two-body interactions (see Notes and Remarks to Section 6.2.1). Thus for this model one expects the low momentum relation $E(p) = cp^2$. Now $E(p)^{-1}$ is integrable at the origin for all $\nu \geq 3$ and hence this intuitive argument indicates the presence of a phase transition in all dimensions greater than or equal to three.

Although this method of infrared bounds is seductively simple in outline, it is nonetheless difficult to apply. The necessary estimates on μ_A are not easily derived. Some results have been obtained through bounds on the finite-volume Gibbs states ω_A which are uniform in Λ. In particular, the method has been successfully used to prove nonuniqueness of (τ^Φ, β)-KMS states for a variety of classical models, for the isotropic Heisenberg antiferromagnet, and the X–Y model for spin greater than one, i.e., $N + 1 \geq 3$ and $\nu \geq 3$.

We conclude this subsection with a few comments on multiplicity of extremal KMS states. The only model for which much information is known is the two-dimensional translationally invariant Ising model. In this model it is known that there is one, and only one, extremal (τ^Φ, β)-KMS state for all positive β if the external field is nonzero or for small positive β if there is no external field. Furthermore in the absence of a field there are exactly two extremal (τ^Φ, β)-KMS states for $\beta > \beta_c$ where β_c is the maximum value of β for which uniqueness occurs. These two states are clearly translationally invariant. In three or more dimensions the situation for the Ising model is known to be more complicated. There is still a unique phase at high temperature or in the presence of an external field but at low temperatures there can be an infinite number of phases which are not necessarily $\mathbb{Z}^\nu$-invariant. This can be partially understood in terms of juxtaposition in the third direction of the two two-dimensional pure phases. Similar easily understood effects occur already for the ground states of the one-dimensional Ising model, as we shall see in the next section.

6.2.7. Ground States

Ground states, or zero-temperature states, were introduced and partially analyzed in Chapter 5, see Definition 5.3.18 and Proposition 5.3.19. These states can be described in various ways, but physically they correspond to the positive energy states associated with a given dynamical group τ. Ground states are sometimes referred to as $(\tau, +\infty)$-KMS states, a notation which is partially justified by Proposition 5.3.23. This proposition establishes that the zero-temperature limits of KMS states are ground states. Nevertheless, the set of τ ground states has affine properties different from the set of (τ, β)-KMS states. The set K_∞ of ground states is always a face in $E_{\mathfrak{A}}$, but it is a simplex if and only if $(\mathfrak{A}, \omega)$ is $\mathbb{R}$-abelian for all $\omega \in K_\infty$, see Corollary 5.3.40. The set K_β of KMS states at finite β is a simplex, but it is a face in $E_{\mathfrak{A}}$ if, and only if, $\pi_\omega(\mathfrak{A})$ is abelian for all $\omega \in K_\beta$ (see Remark 3 after Theorem 5.3.32). In particular, spin systems provide some striking examples of the differences between ground states and finite-temperature equilibrium states.

Consider the one-dimensional quantum spin systems with translationally invariant nearest-neighbor ferromagnetic Ising interaction Φ. This model has a unique (τ^Φ, β)-KMS state ω_β for all $\beta \in \mathbb{R}$ and all values of the external field, by Theorem 6.2.47. These states are automatically $\mathbb{Z}$-invariant. For a nonzero

external field the same remains true for the τ^Φ ground states. If the field is in the positive direction, the ground state is determined by the configuration in which all atomic spins are positively oriented. If the field is in the negative direction, all spins are negatively oriented. But if the external field is zero, a drastic difference occurs. First, there are two extremal $\mathbb{Z}$-invariant τ^Φ ground states, the states with all atoms positively, or negatively, oriented. Second, there are an infinite number of nontranslationally invariant ground states. A typical such state ω_x is determined by positive orientation of all atoms to the left of $x \in \mathbb{Z}$ and negative orientation of those on the right.[5] Thus, the multiplicity and invariance properties of the τ^Φ ground states and the (τ^Φ, β)-KMS states, even with β very large, can be quite different. Furthermore, the states $\omega_x, x \in \mathbb{Z}$, are all extremal τ^Φ ground states which are mutually unitarily equivalent. Extremality follows from purity, and the equivalence arises because one state is transformed into the other by reversal of a finite number of atomic spins (cf. Corollary 5.3.40). But for $\beta \in \mathbb{R}$, extremal (τ^Φ, β)-KMS states are either equal or disjoint, by Theorem 5.3.30, and hence the equivalence is another distinctive feature of zero temperature. Finally, an explicit calculation shows that the finite-temperature KMS states ω_β of the Ising model converge in the weak* topology as $\beta \to \infty$ but the limit state ω is not extremal even among the $\mathbb{Z}$-invariant ground states. It is the average of the spin up and the spin down ground states. Thus, purity properties do not necessarily survive the zero-temperature limit.

Despite the differences illustrated by the Ising interaction there are many similarities between ground states and KMS states, in particular with respect to stability. In Section 5.4 we established various forms of stability for both types of state and we conclude this discussion of spin systems by showing that the ground states can be characterized by stability properties analogous to the maximum entropy principles of Sections 6.2.3 and 6.2.4. This type of principle was expressed as maximality of a functional $S - \beta H_\Phi$ or, equivalently, a functional $\beta^{-1}S - H_\Phi$. Thus, the zero-temperature, $\beta = +\infty$, analogue corresponds to maximization of $-H_\Phi$, i.e., minimization of the energy functional H_Φ. We begin with a zero temperature version of Theorem 6.2.36.

Theorem 6.2.52. *Let Φ be an interaction of a quantum spin system and τ^Λ the corresponding local automorphism group. Assume that:*

(1) *τ^Λ converges strongly to an automorphism group τ, i.e.,*

$$\lim_{\Lambda \to \infty} \|\tau_t^\Lambda(A) - \tau_t(A)\| = 0$$

for all $A \in \mathfrak{A}$ and $t \in \mathbb{R}$.

(2) *The surface energies $W_\Phi(\Lambda)$ are well-defined elements of $\mathfrak{A}$ for all $\Lambda \subset L$.*

[5] It is not immediately evident that the ω_x are ground states but this is an easy consequence of the result we are about to derive, Theorem 6.2.52. See Example 6.2.56.

(3)
$$D = \bigcup_{\Lambda \subset L} \mathfrak{A}_\Lambda$$

is a core for the generator δ of τ.

The following conditions are equivalent for a state ω.

(1)
$$\omega(\tilde{H}_\Phi(\Lambda)) = \inf_{\omega' \in C_\Lambda^\omega} \omega'(\tilde{H}_\Phi(\Lambda))$$

for all $\Lambda \subset L$, where $\tilde{H}_\Phi(\Lambda) = H_\Phi(\Lambda) + W_\Phi(\Lambda)$ is the conditional energy and

$$C_\Lambda^\omega = \{\omega'; \omega' \in E_{\mathfrak{A}}, \omega'|_{\mathfrak{A}_{\Lambda^c}} = \omega|_{\mathfrak{A}_{\Lambda^c}}\} \ .$$

(2) *ω is a τ ground state, i.e.,*

$$-i\omega(A^*\delta(A)) \geq 0$$

for all $A \in D(\delta)$.

(3)
$$\omega(\tilde{H}_\Phi(\Lambda)) \leq \omega(T(\tilde{H}_\Phi(\Lambda)))$$

for all $\Lambda \subset L$ and all positive maps $T : \mathfrak{A} \to \mathfrak{A}$ with the property that $T(A) = A$ for $A \in \mathfrak{A}_{\Lambda^c}$.

Remark. The remark prior to Theorem 6.2.4 is again relevant; an interaction Φ' can always be chosen such that $\delta_{\Phi'} = \delta\,(= \delta_\Phi)$ and the $W_{\Phi'}(\Lambda)$ are well defined. Thus Assumption (2) is partially redundant. Moreover, the results of Section 6.2.1 give various explicit conditions on Φ such that the assumptions of the theorem are valid, e.g.,

$$\|\Phi\|_\lambda = \sum_{n \geq 0} e^{\lambda n} \left(\sup_{x \in L} \sum_{\substack{X \ni x \\ |X| = n+1}} \|\Phi(X)\| \right) < +\infty$$

for some $\lambda > 0$.

Proof. We will prove (1) $\Rightarrow$ (3) $\Rightarrow$ (2) $\Rightarrow$ (1).

(1) $\Rightarrow$ (3) : If $T : \mathfrak{A} \to \mathfrak{A}$ is a positive map with the property $T(A) = A$ for $A \in \mathfrak{A}_{\Lambda^c}$ then $\omega' = \omega \circ T$ is a state in the class C_Λ^ω and hence (3) follows from (1).

(3) $\Rightarrow$ (2) : This is proved in a similar fashion to the implication (1) $\Rightarrow$ (2) of Theorem 6.2.36.

If $A = A^* \in \mathfrak{A}_\Lambda$, then condition (1) implies that

$$\omega(e^{itA}\tilde{H}_\Phi(\Lambda)e^{-itA}) \geq \omega(\tilde{H}_\Phi(\Lambda))$$

and by differentiation at $t = 0$ one deduces that

$$\omega(\delta(A)) = 0 \ .$$

Since D is a core for δ, the state ω must be τ-invariant.

Now reconsider the operator γ_B; $\mathfrak{A} \mapsto \mathfrak{A}$ introduced prior to Theorem 5.3.15,

$$\gamma_B(A) = B^*AB - \{B^*B, A\}/2 \ .$$

It follows from the argument prior to Theorem 5.3.15 that $t \mapsto T_t = \exp\{t\gamma_B\}$ is a semigroup of positive maps. Furthermore, if $B \in \mathfrak{A}_\Lambda$ then $\gamma_B(A) = 0$ for $A \in \mathfrak{A}_{\Lambda^c}$ and hence $T_t(A) = A$. Condition (3) then implies that

$$\omega(T_t(\tilde{H}_\Phi(\Lambda))) \geq \omega(\tilde{H}_\Phi(\Lambda))$$

for all $t \geq 0$. Therefore

$$\omega(\gamma_B(\tilde{H}_\Phi(\Lambda))) \geq 0 \ .$$

But the τ-invariance of ω implies, as in the proof of Theorem 6.2.36, that

$$-i\omega(B^*\delta(B)) = \omega(\gamma_B(\tilde{H}_\Phi(\Lambda)))$$

and hence

$$-i\omega(B^*\delta(B)) \geq 0 \ .$$

Since D is a core for δ, it follows that ω is a τ ground state.

(2) $\Rightarrow$ (1): As there is no analogue of the Gibbs condition for ground states this proof is quite different to the proof of the corresponding implication in Theorem 6.2.36.

We first need a result on extensions of normal states to semi-bounded selfadjoint elements affiliated with a von Neumann algebra. The following lemma is formulated for positive operators but it extends readily to semi-bounded operators.

Lemma 6.2.53. *Let $\mathfrak{M}$ be a von Neumann algebra on a Hilbert space $\mathfrak{H}$, A a positive, selfadjoint operator affiliated with $\mathfrak{M}$, ω a normal state on $\mathfrak{M}$, and $\{\xi_n\}_{n \geq 1}$ a sequence of vectors in $\mathfrak{H}$ such that*

$$\omega = \sum_{n \geq 1} \omega_{\xi_n} \ , \qquad \sum_{n \geq 1} \|\xi_n\|^2 = 1 \ .$$

The following conditions are equivalent:

(1) $\sup\{\omega(B);\ B \in \mathfrak{M}_+,\ B \leq A\} < +\infty$,

(2) $\xi_n \in D(A^{1/2})$ *for all n and*

$$\sum_{n \geq 1} \|A^{1/2}\xi_n\|^2 < +\infty \ .$$

If these conditions are fulfilled, then

$$\sup\{\omega(B);\ B \in \mathfrak{M}_+,\ B \leq A\} = \sum_{n \geq 1} \|A^{1/2}\xi_n\|^2 \ .$$

Remark. Recall from Theorem 2.4.21 that if ω is a normal state on $\mathfrak{M}$, the existence of a sequence $\{\xi_n\}_{n \geq 1}$ with the assumed properties is automatic.

PROOF. Define

$$K_1 = \sup\{\omega(B);\, B \in \mathfrak{M}_+,\ B \leq A\} \ ,$$
$$K_2 = \sum_{n \geq 1} \|A^{1/2}\xi_n\|^2,$$

whenever, the right-hand sides exist and define K_1 and K_2 to be $+\infty$ otherwise.

Let f_n be the sequence of functions over $\mathbb{R}_+$ given by

$$f_n(x) = \begin{cases} x & \text{if } 0 \leq x \leq n \ , \\ n & \text{if} \quad x > n \ , \end{cases}$$

and define A_n by $A_n = f_n(A)$.

It follows from Lemma 2.5.8 that $f_n(A) \in \mathfrak{M}$ for $n = 1, 2, \ldots$, and by spectral theory it follows that the quadratic forms defined by A_n converge monotonically to the form a defined by A, i.e., if $\xi \in \mathfrak{H}$

$$(\xi, A_n\xi) \to a(\xi) = \begin{cases} (A^{1/2}\xi, A^{1/2}\xi) & \text{if } \xi \in D(A^{1/2}) \ , \\ +\infty & \text{if } \xi \notin D(A^{1/2}) \ . \end{cases}$$

Therefore

$$\lim_{n \to \infty} \sum_{k \geq 1} (\xi_k, A_n\xi_k) = \sum_{k \geq 1} (A^{1/2}\xi_k, A^{1/2}\xi_k)$$

whenever the $\xi_k \in D(A^{1/2})$. (See the discussion of quadratic forms prior to Lemma 5.2.13.) Hence

$$K_2 \leq K_1 \ .$$

But conversely if $B \in \mathfrak{M}_+$ and $B \leq A$ in the sense of quadratic forms, then

$$\omega(B) = \sum_{k \geq 1} (\xi_k, B\xi_k) \leq \sum_{k \geq 1} a(\xi_k) = K_2 \ .$$

Hence

$$K_1 \leq K_2 \ .$$

This result indicates a canonical way of extending normal states to semi-bounded operators affiliated with a von Neumann algebra.

Definition 6.2.54. Adopt the assumption and notation of Lemma 6.2.53. The extension of the normal state ω to the semi-bounded operator A affiliated with $\mathfrak{M}$ is defined by

$$\omega(A) = \sup\{\omega(B);\, B \in \mathfrak{M}_+,\, B \leq A\} \ .$$

Hence if $\omega(A) < +\infty$ one has

$$\omega(A) = \sum_{n \geq 1} \|A^{1/2}\xi_n\|^2 \ ,$$

where $\{\xi_n\}_{n \geq 1}$ are the representatives of ω.

Next we need a result which implies that states in C_Λ^ω are quasi-equivalent.

Lemma 6.2.55. *Let $\mathfrak{A}$ be a C^*-algebra of the form*

$$\mathfrak{A} = M_n \otimes \mathfrak{A}_0 \ ,$$

where M_n is the full complex $n \times n$ matrix algebra and $\mathfrak{A}_0$ is an arbitrary C^*-algebra. Let ω_1 and ω_2 be states on $\mathfrak{A}$ such that

$$\omega_1|_{\mathfrak{A}_0} = \omega_2|_{\mathfrak{A}_0} \ .$$

It follows that ω_1 and ω_2 are quasi-equivalent.

PROOF. The proof relies upon a technique similar to that used to deduce Proposition 2.4.27.

Let $(\mathfrak{H}_i, \pi_i, \Omega_i)$ be the cyclic representations associated with $\omega_i, i = 1, 2$ and define $(\mathfrak{H}, \pi, \Omega)$ by

$$\mathfrak{H} = \mathfrak{H}_1 \oplus \mathfrak{H}_2, \quad \pi = \pi_1 \oplus \pi_2, \quad \Omega = \Omega_1 \oplus \Omega_2.$$

Assume, *ad absurdum,* that π_1 and π_2 are not quasi-equivalent. It follows readily from Theorem 2.4.26 that one of the representations, which we may take to be π_1, contains a representation which is disjoint from π_2. If P is the smallest projection in $\pi_1(\mathfrak{A})'' \cap \pi_1(\mathfrak{A})'$ containing the projection onto this subrepresentation, it follows that the projection $P \oplus 0$ on $\mathfrak{H} = \mathfrak{H}_1 \oplus \mathfrak{H}_2$ commutes with $\pi(\mathfrak{A})'$. Hence, $P \oplus 0 \in \pi(\mathfrak{A})'' \cap \pi(\mathfrak{A})'$. The von Neumann density theorem, Corollary 2.4.15, now implies that there exists a net $A_\alpha \in \mathfrak{A}$ such that

$$\pi(A_\alpha) \to P \oplus 0$$

in the strong topology. But this means that

$$\pi_1(A_\alpha) \to P, \quad \pi_2(A_\alpha) \to 0 \ ,$$

and hence

$$\omega_1(A_\alpha) \to (\Omega_1, P\Omega_1) \neq 0, \quad \omega_2(A_\alpha) \to 0 \ .$$

The inequality follows since $P \in \pi_1(\mathfrak{A})'' \cap \pi_1(\mathfrak{A})'$, $P \neq 0$, and Ω_1 is cyclic for π_1. But if $\{E_{ij}\}_{1 \leq i, j \leq n}$ are matrix units of M_n,

$$A \in \mathfrak{A} \mapsto E(A) = \sum_{i=1}^{n} E_{i1} A E_{1i}$$

defines a projection from $\mathfrak{A}$ onto $\mathfrak{A}_0 = M_n' \cup \mathfrak{A}$. (For a similar argument see the proof of Proposition 2.6.9.) As $\pi_1(A_\alpha)$ and $\pi_2(A_\alpha)$ converge to the elements P and 0 of the centers of π_1 and π_2, it follows that

$$\begin{aligned} \lim_\alpha \ \pi_i(E(A_\alpha)) &= \lim_\alpha \sum_{j=1}^{n} \pi_i(E_{j1})\pi_i(A_\alpha)\pi_i(E_{1j}) \\ &= \left(\sum_{j=1}^{n} \pi_i(E_{jj}) \right) \lim_\alpha \pi_i(A_\alpha) = \lim_\alpha \pi_i(A_\alpha) = \delta_{i1} P \ . \end{aligned}$$

But as $E(A_\alpha) \in \mathfrak{A}_0$, we have

$$\omega_1(E(A_\alpha)) = \omega_2(E(A_\alpha)) \ .$$

Taking the limit over α leads to the contradiction

$$(\Omega_1, P\Omega_1) = 0 \ .$$

Therefore π_1 and π_2 are quasi-equivalent.

End of Proof of Theorem 6.2.52. It remains to establish (2) $\Rightarrow$ (1). Assume that ω is a ground state and let ω also denote its normal extension to $\mathfrak{M}_\omega = \pi_\omega(\mathfrak{A})''$. The generator H_ω of the canonical unitary group U_ω which implements τ on $\mathfrak{H}_\omega$ and leaves Ω_ω invariant is positive and H_ω is affiliated with $\mathfrak{M}_\omega$ by Proposition 5.3.19. Now if $\psi \in D(H_\omega)$ and $A \in D(\delta)$, then $\pi_\omega(A)\psi \in D(H_\omega)$. Therefore,

$$\begin{aligned} i[H_\omega - \pi_\omega(\tilde{H}_\Phi(\Lambda)), \pi_\omega(A)]\psi &= (\pi_\omega(\delta(A)) - \pi_\omega(\delta(A)))\psi \\ &= 0 \end{aligned}$$

for $A \in \mathfrak{A}_\Lambda$ and $\psi \in D(H_\omega)$. Thus if $U_\Lambda(t) = \exp\{it(H_\omega - \pi_\omega(\tilde{H}_\Phi(\Lambda)))\}$, one has

$$\begin{aligned} &U_\Lambda(t)\pi_\omega(A)U_\Lambda(t)^{-1}\psi \\ &= \pi_\omega(A)\psi + i\int_0^t ds U_\Lambda(s)[H_\omega - \pi_\omega(\tilde{H}_\Phi(\Lambda)), \pi_\omega(A)]U_\Lambda(s)^{-1}\psi \\ &= \pi_\omega(A)\psi \end{aligned}$$

for all $A \in \mathfrak{A}_\Lambda$ and $\psi \in D(H_\omega)$. Consequently, $U_\Lambda(t) \in \pi_\omega(\mathfrak{A}_\Lambda)'$. But if follows from the Trotter product formula,

$$U_\Lambda(t) = \lim_{n \to \infty} (U_\omega(t/n)\exp\{-it\pi_\omega(\tilde{H}_\Phi(\Lambda))/n\})^n$$

that $U_\Lambda(t) \in \pi_\omega(\mathfrak{A})''$. Thus, $U_\Lambda(t) \in \pi_\omega(\mathfrak{A}_\Lambda)' \cap \pi_\omega(\mathfrak{A})''$ and $H_\omega - \pi_\omega(\tilde{H}_\Phi(\Lambda))$ is affiliated with $\pi_\omega(\mathfrak{A}_\Lambda)' \cap \pi_\omega(\mathfrak{A})''$. But Lemma 2.6.8 and the argument used in the proof of Proposition 2.6.9 imply that

$$\pi_\omega(\mathfrak{A}_\Lambda)' \cap \pi_\omega(\mathfrak{A})'' = \pi_\omega(\mathfrak{A}_{\Lambda^c})'' \ ,$$

i.e., $H_\omega - \pi_\omega(\tilde{H}_\Phi(\Lambda))$ is affiliated with $\pi_\omega(\mathfrak{A}_{\Lambda^c})''$. Now if $\omega' \in C_\Lambda^\omega$, it follows from Lemma 6.2.55 that ω' extends to a normal state of $\mathfrak{M}_\omega$ and $\omega'(H_\omega)$ may be defined. But

$$\omega|_{\pi_\omega(\mathfrak{A}_{\Lambda^c})''} = \omega'|_{\pi_\omega(\mathfrak{A}_{\Lambda^c})''}$$

by continuity and hence

$$\omega(H_\omega - \tilde{H}_\Phi(\Lambda)) = \omega'(H_\omega - \tilde{H}_\Phi(\Lambda)) \qquad (^*)$$

by the monotonic definition of ω on $H_\omega - \pi_\omega(\tilde{H}_\Phi(\Lambda))$. Thus,

$$\omega'(H_\omega - \tilde{H}_\Phi(\Lambda)) = -\omega(\tilde{H}_\Phi(\Lambda)) < +\infty \ .$$

Consequently, the second characterization of $\omega'(H_\omega)$ provided by Lemma 6.2.53 implies that

$$\omega'(\tilde{H}_\Phi(\Lambda)) = \omega'(H_\omega) - \omega'(H_\omega - \tilde{H}_\Phi(\Lambda)) \ .$$

Finally the positivity of H_ω yields

$$0 = \omega(H_\omega) = \inf_{\omega' \in C_\Lambda^\omega} \omega'(H_\omega) \ . \qquad (^{**})$$

Hence, by combination of (*) and (**) one obtains

$$\begin{aligned}\omega(\tilde{H}_\Phi(\Lambda)) &= \omega(H_\omega) - \omega(H_\omega - \tilde{H}_\Phi(\Lambda)) \\ &= \inf_{\omega' \in C_\Lambda^\omega} \{\omega'(H_\omega) - \omega'(H_\omega - \tilde{H}_\Phi(\Lambda))\} = \inf_{\omega' \in C_\Lambda^\omega} \omega'(\tilde{H}_\Phi(\Lambda)) \cdot\end{aligned}$$

EXAMPLE 6.2.56. Let us consider the application of Theorem 6.2.52 to the one-dimensional model with nearest-neighbor ferromagnetic Ising interaction, i.e., an interaction which energetically favours the alignment of spins.

Since the interaction is classical, it can be argued that a state is a ground state if and only if its restriction to the classical subalgebra is a ground state in the classical sense (see Notes and Remarks). It is also evident that these states are characterized by verifying condition (1) of Theorem 6.2.52 for intervals $\Lambda = [a, b] \subset \mathbb{Z}$. But since the only interaction is between nearest neighbors the values of $\omega'(\tilde{H}_\Phi([a, b]))$ for a given state ω' on the classical algebra are governed by the orientations of the spins at the sites $\{a-1, a, a+1, \ldots, b-1, b, b+1\}$, i.e., the only spins external to $[a, b]$ which enter into the minimization problem are those at the neighboring sites a – 1 and b + 1. Now there are two cases to consider, zero external magnetic field and nonzero magnetic field.

First, assume there is a nonzero external field, then the energy contribution of the field is minimized by aligning the spins with the field. Thus, for b – a sufficiently large, $\omega'(\tilde{H}_\Phi([a, b]))$ is minimized by aligning all the spins, at the sites $\{a, a+1, \ldots, b-1, b\}$, with the field. Consequently, there is a unique ground state. This state has all the spins parallel to the external field and consequently is translationally invariant.

Second, consider the case of zero magnetic field. Now the effects of the external spins a – 1 and b + 1 are of greater importance in the minimization problem. There are two basic possibilities:

(1) the spins at $a-1$ and $b+1$ are parallel and $\omega'(\tilde{H}_\Phi([a, b]))$ is minimized by arranging all the spins in $[a-1, b+1]$ to have the same orientation;
(2) the spins at $a-1$ and $b+1$ have opposite orientation and $\omega'(\tilde{H}_\Phi([a, b]))$ is minimized by arranging all spins in $[a-1, x]$ and all spins in $[x+1, b+1]$ to be parallel for any $x \in [a, b]$, i.e., only the pair of spins at the neighboring sites x and $x+1$ are anti-parallel.

Thus the external ground states on the classical algebra now fall into two classes:

(1) One class consists of two translationally invariant states with all spins parallel, either positively or negatively oriented.
(2) The second class consists of an infinite number of states in which the translation symmetry is broken. Each state has the spins to the left of a given site with one orientation and the spins to the right with the opposite orientation.

The translationally invariant states describe the two possible modes of spontaneous magnetization. The nontranslationally invariant states illustrate a form of phase separation; one side of the system has a positive spontaneous magnetization whilst the second has a negative magnetization.

Some properties of these states were discussed at the beginning of the section.

The Ising model without external field is equivalent to a special case of the X–Y model discussed in Examples 6.2.14A and 6.2.14B. Recall that the local X–Y Hamiltonian is given by

$$H_\Phi([-n,n]) = -J\left\{\sum_{x=-n}^{n-1}((1+\gamma)\sigma_1^x\sigma_1^{x+1} + (1-\gamma)\sigma_2^x\sigma_2^{x+1}) + 2\lambda\sum_{x=-n}^{n}\sigma_3^x\right\}$$

and the Ising model corresponds to $|\gamma| = 1$ and $\lambda = 0$. Due to the genuine quantum nature of the X–Y model one would expect the multiplicity of the ground states to be smaller than for the Ising model and this is indeed the case. The number of irreducible ground state representations, up to unitary equivalence, is as follows.

(α) 1 if $|\lambda| \geq 1$, or if $\gamma = 0, |\lambda| < 1$.

In this case there is a unique ground state which is then automatically translation invariant. If $|\lambda| \geq 1$ the external field is dominant and it forces the spins to align along the third axis. If $\gamma = 0$ rotation around the third axis is a symmetry for the system and this symmetry is not broken by the ground state.

(β) 2 if $|\lambda| < 1, \gamma \neq 0$, and $(\lambda, \gamma) \neq (0, \pm 1)$.

In this case the external field is weak and rotation around the third axis is no longer a symmetry. The reflection $\sigma_1^x \to -\sigma_1^x, \sigma_2^x \to -\sigma_2^x, \sigma_3^x \to \sigma_3^x$, i.e., rotation by π around the third axis, is, however, still a symmetry. (This is the automorphism $\Theta(1,0)$ of Example 6.2.14A.) There are only two extremal ground states in this case and they are transformed into each other by the symmetry.

(γ) 4 if $(\lambda, \gamma) = (0, \pm 1)$.

This is the Ising model without external field discussed above. Two of the four representations correspond to the two translationally invariant ground states in class (1) above whilst the other two correspond to the two classes of non-translationally invariant states in class (2). Each of the extremal ground states in each of the two latter classes can be obtained from one of the others by translation composed with certain inner automorphisms defined by a local unitary. Since the state and the transformed state only differ at a finite number of sites the associated representations are unitarily equivalent.

If φ is an extremal ground state for the X–Y model, define locally perturbed states by

$$\varphi_B(A) = \varphi(B^*AB)/\varphi(B^*B)$$

for all $A, B \in \mathfrak{A}^P$ with $\varphi(B^*B) > 0$. Then the state has the return to equilibrium property,

$$\lim_{t\to\infty} \varphi_B(\tau_t(A)) = \varphi(A)$$

for all $A, B \in \mathfrak{A}^P$, if and only if the parameters (γ, λ) are in the region in which the ground state is unique, i.e., if and only if (α) is satisfied.

Recall that all these one-dimensional models with short range interaction have a unique (τ, β)-KMS state for finite β by Theorem 6.2.47. Using the twisted asymptotic abelianness property described in Example 6.2.14B, which is valid in cases (α) and (β), together with extremality one can establish that all these finite temperature states have the property of return to equilibrium.

We conclude with a discussion of $\mathbb{Z}^\nu$-invariant interactions and $\mathbb{Z}^\nu$-invariant ground states. Our aim is to characterize the latter by a minimum energy per

unit volume criterion, i.e., to derive an analogue of the equivalence (1) $\Leftrightarrow$ (3) in Theorem 6.2.42.

First, recall that the mean energy H_Φ of each $\mathbb{Z}^\nu$-invariant interaction Φ was defined as an affine, weak*-continuous functional over the $\mathbb{Z}^\nu$-invariant states $E_{\mathfrak{A}}^{\mathbb{Z}^\nu}$, in Proposition 6.2.39, under the mild assumption that

$$\|\Phi\| = \sum_{X \ni 0} \frac{\|\Phi(X)\|}{|X|} < +\infty \ .$$

One has

$$H_\Phi(\omega) = \sum_{X \ni 0} \frac{\omega(\Phi(X))}{|X|} \ ,$$

and hence $|H_\Phi(\omega)| \leq \|\Phi\|$ for all $\omega \in E_{\mathfrak{A}}^{\mathbb{Z}^\nu}$. Let $\mathfrak{B}$ again denote the Banach space of $\mathbb{Z}^\nu$-invariant interactions equipped with the foregoing norm and define the functional $\Phi \in \mathfrak{B} \mapsto H(\Phi) \in [-\|\Phi\|, \|\Phi\|]$ by

$$H(\Phi) = \inf_{\omega \in E_{\mathfrak{A}}^{\mathbb{Z}^\nu}} H_\Phi(\omega) \ .$$

It follows immediately that $\Phi \in \mathfrak{B} \mapsto H(\Phi)$ is concave. But

$$\begin{aligned} H(\Phi) &= \inf_{\omega \in E_{\mathfrak{A}}^{\mathbb{Z}^\nu}} \{H_\Psi(\omega) + H_{\Phi-\Psi}(\omega)\} \\ &\leq \inf_{\omega \in E_{\mathfrak{A}}^{\mathbb{Z}^\nu}} \{H_\Psi(\omega) + \|\Phi - \Psi\|\} = H(\Psi) + \|\Phi - \Psi\| \ . \end{aligned}$$

Hence, by interchange of Φ and Ψ one obtains

$$|H(\Phi) - H(\Psi)| \leq \|\Phi - \Psi\| \ ,$$

and in particular H is continuous. The energy function $-H$ is the zero-temperature analogue of the thermodynamic free energy discussed in Theorem 6.2.40. This is made more precise by the following proposition which is not essential for the sequel.

Proposition 6.2.57. *Let $\mathfrak{B}$ denote the Banach space of $\mathbb{Z}^\nu$-invariant interactions with norm*

$$\|\Phi\| = \sum_{X \ni 0} \frac{\|\Phi(X)\|}{|X|} < +\infty \ .$$

Let $\Phi \mapsto F(\Phi)$ denote the thermodynamic free energy

$$F(\Phi) = \lim_{\Lambda \rightsquigarrow \infty} |\Lambda|^{-1} \log \operatorname{Tr}_{\mathfrak{H}_\Lambda}(e^{-H_\Phi(\Lambda)})$$

and $\Phi \mapsto H(\Phi)$ the mean energy

$$H(\Phi) = \inf_{\omega \in E_{\mathfrak{A}}^{\mathbb{Z}^\nu}} \sum_{X \ni 0} \frac{\omega(\Phi(X))}{|X|} \ .$$

It follows that

$$H(\Phi) = \lim_{\beta \to \infty} (-\beta^{-1} F(\beta\Phi))$$

for all $\Phi \in B$.

PROOF. From Theorem 6.2.40

$$F(\beta\Phi) = \sup_{\omega \in E_{\mathfrak{A}}^{\mathbb{Z}^\nu}} \{S(\omega) - \beta H_\Phi(\omega)\} .$$

Now for each $\beta > 0$, choose an ω_β such that the supremum is attained. This is possible because $S - \beta H_\Phi$ is upper semi-continuous. Now choose a sequence β_n such that $-\beta_n^{-1} F(\beta_n \Phi)$ converges and a subsequence n' such that $\omega_{\beta_{n'}}$ converges in the weak* topology to a state ω.

By continuity of H_Φ one has

$$\lim_{n' \to \infty} H_\Phi(\omega_{\beta_{n'}}) = H_\Phi(\omega) .$$

But

$$|-\beta_{n'}^{-1} F(\beta_{n'}\Phi) - H_\Phi(\omega_{\beta_{n'}})| = \beta_{n'}^{-1} S(\omega_{\beta_{n'}}) \leq \beta_{n'}^{-1} \log(N+1) ,$$

and hence

$$\lim_{n \to \infty} -\beta_n^{-1} F(\beta_n \Phi) = H_\Phi(\omega) .$$

But as the mean entropy S is positive

$$-\beta^{-1} F(\beta\Phi) \leq H_\Phi(\omega')$$

for all $\omega' \in E_{\mathfrak{A}}^{\mathbb{Z}^\nu}$. This implies that

$$\lim_{n \to \infty} -\beta_n^{-1} F(\beta_n \Phi) = \inf_{\omega \in E_{\mathfrak{A}}^{\mathbb{Z}^\nu}} H_\Phi(\omega) = H(\Phi) .$$

Thus, all limit points of $-\beta^{-1} F(\beta\Phi)$ are equal to $H(\Phi)$ as $\beta \to \infty$. Hence the limit exists and is equal to $H(\Phi)$.

The zero-temperature analogue of Theorem 6.2.42 is derived by the same arguments used to prove (3) $\Rightarrow$ (1) in this theorem coupled with the previous stability result, Theorem 6.2.52.

Theorem 6.2.58. *Let* Φ *be a* $\mathbb{Z}^\nu$*-invariant interaction such that*

$$\|\Phi\|_\lambda = \sum_{X \ni 0} \|\Phi(X)\| e^{\lambda |X|} < +\infty$$

for some $\lambda > 0$ *and let* τ^Φ *denote the associated dynamical group.*

If ω *is a* $\mathbb{Z}^\nu$*-invariant state the following are equivalent:*

(1) ω *is a* τ^Φ *ground state.*
(2) ω *minimizes* H_Φ.

PROOF. (1) $\Rightarrow$ (2): Let ω be a $\mathbb{Z}^\nu$-invariant τ^Φ ground state. Theorem 6.2.52 implies that

$$\omega(\tilde{H}_\Phi(\Lambda)) \leq \omega'(\tilde{H}_\Phi(\Lambda))$$

for all $\omega' \in C_\Lambda^\omega$. Now let $\sigma \in E_{\mathfrak{A}}^{\mathbb{Z}^\nu}$ and define ω' by

$$\omega' = \sigma|_{\mathfrak{A}_\Lambda} \otimes \omega|_{\mathfrak{A}_{\Lambda^c}} .$$

Thus, $\omega' \in C_\Lambda^\omega$ and

$$\omega(\tilde{H}_\Phi(\Lambda)) \leq \omega'(\tilde{H}_\Phi(\Lambda)) .$$

But as $\tilde{H}_\Phi(\Lambda) = H_\Phi(\Lambda) + W_\Phi(\Lambda)$ and $\sigma(H_\Phi(\Lambda)) = \omega'(H_\Phi(\Lambda))$, this gives

$$\begin{aligned}\omega(H_\Phi(\Lambda)) &\leq \sigma(H_\Phi(\Lambda)) + \omega'(W_\Phi(\Lambda)) - \omega(W_\Phi(\Lambda)) \\ &\leq \sigma(H_\Phi(\Lambda)) + 2\|W_\Phi(\Lambda)\| .\end{aligned}$$

Now we already observed in the proof of Theorem 6.2.42 that $\|W_\Phi(\Lambda)\|/|\Lambda| \to 0$ as $\Lambda \rightsquigarrow \infty$. Hence, dividing both sides of the last relation by $|\Lambda|$ and taking the limit $\Lambda \rightsquigarrow \infty$ yields

$$H_\Phi(\omega) \leq H_\Phi(\sigma) .$$

Thus

$$H_\Phi(\omega) = \inf_{\sigma \in E_{\mathfrak{A}}^{\mathbb{Z}^\nu}} H_\Phi(\sigma) = H(\Phi) .$$

(2) $\Rightarrow$ (1): The proof of this implication is a repetition of the convexity argument used to prove (3) $\Rightarrow$ (1) in Theorem 6.2.42. One simply replaces the free energy $F(\Phi)$ by the mean energy $-H(\Phi)$.

The foregoing theorems give general characterizations of ground states and invariant ground states but in particular models one can give a much more detailed and precise description. In Example 6.2.56 we described all ground states of the one-dimensional ferromagnetic Ising and X–Y models and we end this discussion of spin systems with some comments on the translationally invariant ground states of the one-dimensional ferromagnetic Heisenberg model. If there is a nonzero external magnetic field, it follows from Theorem 6.2.52, by the argument used for the Ising model in Example 6.2.56, that there is a unique ground state and this state is translationally invariant. If, on the other hand, there is no external field, then there exists a continuum of invariant ground states. Each of these states is a product state in which all the spins are parallel but there is a continuum of possible orientations. Let us briefly describe one of these states and the corresponding dynamics.

We consider the state ω determined by the configuration in which all spins are down and we begin by describing the associated representation $(\mathfrak{H}_\omega, \pi_\omega, \Omega_\omega)$ but, for notational simplicity, we drop the symbol π_ω, i.e., we identify $\pi_\omega(A)$ and A. Since all spins are down the cyclic vector Ω_ω is a simultaneous eigenfunction of all the σ_3^x, $x \in \mathbb{Z}$, with eigenvalue -1. Next reintroduce the spin raising and lowering operators $\sigma_\pm^x = (\sigma_1^x \pm \sigma_2^x)/2$ of Example 6.2.13. One has

$$[\sigma_\pm^x, \sigma_3^x] = \mp 2\sigma_\pm^x, \qquad [\sigma_+^x, \sigma_-^x] = \sigma_3^x$$

and the σ corresponding to different $x, y \in \mathbb{Z}$ mutually commute. It follows readily that $\sigma_-^x \Omega_\omega = 0$, for all $z \in \mathbb{Z}$, and the vectors $|X\rangle$ defined by $|\emptyset\rangle = \Omega_\omega$ and

$$|X\rangle = \left(\prod_{x \in X} \sigma_+^x\right)|\varnothing\rangle$$

form an orthonormal basis of $\mathfrak{H}_\omega$. This basis was used earlier in the proof of Theorem 6.2.48. Thus if $\mathfrak{H}_\omega^{(n)}$ denotes the subspace spanned by the vectors $\{|X\rangle; X \subset \mathbb{Z}, |X| = n\}$ one has

$$\mathfrak{H}_\omega = \bigoplus_{n \geq 0} \mathfrak{H}_\omega^{(n)} .$$

The vector Ω_ω describes the configuration with all spins down and the vectors in $\mathfrak{H}_\omega^{(n)}$ correspond to configurations in which exactly n spins are up. Note that the representation $(\mathfrak{H}_\omega, \pi_\omega, \Omega_\omega)$ is analogous to the Fock representation of the CCR and CAR algebras described in Chapter 5 with the spin raising and lowering operators replacing the particle creation and annihilation operators, the n-spin subspaces $\mathfrak{H}_\omega^{(n)}$ replacing the n-particle subspaces, and the raised spins analogous to the particles. Analysis of the Heisenberg dynamics exploits this analogy and interprets the raised spins as some form of quasi-particle. These quasi-particles are usually referred to as *spin waves* or *spin excitations*.

The dynamical group τ corresponding to the Heisenberg dynamics is represented on $\mathfrak{H}_\omega$ by

$$A \mapsto \tau_t(A) = e^{itH_\omega} A e^{-itH_\omega} ,$$

where the selfadjoint Hamiltonian H_ω is defined as the direct sum

$$H_\omega = \bigoplus_{n \geq 0} H_\omega^{(n)}$$

of bounded selfadjoint Hamiltonians $H_\omega^{(n)}$ whose action on $\mathfrak{H}_\omega^{(n)}$ is given by

$$H_\omega^{(n)}|X\rangle = -J \sum_{x \in \mathbb{Z}} (\sigma^x \cdot \sigma^{x+1} - \mathbb{1})|X\rangle .$$

(The infinite sum causes no difficulty since the σ at different points commute and $(\sigma^x \cdot \sigma^{x+1} - \mathbb{1})|\varnothing\rangle = 0$. Moreover, $H_\omega^{(n)} \geq 0$ for $J \geq 0$ because $\mathbb{1} - \sigma^x \cdot \sigma^{x+1}$ has eigenvalues 0 and 4.) The action of $H_\omega^{(1)}$ is particularly simple. One has

$$\begin{aligned} H_\omega^{(1)}|x\rangle &= [H_\omega^{(1)}, \sigma_+^x]\,|\varnothing\rangle \\ &= -2J(\sigma_+^{x+1} - 2\sigma_+^x + \sigma_+^{x-1})|\varnothing\rangle \\ &= -2J(|x+1\rangle - 2|x\rangle + |x-1\rangle) , \end{aligned}$$

i.e., $H_\omega^{(1)}$ acts like a multiple of a double difference operator. Hence, the evolution of the one spin vectors, i.e., the elements of $\mathfrak{H}_\omega^{(1)}$, is a lattice analogue of the free evolution of point particles discussed on Fock space in Chapter 5. In particular if $f \in \ell^2(\mathbb{Z})$ and

$$\sigma_+(f) = \sum_{x \in \mathbb{Z}} f(x)\sigma_+^x ,$$

one calculates by Fourier transformation that

$$e^{itH_\omega}\sigma_+(f)|\varnothing\rangle = e^{itH_\omega^{(1)}}\sigma_+(f)|\varnothing\rangle = \sigma_+(f_t)|\varnothing\rangle$$

where

$$f_t(x) = \sum_{y\in\mathbb{Z}} G_t(x-y)f(y)$$

and

$$G_t(x) = \frac{1}{2\pi}\int_0^{2\pi} d\theta\, e^{4itJ(1-\cos\theta)}e^{i\theta x} .$$

Thus the one-spin evolution is a free motion with lattice momentum $\theta \in [0, 2\pi]$ and a corresponding energy $4J(1-\cos\theta)$. Comparison with Example 6.2.14 shows that this is essentially the evolution of the X–Y model with an additional energy $4J$ contributed by the Ising interaction. The evolution of the multispin states is more complex but can be thought of as a free evolution stemming from the X–Y contribution to the Hamiltonian together with a spin interaction arising from the Ising contribution. Adopting this point of view one defines a free multispin evolution $t \in \mathbb{R} \mapsto U_t^0$ by setting

$$U_t^0\sigma_+(f^{(1)})\cdots\sigma_+(f^{(n)})|\varnothing\rangle = \sigma_+(f_t^{(1)})\cdots\sigma_+(f_t^{(n)})|\varnothing\rangle ,$$

where $t \mapsto f_t^{(i)}$ is the one-spin evolution introduced above and U_t^0 is extended by linearity. One then exploits scattering theory methods to obtain properties of the Heisenberg evolution $U_t = \exp\{itH_\omega\}$ by reference to the free evolution U_t^0. Both groups describe the total evolution of complexes of spin excitations together with the relative motion of these excitations. The Ising contribution to H_ω appears as an interaction between the various excitations. This interaction leads to a variety of phenomena, binding of two or more spin excitations, scattering of bound or unbound complexes, etc. We will not enter into more details of the mathematical description of these problems but remark that the physical picture of spin excitations, or spin waves, has been fruitful both conceptually and analytically. For example, the realization that H_ω describes an overall free motion of a system of interacting spin waves indicates that H_ω has absolutely continuous spectrum, on the orthogonal complement of Ω_ω. This has indeed been verified (see Notes and Remarks) and consequently

$$\lim_{|t|\to\infty}(\psi, e^{itH_\omega}\varphi) = (\varphi, \Omega_\omega)(\Omega_\omega, \varphi)$$

for all $\varphi, \psi \in \mathfrak{H}_\omega$. Alternatively stated,

$$\lim_{|t|\to\infty}\omega(A\tau_t(B)) = \omega(A)\omega(B)$$

for all A and B in the spin algebra, i.e., the ground state ω is strongly mixing in the sense of Chapter 4.

Despite a great deal of analysis of the translationally invariant ground states of the Heisenberg model, little attention has apparently been paid to the examination of nontranslationally invariant states and even a proof of existence

or absence of such states appears to be lacking. If one considers the state ω determined by the configuration in which all spins to the left of $0 \in \mathbb{Z}$ are down and the 0 spin and all spins to the right of 0 are up, then this state is not a ground state of the Heisenberg dynamics but is a ground state for the dynamics obtained by removing the interaction between the 0th spin and the 1st spin. Since this interaction is given by a bounded element of the spin algebra, one can use the perturbation techniques developed in Chapter 5, e.g., Corollary 5.4.2, to deduce that the full Heisenberg dynamics is covariantly implemented in the representation $(\mathfrak{H}_\omega, \pi_\omega, \Omega_\omega)$, i.e., there is a selfadjoint operator H_ω such that

$$\pi_\omega(\tau_t(A)) = e^{itH_\omega}\pi_\omega(A)e^{-itH_\omega} ,$$

where τ denotes the Heisenberg group. Since H_ω is constructed as a bounded perturbation of the positive ground-state Hamiltonian of the decoupled systems one deduces that H_ω is lower semi-bounded. In fact H_ω may be explicitly computed. The state ω has the form $\otimes_{x \in Z}\varphi_x$ where $\varphi_x = \varphi_-$ for $x < 0$ and $\varphi_x = \varphi_+$ for $x \geq 0$. The corresponding representation space is the incomplete tensor product

$$\mathfrak{H}_\omega = \otimes_{x \in Z}(\mathbb{C}^2, \Omega_x) .$$

Now the nearest neighbor operator $\mathbb{1} - \sigma^x \cdot \sigma^{x+1}$ has eigenvalues 0 and 4 on $\mathbb{C}^2 \otimes \mathbb{C}^2$ and the operator is in fact $4P_-$ where P_- is the orthogonal projection onto the antisymmetric subspace of $\mathbb{C}^2 \otimes \mathbb{C}^2$. Thus the formal Hamiltonian, i.e., the sum of the translates of the $\mathbb{1} - \sigma^x.\sigma^{x+1}$, converges on the set of vectors differing from the reference vector $\otimes_x \Omega_x$ at only a finite number of sites. (On the reference vector itself, except at the kink $x = 0, -1$, one obtains zero.) This space is a core for H_ω. Thus H_ω expressed in this form is positive. But H_ω does not have zero as an eigenvalue because the corresponding vector would have to minimize each single term of the interaction and thus be permutation invariant. But zero is the infimum of the spectrum of H_ω. To deduce this consider product vectors coinciding with Ω_- on the left of a finite set of N consecutive points, with Ω_+ to the right of the set and rotating through an angle π/N between neighboring points of the set. The contribution to the energy of two neighboring points is proportional to $\sin^2(\pi/N)$. Hence the total energy is proportional to $N \sin^2(\pi/N)$ which tends to zero as $N \to \infty$. This argument indicates that there may not be any non-translationally invariant ground states for the one-dimensional Heisenberg ferromagnet.

6.3. Continuous Quantum Systems. II

Quantum spin systems give a relatively simple explanation of the most important magnetic phenomena. In Section 6.2.2 we demonstrated that the Ising model exhibits ferromagnetic behavior if the interparticle forces favor spin alignment and antiferromagnetic behavior if it is energetically more favorable to have anti-parallel neighboring spins. If one reinterprets this model in the lattice gas language described at the beginning of Section 6.2.1, one obtains a rudimentary description of liquid-gas and solid-liquid phase transitions. In this language a positively oriented spin corresponds to a lattice point occupied by a particle and a negatively oriented spin corresponds to an unoccupied site. Thus, the ferromagnetic phenomenon, the favoring of large blocks of parallel spins, can be interpreted as the formation of large blocks of occupied sites, "liquid droplets," interspersed between large blocks of empty sites, "gaseous regions." On the other hand, anti-ferromagnetism corresponds to the formation of a periodic structure in which one sublattice is occupied by particles and the other sublattice is empty. Thus, one obtains a primitive version of crystalline structure. Note that the ferromagnetic case corresponds to an attractive interaction between neighboring particles while the anti-ferromagnetic case corresponds to repulsive forces.

It is widely believed that a more realistic and detailed description of the solid-liquid-gas transitions should be obtainable from analysis of continuous models with interparticle interactions which are partly attractive and partly repulsive. Unfortunately, there are few rigorous results to substantiate this belief. Typical interatomic, or intermolecular, forces are attractive at large distances and repulsive at short distances. Thus, it is plausible to suppose that at low densities, for which the interparticle spacing is on average large, the attractive forces would give rise to the formation of liquid droplets in the manner observed for the lattice gas. Alternatively, at high densities for which the interparticle spacing is small one could well expect the interparticle repulsion to force the formation of a periodic, or crystalline, structure. Unfortunately, one is far from a quantitative justification of these simple qualitative ideas. In fact, the only transition phenomenon which has been rigorously derived for nonrelativistic continuous particle systems of the type we consider is the Bose-Einstein condensation of the noninteracting Bose gas. This was described in detail in Chapter 5, Section 5. It is an effect of quantum statistics and not of particle interaction. It is believed that this type of con-

densation will still prevail in interacting systems and that it is directly related to another important physical effect, superfluidity. Unfortunately even the existence of Bose–Einstein condensation in interacting systems has resisted proof. Thus, the rigorous theory of equilibrium states of continuous systems is much less complete than the corresponding theory for spin systems. Nevertheless, some results are known about existence of equilibrium states at high temperatures and low densities. The purpose of this section is to partially review these results and some of the new methods which have been used to obtain them.

In Section 5.2 we studied the equilibrium states of quantum systems of noninteracting point particles in $\mathbb{R}^\nu$. The description of the Fermi gas was particularly simple because the time development is given by a strongly continuous one-parameter group of *-automorphisms τ of the CAR algebra and the Gibbs equilibrium states coincide with the (τ, β)-KMS states where $\beta \in \mathbb{R} \cup \{\pm\infty\}$ is the inverse temperature. These states are readily computable, see Examples 5.3.2 and 5.3.20, and one finds that there is a unique equilibrium state for each β. The situation for the noninteracting Bose gas was much more complex because the time development is given by a discontinuous group of *-automorphisms τ of the CCR algebra. To make global statements about the set of equilibrium states (see Example 5.3.2), it was necessary to impose some extra continuity conditions. Within this framework, however, the equilibrium states once more correspond to the (τ, β)-KMS states. Moreover, no KMS state occurs for $\beta < 0$, there is a unique KMS state for $\beta = 0$, and nonuniqueness arises if $\beta > 0$. This nonuniqueness corresponds to the Bose–Einstein condensation.

The situation for interacting quantum systems is certainly much more complex. First, no global statement of the time development as a group of *-automorphisms of an appropriate C^*-algebra has been obtained and, second, there are plausible physical reasons for believing that such a development, if it existed, would be discontinuous in the norm topology. The problem is that a norm-continuous time development would imply that every state of the system evolves continuously throughout time. Nevertheless, one can easily envisage states for which discontinuous phenomena occur after a finite time, e.g., states for which an arbitrarily large local density or an arbitrarily large local accumulation of energy occurs. Thus, in this respect the noninteracting Fermi gas appears to be atypical.

These problems with the time development can be partially circumvented by using the thermodynamic limit procedures employed in Theorems 5.2.24 and 5.2.32 and the associated remarks. The idea is to examine the limits of the finite-volume Gibbs states and the associated time-dependent Green's functions. If ω_Λ denotes the Gibbs state of a noninteracting gas in the bounded set Λ, ω an infinite-volume limit, τ^Λ the local time development, and τ the corresponding thermodynamic limit, then we established that the Green's functions

$$\omega(A_0 \tau_{t_1}(A_1) \cdots \tau_{t_n}(A_n)) = \lim_{\Lambda \to \infty} \omega_\Lambda(A_0 \tau^\Lambda_{t_1}(A_1) \cdots \tau^\Lambda_{t_n}(A_n))$$

exist for all $A_0, \ldots, A_n \in \mathfrak{A}$ and $t_1, \ldots, t_n \in \mathbb{R}$. Now if one considers interacting particles, then it is possible to examine the thermodynamic Green's functions and to obtain some information about equilibrium phenomena and the time development of states near equilibrium. We will discuss these questions in more detail in Section 6.3.3. Prior to this however we discuss the general definition of the interacting system and its equilibrium states. We also introduce and analyze various functional integration techniques which are of great use for the analysis of these states.

6.3.1. The Local Hamiltonians

We first discuss the existence of dynamics and the Gibbs equilibrium states for systems of interacting particles confined to a bounded open subset Λ of the configuration space $\mathbb{R}^\nu$. Since the discussions of the Fermi gas and the Bose gas are very similar, we treat the two cases simultaneously. For simplicity we consider identical spinless particles although there is no difficulty in principle in considering several species of particle or particles with spin but with spin-independent interactions.

Let $L^2(\Lambda)^n_\pm$ denote the subspaces of $L^2(\Lambda^n)$ formed by the totally symmetric (plus sign) and totally anti-symmetric (minus sign) functions of n variables $x \in \Lambda$. These Hilbert spaces describe the quantum states of n point particles obeying Bose statistics (plus sign) or Fermi statistics (minus sign). The associated Fock spaces

$$\mathfrak{F}_\pm(\Lambda) = \bigoplus_{n \geq 0} L^2(\Lambda)^n_\pm$$

describe the states of an arbitrary number of particles (for more details see Section 5.2.1 and in particular Example 5.2.1). Next let $\mathfrak{A}_\pm(\Lambda)$ denote the CCR algebra (plus sign) and the CAR algebra (minus sign) over the one-particle space $L^2(\Lambda)$. The action of these algebras on $\mathfrak{F}_\pm(\Lambda)$ is described and discussed in Section 5.2.

The time evolution τ^Λ of a system of noninteracting particles is a one-parameter group of *-automorphisms of $\mathfrak{A}_\pm(\Lambda)$ implemented by a unitary group

$$t \mapsto \exp\{itd\Gamma(T^{(1)}_\Lambda)\} ,$$

where $T^{(1)}_\Lambda$ is a selfadjoint extension of the Laplacian $-\nabla^2$ on $C^\infty_0(\Lambda)$. One can consider a wide variety of $T^{(1)}_\Lambda$ corresponding to different boundary conditions, i.e., corresponding to different dynamical behavior of the particles at the boundary $\partial\Lambda$ of Λ, but for simplicity we restrict our attention to the classical boundary conditions described in Example 5.2.26. In particular we now use $T^{(1)}_{\sigma,\Lambda}$ to denote the selfadjoint extension of $-\nabla^2$ corresponding to the conditions $\partial\psi/\partial n = \sigma\psi$ where $\sigma \in C^1(\partial\Lambda)$ and we assume that the boundary $\partial\Lambda$ of Λ is piecewise differentiable. Moreover, we also assume that σ is non-negative and

this ensures that $T^{(1)}_{\sigma,\Lambda} \geq 0$. This last result is an easy consequence of the quadratic form characterization of $T^{(1)}_{\sigma,\Lambda}$ given in Example 5.2.26, i.e., for $\psi \in D(T^{(1)}_{\sigma,\Lambda})$

$$\begin{aligned}(\psi, T^{(1)}_{\sigma,\Lambda}\psi) &= \int_\Lambda dx|\nabla\psi(x)|^2 + \int_{\partial\Lambda} dx\,\sigma(x)|\psi(x)|^2 \\ &\geq 0\ .\end{aligned}$$

Finally, we let $T^{(1)}_{\infty,\Lambda}$ denote the selfadjoint extension of $-\nabla^2$ corresponding to the Dirichlet boundary condition $\psi = 0$ on $\partial\Lambda$. For this latter extension it is not necessary to assume smoothness of $\partial\Lambda$.

Next define, $T_{\sigma,\Lambda}$ by

$$T_{\sigma,\Lambda} = d\Gamma(T^{(1)}_{\sigma,\Lambda})$$

and let

$$T_{\sigma,\Lambda} = \bigoplus_{n\geq 0} T^{(n)}_{\sigma,\Lambda}$$

be the decomposition of $T_{\sigma,\Lambda}$ corresponding to the direct sum decomposition of $\mathfrak{F}_\pm(\Lambda)$ into the n-particle subspaces $L^2(\Lambda)^n_\pm$, i.e., $T^{(n)}_{\sigma,\Lambda}$ is the restriction of $T_{\sigma,\Lambda}$ to $L^2(\Lambda)^n_\pm$. Alternatively stated, $T^{(n)}_{\sigma,\Lambda}$ is the restriction to $L^2(\Lambda)^n_\pm$ of the closure of the operator.

$$(T^{(1)}_{\sigma,\Lambda} \otimes \mathbb{1} \otimes \cdots \otimes \mathbb{1}) + (\mathbb{1} \otimes T^{(1)}_{\sigma,\Lambda} \otimes \cdots \otimes \mathbb{1}) + \cdots + (\mathbb{1} \otimes \mathbb{1} \otimes \cdots \otimes T^{(1)}_{\sigma,\Lambda})$$

acting on $L^2(\Lambda)^n$. Thus, $T^{(n)}_{\sigma,\Lambda}$ is the non-negative selfadjoint operator associated with the positive closed quadratic form defined by

$$t^{(n)}_{\sigma,\Lambda} = t^{(n)}_{0,\Lambda} + s^{(n)}_{\sigma,\Lambda}\ ,$$

where

$$t^{(n)}_{0,\Lambda}(\psi) = \int_{\Lambda^n} dx_1 \ldots dx_n \sum_{i=1}^n |(\nabla_{x_i}\psi)(x_1,\ldots,x_n)|^2\ ,$$

$$s^{(n)}_{\sigma,\Lambda}(\psi) = \sum_{i=1}^n \int_\Lambda dx_1 \ldots \int_{\partial\Lambda} dx_i \ldots \int_\Lambda dx_n\, \sigma(x_i)|\psi(x_1,\ldots,x_n)|^2\ ,$$

and $D(t^{(n)}_{\sigma,\Lambda})$ consists of the $\psi \in L^2(\Lambda)^n_\pm$ for which each derivative lies in $L^2(\Lambda)^n_\pm$. The fact that $t^{(n)}_{\sigma,\Lambda}$ is a positive form is evident from the assumption $\sigma \geq 0$ but it requires some work to prove that it is closed. In the case $n = 1$, this is a standard result of partial differential equations that we already mentioned in Example 5.2.26. The argument for general n is very similar and we omit the details.

Next, we wish to introduce particle interactions by the addition of an operator corresponding to the potential energy. Thus we try to define a selfadjoint Hamiltonian.

$$H_{\sigma,\Lambda} = T_{\sigma,\Lambda} + U_\Lambda$$

and then the evolution of an observable $A \in \mathfrak{A}_{\pm}(\Lambda)$ is defined by

$$\tau_t^{\Lambda}(A) = e^{itH_{\sigma,\Lambda}} A e^{-itH_{\sigma,\Lambda}} .$$

We will only consider interactions coming from potentials and hence the number of particles is conserved. Thus, the total Hamiltonian has a decomposition

$$H_{\sigma,\Lambda} = \bigoplus_{n \geq 0} H_{\sigma,\Lambda}^{(n)}$$

in terms of n-particle Hamiltonians $H_{\sigma,\Lambda}^{(n)}$ on $L^2(\Lambda)_{\pm}^n$. These latter operators have the form

$$H_{\sigma,\Lambda}^{(n)} = T_{\sigma,\Lambda}^{(n)} + U_{\Lambda}^{(n)} ,$$

where the interaction operator $U_{\Lambda}^{(n)}$ is an operator of multiplication,

$$(U_{\Lambda}^{(n)}\psi)(x_1, \ldots, x_n) = U^{(n)}(x_1, \ldots, x_n)\psi(x_1, \ldots, x_n)$$

by a real function whose values $U^{(n)}(x_1, \ldots, x_n)$ correspond to the potential energy of n particles at the points $x_1, x_2, \ldots, x_n$. Note that for $U^{(n)}$ to preserve the symmetry, or anti-symmetry, properties of the elements in $L^2(\Lambda)_{\pm}^n$ it is necessary that it is a totally symmetric function i.e.,

$$U^{(n)}(x_1, \ldots, x_n) = U^{(n)}(x_{\pi(1)}, \ldots, x_{\pi(n)})$$

for all $x_i \in \mathbb{R}^{\nu}$ and all permutations π of $\{1, 2, \ldots, n\}$.

In order to be more precise in this formulation one must consider several different details. It is necessary that $H_{\sigma,\Lambda}$ is selfadjoint and for this one must specify the interaction $U^{(n)}$ and the meaning of the sum $T_{\sigma,\Lambda}^{(n)} + U_{\Lambda}^{(n)}$ in such a way that $H_{\sigma,\Lambda}^{(n)}$ is selfadjoint. One must also clarify the meaning of the infinite direct sum of the selfadjoint $H_{\sigma,\Lambda}^{(n)}$. This latter point is, however, straightforward.

Let $\{H^{(n)}\}_{n \geq 1}$ be an infinite sequence of selfadjoint operators with domains $\{D(H^{(n)})\}_{n \geq 1}$ in the Hilbert spaces $\{\mathfrak{H}^{(n)}\}_{n \geq 1}$. We define the infinite direct sum

$$H = \bigoplus_{n \geq 1} H^{(n)}$$

by

$$D(H) = \left\{ \psi = \{\psi^{(n)}\}_{n \geq 1}; \psi^{(n)} \in D(H^{(n)}), \sum_{n \geq 1} \|H^{(n)}\psi^{(n)}\|^2 < +\infty \right\}$$

and

$$H\psi = \left\{ H^{(n)}\psi^{(n)} \right\}_{n \geq 1}$$

for $\psi = \{\psi^{(n)}\}_{n \geq 1} \in D(H)$. It follows that H is selfadjoint. To deduce this, first remark that H is obviously a densely defined symmetric operator. But the graph of H is closed by the standard argument that proves that the infinite

direct sum of Hilbert spaces is complete. Thus, H is closed. Finally, the range of $\lambda\mathbb{1} - H$ is equal to $\mathfrak{H}$ for each $\lambda \in \mathbb{C}\backslash\mathbb{R}$ because $R(\lambda\mathbb{1} - H^{(n)}) = \mathfrak{H}^{(n)}$ for each n, i.e.,

$$R(\lambda\mathbb{1} - H) = \bigoplus_{n\geq 1} R(\lambda\mathbb{1} - H^{(n)}) = \bigoplus_{n\geq 1} \mathfrak{H}^{(n)} = \mathfrak{H} \ .$$

This establishes the selfadjointness of the direct sum. Hence, the initial problem of existence of dynamics is reduced to the discussion of selfadjointness of the n-particle Hamiltonians $H^{(n)}_{\sigma,\Lambda}$.

There is a wide variety of methods for defining Hamiltonians of the type under consideration and studying their selfadjointness, e.g., quadratic-form techniques, pointwise positivity arguments, perturbation theory, and functional integration. Each method has its own peculiar advantages and the appropriateness of any given technique is governed by the properties of the interaction in question and the specific problem under consideration. In the remainder of this section we discuss various aspects of the selfadjointness problem for the $H^{(n)}_{\sigma,\Lambda}$ by use of form techniques and perturbation theory. In the subsequent description of equilibrium states, it is however more appropriate to define the Hamiltonian by an implicit functional integration technique. Under suitable restrictions on the interaction these methods all lead to the same Hamiltonian and one can then pass from one method to the other. This will be discussed in the next section but first it is necessary to be more specific concerning the interaction.

The most commonly studied interactions are those that arise from translationally invariant two-body potentials. A *two body potential* is a real function Φ over $\mathbb{R}^\nu \times \mathbb{R}^\nu$ whose values $\Phi(x_1, x_2)$ represent the potential energy of interaction between a particle at the point x_1 and a second particle at the point x_2. Thus, the total interaction energy of n particles at the points $x_1, x_2, \ldots, x_n$ is given by

$$U^{(n)}(x_1, \ldots, x_n) = \sum_{1\leq i<j\leq n} \Phi(x_i, x_j) \ .$$

Note that the symmetry of $U^{(n)}$ is reflected by the symmetry property

$$\Phi(x_i, x_j) = \Phi(x_j, x_i)$$

of Φ. The potential is said to be *translationally invariant* if $\Phi(x_i, x_j)$ is a function of the interparticle position $x_i - x_j$. Thus a translationally invariant two-body potential is a real symmetric function Φ over $\mathbb{R}^\nu$ and the associated interaction energy $U^{(n)}$ is given by

$$U^{(n)}(x_1, \ldots, x_n) = \sum_{1\leq i<j\leq n} \Phi(x_i - x_j) \ .$$

The total interaction energy is then formally given by

$$U_\Lambda = \frac{1}{2}\int_\Lambda dx_1 \int_\Lambda dx_2\, \Phi(x_1 - x_2) a^*(x_1) a^*(x_2) a(x_2) a(x_1) \ ,$$

where we use the notation of Example 5.2.1. Similarly, one can define a (*translationally invariant*) *k-body potential* as a real-valued totally symmetric function $\Phi^{(k)}$ over $(\mathbb{R}^\nu)^k$ (invariant under simultaneous translations of all k variables in $\mathbb{R}^\nu$) and then

$$U^{(n)}(x_1, \ldots, x_n) = \sum_{k=1}^{n} \sum_{1 \le i_1 \le i_2 \le \cdots \le i_k \le n} \Phi^{(k)}(x_{i_1}, \ldots, x_{i_k}) \ .$$

The sequence $\Phi = \{\Phi^{(k)}\}_{k \ge 1}$ is the analogue of the interactions introduced for quantum spin systems.

Note that there is a converse to the above construction. If one is given a sequence $U = \{U^{(n)}\}_{n \ge 1}$ of real totally symmetric functions $U^{(n)}$ over $(\mathbb{R}^\nu)^n$ representing the interaction energies, then one may introduce k-body potentials by recursion, e.g.,

$$\Phi^{(1)}(x) = U^{(1)}(x) \ ,$$
$$\Phi^{(2)}(x_1, x_2) = U^{(2)}(x_1, x_2) - U^{(1)}(x_1) - U^{(1)}(x_2) \ ,$$

etc.

A typical translationally invariant two-body potential which occurs in atomic and molecular physics is the *Lennard–Jones potential*

$$\Phi(x) = \frac{a}{|x|^{12}} - \frac{b}{|x|^6} \ ,$$

where $a, b > 0$. The positive term $a/|x|^{12}$ predominates when two atoms are close, i.e., when $|x|$ is small, and this corresponds to a repulsive force arising from the interaction of the atomic nuclei. The negative term $-b/|x|^6$ predominates at large interatomic spacing and this corresponds to an attractive force originating in the electrostatic interaction of the charged subatomic particles which build the atom. This attraction at large distances is called the van der Waal's force. The principle features of this potential which we abstract in the following are that it is lower semi-bounded and locally integrable away from the origin.

The lower-semi-boundedness property is of importance because it allows the application of quadratic form techniques in the definition of the local Hamiltonians $H^{(n)}_{\sigma,\Lambda}$. There are however important physical potentials which do not have this property. The Coulomb potential between two particles with charges e_i, e_j, at the points $x_i, x_j, \in \mathbb{R}^\nu$ is given by

$$\Phi_{ij}(x_i - x_j) = \frac{e_i e_j}{|x_i - x_j|}$$

and this can be arbitrarily negative if the charges are of the opposite sign. Nevertheless, effects of this kind can be handled by perturbation techniques. First, however, let us consider the lower-semi-bounded case.

Throughout the sequel it is of importance to recall that there is a one-to-one correspondence between positive selfadjoint operators T on the Hilbert space

$\mathfrak{H}$ and positive, densely defined, closed, quadratic forms t. This correspondence is given by

$$t(\psi) = \|T^{1/2}\psi\|^2$$

with $D(t) = D(T^{1/2})$. Furthermore, by the addition of a constant multiple of the identity $\mathbb{1}$ this correspondence may be extended to a correspondence between lower-semi-bounded T, and lower-semi-bounded t, i.e., if $T \geq -c\mathbb{1}$, then the correspondence is given by

$$t(\psi) = \|(T + c\mathbb{1})^{1/2})\psi\|^2 - c\|\psi\|^2$$

with $D(t) = D((T + c\mathbb{1})^{1/2})$ and one has $t \geq -c$.

We define a *lower-semi-bounded interaction energy* to be a real-valued totally symmetric function $U^{(n)}$ of n variables in $\mathbb{R}^\nu$ satisfying the two conditions.

(1) $U^{(n)}(x_1, \ldots, x_n) \geq -c_n$ for some $c_n \geq 0$ and all $x_1, \ldots, x_n \in \mathbb{R}^\nu$,

(2) $U^{(n)} \in L^1_{\text{loc}}(\mathbb{R}^{\nu n} \backslash S_n)$ where S_n is a closed set of Lebesgue measure zero.

If the constant c_n can be chosen to be zero, we call $U^{(n)}$ a positive interaction Note that the second condition means

$$\int_K dx_1 \ldots dx_n |U^{(n)}(x_1, \ldots, x_n)| < +\infty$$

for each compact subset $K \subset \mathbb{R}^{\nu n} \backslash S_n$. The set S_n allows possible singularities in the interaction potential. For example, the interaction energy arising from the Lennard – Jones potential satisfies these conditions with

$$S_n = \{(x_1, \ldots, x_n);\ x_i \in \mathbb{R}^\nu \text{ and } x_i = x_j \text{ for some } i \neq j\}\ .$$

The requirement that S_n should have Lebesgue measure zero excludes particles with hard cores. As the inclusion of hard cores entails additional discussion of the boundary conditions imposed upon the cores we have made the restriction on S_n to avoid irrelevant details. In fact, the discussion of hard-core particles is easier in some respects than the discussion of point particles because the hard core prevents a large number of particles collapsing into a small volume.

Next we associate to each lower-semi-bounded interaction energy $U^{(n)}$ and each $\Lambda \subset \mathbb{R}^\nu$ a selfadjoint interaction operator $U^{(n)}_\Lambda$ by use of the quadratic-form techniques described above and in Section 5.2.3. First, define the quadratic form

$$u^{(n)}_\Lambda(\psi) = \int_{\Lambda^n} dx_1 \ldots dx_n\, U^{(n)}(x_1, \ldots, x_n)|\psi(x_1, \ldots, x_n)|^2$$

where the domain $D(u^{(n)}_\Lambda)$ of the form consists of all $\psi \in L^2(\Lambda)^n_\pm$ for which the integral is finite. This form is lower semi-bounded, $u^{(n)}_\Lambda \geq -c_n$, and closed. But it is also densely defined since $D(u^{(n)}_\Lambda)$ contains all bounded functions with compact support in $(\mathbb{R}^{\nu n} \backslash S_n) \cap \Lambda^n$. Thus, there exists a lower-semi-bounded selfadjoint operator $U^{(n)}_\Lambda \geq -c_n\mathbb{1}$ such that $D(u^{(n)}_\Lambda) = D((U^{(n)}_\Lambda + c_n\mathbb{1})^{1/2})$ and

$$u^{(n)}_\Lambda(\psi) = \|(U^{(n)}_\Lambda + c_n\mathbb{1})^{1/2}\psi\|^2 - c_n\|\psi\|^2\ .$$

We refer to $U_\Lambda^{(n)}$ as the interaction operator. It is the operator of multiplication by $U^{(n)}$ on $L^2(\Lambda)_\pm^n$. Now we can define a total Hamiltonian by summing quadratic forms.

First, note that the sum of two lower-semi-bounded closed quadratic forms is automatically lower semi-bounded and closed. Thus, if $t_{\sigma,\Lambda}^{(n)}$ denotes the positive closed quadratic form associated with the noninteracting Hamiltonian $T_{\sigma,\Lambda}^{(n)}$, then the sum

$$h_{\sigma,\Lambda}^{(n)} = t_{\sigma,\Lambda}^{(n)} + u_\Lambda^{(n)}$$

is lower semi-bounded and closed. But it is also densely defined because its domain contains the once continuously differentiable functions with compact support in $(\mathbb{R}^{\nu n}\backslash S_n)\cap\Lambda^n$. Thus, $h_{\sigma,\Lambda}^{(n)}$ also determines a lower-semi-bounded selfadjoint operator $H_{\sigma,\Lambda}^{(n)} \geq -c_n\mathbb{1}$ in the canonical fashion. This Hamiltonian operator $H_{\sigma,\Lambda}^{(n)}$ is called the form sum of $T_{\sigma,\Lambda}^{(n)}$ and $U_\Lambda^{(n)}$ and we write

$$H_{\sigma,\Lambda}^{(n)} = T_{\sigma,\Lambda}^{(n)} \dot{+} U_\Lambda^{(n)} .$$

The form sum differs in general from the operator sum. In the case at hand it could well occur that $D(T_{\sigma,\Lambda}^{(n)}) \cap D(U_\Lambda^{(n)})$ is empty and hence the operator sum would have no nonzero vector in its domain of definition. To ensure that the operator sum is densely defined it is necessary to place more stringent restrictions on $U^{(n)}$. Then it is often possible to prove equality of the two types of sum. For example, if $U^{(n)} \in L^2(\Lambda)^n$ and $U^{(n)} \geq 0$, one can establish that $T_{\sigma,\Lambda}^{(n)} + U_\Lambda^{(n)}$ is essentially selfadjoint on $C^\infty(\Lambda^n) \cap D(T_{\sigma,\Lambda})$ and hence the form sum and the (closure of the) operator sum coincide. (See Notes and Remarks.)

In Section 3.1.4 we considered relatively bounded perturbations of generators of semigroups and in the present context we specialize to perturbations of a selfadjoint operator. Let S be a selfadjoint operator and P a closed symmetric operator on the Hilbert space $\mathfrak{H}$, then P is defined to be relatively bounded with respect to S, or S-bounded, if $D(S) \subset D(P)$ and

$$\|P\psi\| \leq a\,\|\psi\| + b\|S\psi\|$$

for all $\psi \in D(S)$ and for some $a, b \geq 0$. The relative bound of P with respect to S is the infimum over all b for which a bound of this type is valid. It is now an easy consequence of Theorem 3.1.32 that $S + P$ is selfadjoint whenever the relative bound is less than one, i.e., the above inequality is valid with $b < 1$. Moreover, if $S \geq 0$, then $S + P$ is lower semi-bounded. This follows from the perturbation series definition of the resolvent of $S+P$,

$$(S+P+\alpha\mathbb{1})^{-1} = (S+\alpha\mathbb{1})^{-1}\sum_{n\geq 0}(-P(S+\alpha\mathbb{1})^{-1})^n$$

for $\alpha > 0$, and the relative bound which gives

$$\|P(S+\alpha\mathbb{1})^{-1}\| < b + a/\alpha .$$

Thus, one has convergence of the perturbation series for all sufficiently large α.

Now let us consider interaction operators $U_\Lambda^{(n)}$ of multiplication by real functions $U^{(n)}$ on $L^2(\Lambda)_\pm^n$. If $U_\Lambda^{(n)}$ is relatively bounded with respect to $T_{0,\Lambda}^{(n)}$, i.e.,

$$\|U_\Lambda^{(n)}\psi\| \leq a\,\|\psi\| + b\|T_{0,\Lambda}^{(n)}\psi\| ,$$

then by choosing ψ to be a constant one deduces that $U^{(n)} \in L^2(\Lambda)_+^n$. Similarly, if $U_\Lambda^{(n)}$ is bounded with respect to one of the other classical kinetic energy operators $T_{\sigma,\Lambda}^{(n)}$, it is certainly square integrable in compact subsets of the interior of Λ^n. Thus, some form of square integrability is necessary for the $U_\Lambda^{(n)}$ to be relatively bounded by the $T_{\sigma,\Lambda}^{(n)}$, but no sufficient conditions appear to be known. It is possible, for translationally invariant two-body interactions in low dimensions, that square integrability is both necessary and sufficient for relative boundedness with respect to the Neumann operator. This is indicated by the following.

Proposition 6.3.1. *Let U_Λ, where $\Lambda \subset \mathbb{R}^\nu$, be an operator of multiplication by a real function U on $L^2(\Lambda)$, i.e., $(U_\Lambda\psi)(x) = U(x)\psi(x)$.*

If $\nu \leq 3$ then the following conditions are equivalent:

(1) $U \in L^2(\Lambda)$.

(2) U_Λ is $T_{0,\Lambda}^{(1)}$*-bounded.*

(3) U_Λ is $T_{0,\Lambda}^{(1)}$*-bounded with relative bound zero.*

Proof. Condition (3) obviously implies (2) and this latter implies (1) by the preceding discussion. Thus, it remains to prove that (1) $\Rightarrow$ (3).

If $\psi \in C^\infty(\Lambda)$, then

$$\|U_\Lambda\psi\| \leq \|U\|_2 \sup_{x\in\Lambda} |\psi(x)| .$$

Next let $\{\psi_i\}_{i\geq 1}$ denote a complete orthonormal family of eigenfunctions of $T_{0,\Lambda}^{(1)}$ with corresponding eigenvalues $\{\varepsilon_i\}_{i\geq 1}$. One has

$$\psi(x) = \sum_{i\geq 1} \frac{\psi_i(x)}{\varepsilon_i + \alpha} (\psi_i, (T_{0,\Lambda}^{(1)} + \alpha\mathbb{1})\psi)$$

for each $\alpha > 0$. Therefore,

$$|\psi(x)|^2 \leq \sum_{i\geq 1} \frac{|\psi_i(x)|^2}{(\varepsilon_i + \alpha)^2} \|(T_{0,\Lambda}^{(1)} + \alpha\mathbb{1})\psi\|^2$$

by the Cauchy–Schwarz inequality. Thus

$$\|U_\Lambda\psi\| \leq c_\alpha \|U_\Lambda\|_2 (\alpha\|\psi\| + \|T_{0,\Lambda}^{(1)}\psi\|) ,$$

where

$$C_\alpha = \sup_{x\in\Lambda} \left(\sum_{i\geq 1} \frac{|\psi_i(x)|^2}{(\varepsilon_i + \alpha)^2} \right)^{1/2} .$$

This inequality immediately extends to all of $D(T^{(1)}_{0,\Lambda})$ by closure. Thus, $D(T^{(1)}_{0,\Lambda}) \subseteq D(U_\Lambda)$, if $c_\alpha < +\infty$, and the proof is complete if one can show that $c_\alpha \to 0$ as $\alpha \to \infty$.

This last point is particularly easy for special choices of Λ, e.g., parallelepipeds, spheres, etc., because the ψ_i and ε_i can be explicitly computed. To handle the general case we remark that

$$\sum_{i \geq 1} \frac{|\psi_i(x)|^2}{(\varepsilon_i + \alpha)^2} = \int_0^x d\beta\ \beta e^{-\beta x}\ p_{0,\Lambda}(x,x;\beta)\ ,$$

where $p_{0,\Lambda}(x,y;\beta)$ denotes the kernel of the semigroup $\beta \mapsto \exp\{-\beta T^{(1)}_{0,\Lambda}\}$. But it is known[6] that there exist positive constants $c^{(1)}_\Lambda$ and $c^{(2)}_\Lambda$ such that

$$0 \leq p_{0,\Lambda}(x,x;\beta) \leq c^{(1)}_\Lambda \beta^{-\nu 2} + c^{(2)}_\Lambda$$

for all $x \in \Lambda$ and hence one estimates that $c_\alpha \to 0$ as $\alpha \to \infty$.

This result does not immediately extend to all classical boundary conditions, e.g., for Dirichlet boundary conditions it is possible for U to have a singularity on the boundary $\partial\Lambda$ of Λ. Nevertheless the same argument shows that $U \in L^2(\Lambda)$ is sufficient for U_Λ to be $T^{(1)}_{\sigma,\Lambda}$-bounded with relative bound zero.

Now let us return to the discussion of n-particle Hamiltonians.

One can now define more general interaction Hamiltonians by combination of the two foregoing techniques. If $U^{(n)}_\Lambda$ is a $T^{(n)}_{\sigma,\Lambda}$ relatively bounded interaction with relative bound less than one and if $V^{(n)}_\Lambda$ is a lower-semi-bounded interaction defined by form methods, then one can introduce a selfadjoint total Hamiltonian

$$H^{(n)}_{\sigma,\Lambda} = (T^{(n)}_{\sigma,\Lambda} + U^{(n)}_\Lambda) \dotplus V^{(n)}_\Lambda$$

by first taking the operator sum of $T^{(n)}_{\sigma,\Lambda}$ and $U^{(n)}_\Lambda$ and subsequently the form sum with $V^{(n)}_\Lambda$. For this it is important that $T^{(n)}_{\sigma,\Lambda} + U^{(n)}_\Lambda$ is lower semi-bounded and $D(T^{(n)}_{\sigma,\Lambda} + U^{(n)}_\Lambda) = D(T^{(n)}_{\sigma,\Lambda})$. This last property ensures that the form sum is densely defined.

It is possible to introduce more general Hamiltonians by use of additional techniques such as relatively bounded forms, etc., but for brevity we restrict ourselves to the above class.

Selfadjointness of each $H^{(n)}_{\sigma,\Lambda}$ ensures that the total Hamiltonian

$$H_{\sigma,\Lambda} = \bigoplus_{n \geq 0} H^{(n)}_{\sigma,\Lambda}$$

is selfadjoint and this is sufficient to define the time development of each observable $A \in \mathfrak{A}_\pm(\Lambda)$. It is not however sufficient for defining the local Gibbs equilibrium state. For this it is necessary that $\exp\{-\beta(H_{\sigma,\Lambda} - \mu N_\Lambda)\}$ is of trace-class[7] for a sufficiently large set of values of $\beta > 0$ and $\mu \in \mathbb{R}$. Hence it is

[6]For more details on this and related semigroups see Section 6.3.2, in particular Theorem 6.3.8, and the references cited in the corresponding Notes and Remarks.

[7]Here we have reintroduced the number operator N_Λ on Fock space. Since N_Λ is a direct sum of multiples $n\mathbb{1}$ of the identity $\mathbb{1}$ on $L^2(\Lambda)^n_\pm$ the sum $H_{\sigma,\Lambda} - \mu N_\Lambda$ is automatically selfadjoint.

at least necessary that $H_{\sigma,\Lambda} - \mu N_\Lambda$ is, lower semi-bounded. But this does not follow from our present assumptions on the interaction. Although each $H^{(n)}_{\sigma,\Lambda}$ is bounded below, the direct sum could fail to be semi-bounded if the bounds $c_n \mathbb{1}$ on $H^{(n)}_{\sigma,\Lambda}$ are not sufficiently uniform. In a physically stable system one expects the energy per particle to be bounded below since if no such bound existed, the system would collapse into a bound state with large negative energy. Thus one expects

$$H^{(n)}_{\sigma,\lambda} \geq -Bn\mathbb{1}$$

for some $B \geq 0$, or, equivalently,

$$H_{\sigma,\Lambda} \geq -BN_\Lambda \ .$$

Since the kinetic energy $T_{\sigma,\Lambda}$ is positive, this stability condition would be ensured if the interaction satisfied the conditions

$$U^{(n)}(x_1, \ldots, x_n) \geq -Bn$$

for all $n = 1, 2, \ldots$, and all $x_i \in \mathbb{R}^\nu$. Interactions with this property are called *stable interactions*.

The simplest type of stable interactions arise from positive potentials but there also many interactions with partially negative potentials which are nevertheless stable.

EXAMPLE 6.3.2. Assume the interaction $U^{(n)}$ is defined by a translationally invariant two-body interaction potential Φ, i,e.,

$$U^{(n)}(x_1, \ldots, x_n) = \sum_{1 \leq i < j \leq n} \Phi(x_i - x_j) \ ,$$

and that Φ is bounded below. Furthermore, assume there exist numbers $0 < a_1 < a_2$ and positive decreasing functions Φ_1 and Φ_2, on $\langle 0, a_1 \rangle$ and $\langle a_2, \infty \rangle$, respectively, such that

$$\int_0^{a_1} dt\, \Phi_1(t) t^{\nu-1} = +\infty, \qquad \int_{a_2}^{\infty} dt\, \Phi_2(t) t^{\nu-1} < +\infty \ .$$

If

$$\Phi(x) \geq \Phi_1(|x|) \quad \text{for} |x| < a_1$$

and

$$\Phi(x) \geq -\Phi_2(|x|) \quad \text{for} |x| > a_2 \ ,$$

then $U^{(n)}$ is stable. In fact, more is true. The interaction is *superstable* in the sense that if Λ is a cube of sufficiently large volume $|\Lambda|$ and $x_1, \ldots, x_n \in \Lambda$, then

$$U^{(n)}(x_1, \ldots, x_n) \geq C \frac{n^2}{|\Lambda|} - Bn$$

where $B, C > 0$. (See Notes and Remarks.)

One important interaction (for several species of particles) which is not stable is the Coulomb interaction. Consider a system of n particles with charges

$e_i = \pm 1$ and for simplicity assume it is neutral, i.e., the total charge $e_1 + e_2 + \cdots + e_n$ is zero. Then the Coulomb interaction

$$U^{(n)}(x_1, \ldots, x_n) = \sum_{1 \le i < j \le n} \frac{e_i e_j}{|x_i - x_j|}$$

is not stable. Nevertheless, quantum statistics can ensure that the total Hamiltonian is stable. This is the case, for example, if all the negatively charged particles satisfy Fermi statistics. (See Notes and Remarks.) In classical statistical mechanics the situation is somewhat different and stability is essentially a necessary and sufficient condition for the existence of the Gibbs formalism.

EXAMPLE 6.3.3. Let $U^{(n)}$ be the interaction energy arising from a translationally invariant two-body potential Φ which is upper semi-continuous. The following conditions are equivalent:

(1) Φ is stable.
(2) $\Sigma_{i=1}^n \Sigma_{j=1}^n \Phi(x_i - x_j) \ge 0$ for all $n \ge 1$ and all $x_1, \ldots, x_n \in \mathbb{R}^\nu$.
(3) The classical partition function

$$\Xi_\Lambda = 1 + \sum_{n \ge 1} \frac{z^n}{n!} \int_{\Lambda^n} dx_1 \cdots dx_n \exp\{-\beta U^{(n)}(x_1, \ldots, x_n)\}$$

converges for all $z > 0$, $\beta > 0$, and all bounded regions Λ.

Stability of the interaction is sufficient for the existence of the local Gibbs states as a consequence of the results of Section 5.2 and the following *minimax principle.*

Proposition 6.3.4. *Let t be a densely defined, closed, lower-semi-bounded quadratic form and let T be the associated selfadjoint operator. Further, let D be a core of t and for every finite-dimensional subspace $M \subset D$ define*

$$\lambda(M) = \sup_{\psi \in M, \|\psi\| = 1} t(\psi)$$

and for every integer $m \le 1$ define

$$\lambda_m = \inf_{\dim M = m} \lambda(M) \ .$$

It follows that $\lambda_m \to \infty$ as $m \to \infty$ if and only if the spectrum of T consists of discrete eigenvalues of finite multiplicity and each eigenvalue is isolated in the spectrum of T. In this case the eigenvalues are given in increasing order, repeated according to multiplicity, by the λ_m.

This is a basically standard result in operator theory whose proof we omit (see Notes and Remarks). It does have many interesting applications. For example, if t_1 and t_2 are two forms of the kind considered in the proposition and λ_m^1 and λ_m^2 the corresponding numbers defined by the minimax principle,

then $t_1 \geq t_2$ implies that $\lambda_m^1 \geq \lambda_m^2$ and in particular if $\lambda_m^2 \to \infty$, then $\lambda_m^1 \to \infty$. Now if T_1 and T_2 are the selfadjoint operators associated with t_1 and t_2, the condition $t_1 \geq t_2$ corresponds to $T_1 \geq T_2$ and to prove that T_1 has purely discrete spectrum with finite multiplicity it suffices to prove the same property for T_2. In fact, more is true. If $\exp\{-\beta T_2\}$ is of trace-class for some $\beta > 0$, then $\exp\{-\beta T_1\}$ is of trace-class and

$$\mathrm{Tr}(e^{-\beta T_1}) = \sum_{m \geq 1} e^{-\beta \lambda_m^1} \leq \sum_{m \geq 1} e^{-\beta \lambda_m^2} = \mathrm{Tr}(e^{-\beta T_2}) \ .$$

Now utilizing the minimax principle together with Propositions 5.2.22 and 5.2.27 and the fact that $\exp\{-\beta\, T_{\sigma,\Lambda}^{(1)}\}$ is trace-class for all $\beta > 0$ one obtains the following result.

Proposition 6.3.5. *Let*

$$H_{\sigma,\Lambda}^{(n)} = (T_{\sigma,\Lambda}^{(n)} + U_\Lambda^{(n)}) \dotplus V_\Lambda^{(n)}$$

be a selfadjoint Hamiltonian constructed from a $T_{\sigma,\Lambda}^{(n)}$ -bounded interaction $U_\Lambda^{(n)}$, with relative bound less than one, and a lower-semi-bounded interaction $V_\Lambda^{(n)}$. Assume that $U^{(n)} + V^{(n)}$ is stable, i.e., for all $n \geq 1$ and $x_i \in \mathbb{R}^\nu$

$$U^{(n)}(x_1, \ldots, x_n) + V^{(n)}(x_1, \ldots, x_n) \geq -Bn \ .$$

It follows that the spectrum of $H_{\sigma,\Lambda}^{(n)}$ consists of discrete eigenvalues with finite multiplicity and

$$\lambda_m(H_{\sigma,\Lambda}^{(n)}) \ \geq \ \lambda_m(T_{\sigma,\Lambda}^{(n)}) - Bn$$

for $m = 1, 2 \ldots$, where $\{\lambda_m(X)\}_{m \geq 1}$ denotes the eigenvalues of X in increasing order and repeated according to multiplicity.

In particular $\exp\{-\beta(H_{\sigma,\Lambda} - \mu N_\Lambda)\}$ is of trace-class for all $\beta > 0$ and all $\mu \in \mathbb{R}$ for Fermi statistics, and all $\mu < -B$ for Bose statistics.

6.3.2. The Wiener Integral

The Wiener integral, as we shall use it, is a technical tool to prove the existence of thermodynamic limit functions, but it has its origin in attempts to understand Brownian motion. Brownian motion is the thermal motion of very small particles immersed in a heat bath. If $\rho(x, t)$ is the density of particles at the point $x \in \mathbb{R}^\nu$ at time t, it is well known that ρ is governed by the diffusion equation

$$\frac{\partial \rho}{\partial t} = \nabla^2 \rho$$

(in suitable units). If the initial density distribution $x \to \rho(x, 0)$ is given (and is sufficiently tempered as $|x| \to \infty$), this equation has a unique solution for all $t \geq 0$ given by

$$\rho(x,t) = \int dy \; p(x,y;t)\rho(y,0) \; ,$$

where

$$p(x,y;t) = (4\pi t)^{-\nu/2} e^{-|x-y|^2/4t} \; .$$

We use the convention $p(x,y;0) = \delta(x-y)$, where δ is the Dirac measure. It follows that if a Brownian particle starts at a point y at time t_0, then

$$p(x,y;t-t_0)dx$$

is the probability that the particle will be in the volume element dx near x at time $t > t_0$. The philosophy behind the Wiener integral is that the particle in moving from y to x must have followed a continuous trajectory, and therefore there should be a probability measure $\mu_{x,y}^{t-t_0}$ on the set $\Omega_{x,y}$ of continuous trajectories starting at y at time t_0 and ending at x at time t, such that $\mu_{x,y}^{t-t_0}$ applied to some subset K of $\Omega_{x,y}$ gives the probability that the particle has followed one of the trajectories in K. In the following paragraphs we will show that modulo the problem of giving $\Omega_{x,y}$ (or a related set) a reasonable Borel structure such a measure exists.

By translation invariance it is enough to consider $t_0 = 0$ and with subsequent applications in mind we set $t = \beta$. For technical reasons we will assume that the orbits are functions from $[0,\beta]$ into $\mathbb{R}^\nu$, where $\mathbb{R}^\nu$ is the one-point compactification of $\mathbb{R}^\nu$. At the outset we put no continuity restrictions on the trajectories, i.e., we take

$$\Omega_\beta = \bigtimes_{0 \le t \le \beta} \dot{\mathbb{R}}^\nu = (\dot{\mathbb{R}}^\nu)^{[0,\beta]}$$

as our *space of trajectories,* or *paths.* (*A posteriori* the Wiener measures will be supported on "nice " subsets of Ω_β, see Theorem 6.3.6.) Equip Ω_β with the product topology, i.e., the topology of pointwise convergence, then Ω_β is a compact Hausdorff space by the Tychonoff theorem. Obviously, Ω_β is so large a space that not all Borel sets are Baire. We shall define $\mu_{x,y}^\beta$ as a Baire measure on Ω_β, and hence by the discussion at the beginning of Section 4.1.2, it is enough to define $\mu_{x,y}^\beta$ as a Radon measure.

We first define $\mu_{x,y}^\beta$ on a special *-subalgebra $C_{\text{fin}}(\Omega_\beta)$ of the C^*-algebra $C(\Omega_\beta)$ of continuous functions on Ω_β. This algebra[8] consists of functions of the form

$$\omega \in \Omega_\beta \mapsto \varphi(\omega) = F(\omega(t_1), \omega(t_2), \ldots, \omega(t_m))$$

where $0 \le t_1 < t_2 < \cdots < t_m \le \beta$ are fixed real numbers, and $F\colon (\dot{\mathbb{R}}^\nu)^m \mapsto \mathbb{C}$ is a continuous function. Thus φ is a continuous function on Ω_β by the definition of the product topology. In evaluating $\mu_{x,y}^\beta(\varphi)$ it is useful to notice that if $K_1, K_2, \ldots, K_m$ are Borel subsets of $\mathbb{R}^\nu$, then

[8]The suffix fin is an abbreviation for finite. This nomenclature is apposite since each function $\varphi \in C_{\text{fin}}(\Omega_\beta)$ depends only on a finite number of points $\omega(t_i)$ on the paths.

$$dy \int_{K_m} \cdots \int_{K_1} p(x, x_1; t_1)\, p(x_1, x_2; t_2 - t_1)$$
$$\cdots p(x_{m-1}, x_m; t_m - t_{m-1})\, p(x_m, y; \beta - t_m) dx_1 \ldots dx_m$$

is the probability that a Brownian particle starting at x at time $t = 0$ is in the set K_l at time t_l for all $l = 1, 2, \ldots, m$ and is in the volume element dy around y at time β. The following definition of $\mu^{\beta}_{x,y}(\varphi)$ is therefore perfectly natural.

$$\mu^{\beta}_{x,y}(\varphi) = \int_{\mathbb{R}^v} \cdots \int_{\mathbb{R}^v} F(x_1, \ldots, x_m)\, p(x, x_1;\, t_1)\, p(x_1, x_2;\, t_2 - t_1)$$
$$\cdots p(x_{m-1}, x_m;\, t_m - t_{m-1})\, p(x_m, y;\, \beta - t_m) dx_1 \cdots dx_m \ .$$

Now $\mu^{\beta}_{x,y}(\varphi)$ is independent of the particular representation used for φ because if, for example, F does not depend on x_k one can use the semigroup property of the solutions to the diffusion equation,

$$\int_{\mathbb{R}^v} p(x_{k-1}, x_k;\, t_k - t_{k-1})\, p(x_k, x_{k+1};\, t_{k+1} - t_k) dx_k$$
$$= p(x_{k-1}, x_{k+1};\, t_{k+1} - t_{k-1}) \ ,$$

to integrate out the variable x_k. Thus $\mu^{\beta}_{x,y}$ is a well-defined linear functional on $C_{\text{fin}}(\Omega_\beta)$. Using the semigroup property just mentioned on all the variables $x_1, \ldots, x_m$ one immediately derives the estimate

$$|\mu^{\beta}_{x,y}(\varphi)| \leq p(x, y; \beta) \|F\|_\infty = p(x, y;\, \beta) \|\varphi\|_\infty \ ,$$

i.e., $\mu^{\beta}_{x,y}$ is bounded with norm less than or equal to $p(x, y; \beta)$. But the Stone-Weierstrass theorem implies that $C_{\text{fin}}(\Omega_\beta)$ is a norm-dense subalgebra of $C(\Omega_\beta)$, and hence $\mu^{\beta}_{x,y}$ extends by continuity to a Radon measure on $C(\Omega_\beta)$. Since $\|\mu^{\beta}_{x,y}\| \leq p(x, y; \beta)$ and $\mu^{\beta}_{x,y}(\mathbb{1}) = p(x, y;\, \beta)$ it follows from Proposition 2.3.11 that $\mu^{\beta}_{x,y}$ is a positive Radon measure. Finally, by the Riesz representation theorem, there exists a regular Borel measure, also denoted by $\mu^{\beta}_{x,y}$ on Ω_β, such that

$$\mu^{\beta}_{x,y}(\varphi) = \int_{\Omega_\beta} \varphi(\omega) du^{\beta}_{x,y}(\omega)$$

for all $\varphi \in C(\Omega_\beta)$. The measure $\mu^{\beta}_{x,y}$ is called the *conditional Wiener measure* on Ω_β.

The qualification conditional in the definition of $\mu^{\beta}_{x,y}$ stems from the specification that a path starting at x at time 0 shall end in y at time β. Alternatively one could place no restriction on the path at time β, i.e., one could consider the compact space

$$\Omega = \bigtimes_{t \geq 0} \dot{\mathbb{R}}^v = (\dot{\mathbb{R}}^v)^{[0, \infty\rangle} \ ,$$

and if $\varphi \in C(\Omega)$ is a function of the form

$$\varphi(\omega) = F(\omega(t_1), \omega(t_2), \ldots, \omega(t_m)) \ ,$$

where $F : (\dot{\mathbb{R}}^v)^m \mapsto \mathbb{C}$ is continuous and $0 \leq t_1 < t_2 < \cdots < t_m$, one may define

$$\mu_x(\varphi) = \int_{\mathbb{R}^\nu} \cdots \int_{\mathbb{R}^\nu} F(x_1, \ldots, x_m)\, p(x, x_1; t_1)\, p(x_1, x_2; t_2 - t_1)$$
$$\cdots\, p(x_{m-1}, x_m; t_m - t_{m-1}) dx_1 dx_2 \ldots dx_m \ .$$

This time μ_x extends by continuity to a Radon probability measure on $C(\Omega)$, and the associated regular Borel measure is called a *Wiener measure*. If K is a Borel subset, $\mu_x(K)$ is the probability that a particle starting at x at time zero shall follow one of the trajectories in K. If μ_x is restricted to $C(\Omega_\beta)$ in the obvious way, one clearly has the connection

$$\mu_x(\varphi) = \int_{\mathbb{R}^\nu} \mu^\beta_{x,y}(\varphi) dy$$

for all $\varphi \in C(\Omega_\beta)$. This corresponds to the fact that a path starting at x at time zero has to end up somewhere at time β.

It is well known in the elementary theory for Brownian motion that if a particle is at the point x at the time zero, then its mean distance from x at time $t \geq 0$ is proportional to $t^{1/2}$. This indicates that the Wiener measures should be supported on continuous paths, and even paths which are Hölder continuous of order less than $\frac{1}{2}$. Recall that a mapping $\omega : [0, \infty\rangle \mapsto \mathbb{R}^\nu$ is said to be Hölder continuous of order $\alpha, 0 < \alpha < 1$, if for all $m > 0$ there exists an $M > 0$ such that

$$|\omega(s) - \omega(t)| < M|s - t|^\alpha, \quad 0 \leq s,\, t \leq m \ .$$

Let Ω^α be the set of such paths in Ω and Ω^α_β the set of such paths in Ω_β. The following theorem states that the Wiener measure really can be viewed as a measure on continuous trajectories.

Theorem 6.3.6 *For $0 < \alpha \leq 1$ the set Ω^α of Hölder continuous paths of order α is a Borel subset of Ω and Ω^α_β is a Borel subset of Ω_β.*

If $0 < \alpha < \frac{1}{2}$, then $\mu_x(\Omega^\alpha) = 1$ for all $x \in \mathbb{R}^\nu$. If $\frac{1}{2} \leq \alpha < 1$, then $\mu_x(\Omega^\alpha) = 0$ for all $x \in \mathbb{R}^\nu$. Furthermore, μ_x is supported by the paths ω such that $\omega(0) = x$.

If $0 < \alpha < \frac{1}{2}$, then

$$\mu^\beta_{x,y}(\Omega^\alpha_\beta) = p(x, y; \beta)$$

for all $x, y \in \mathbb{R}^\nu$ and $\beta > 0$, and if $\frac{1}{2} \leq \alpha < 1$, then $\mu^\beta_{x,y}(\Omega^\alpha_\beta) = 0$. Furthermore, $\mu^\beta_{x,y}$ is supported by the paths $\omega(0) = x$ and $\omega(\beta) = y$.

PROOF. See Notes and Remarks.

The main reason for introducing the Wiener measure, from a statistical mechanics point of view, is that one can derive an integral formula for the semigroup

$$\beta \mapsto \exp\{-\beta(-\nabla^2 + U)\} \ ,$$

where $-\nabla^2$ is the selfadjoint Laplacian operator on $L^2(\mathbb{R}^\nu)$ and U is a sufficiently well behaved real function. This formula is usually referred to as the *Feynman–Kac formula* and it is a consequence of the Trotter product formula of Corollary 3.1.31. It is very convenient in making estimates on the kernel of the semigroup.

Theorem 6.3.7 *Let U, V be operators of multiplication by real functions on $L^2(\mathbb{R}^\nu)$. Assume that U is relatively bounded by the selfadjoint Laplacian operators $H_0 = -\nabla^2$, with relative bound $b < 1$, and that $V \in L^1_{\mathrm{loc}}(\mathbb{R}^\nu)$ is bounded below. If*

$$H = (H_0 + U) \dot{+} V$$

then[9]

$$\begin{aligned}(e^{-\beta H}\psi)(x) &= \int_\Omega d\mu_x(\omega)\, \exp\left\{-\int_0^\beta dt\,[U(\omega(t)) + V(\omega(t))]\right\}\psi(\omega(\beta)) \\ &= \int_{\mathbb{R}^\nu} dy \int_{\Omega_\beta} d\mu^\beta_{x,y}(\omega)\exp\left\{-\int_0^\beta dt\,[U(\omega(t)) + V(\omega(t))]\right\}\psi(y)\ .\end{aligned}$$

Proof. We begin by proving the first statement of the theorem with U and V replaced by real bounded continuous functions and then we make a series of approximation arguments to obtain the general case. The second statement then follows because

$$\mu_x(\varphi) = \int_{\mathbb{R}^\nu} dy\, \mu^\beta_{x,y}(\varphi)$$

and $\mu^\beta_{x,y}$ is supported by trajectories ω such that $\omega(\beta) = y$.

Let $H = H_0 + W$ where W is a real bounded continuous function. Consequently, the Trotter product formula

$$e^{-\beta H}\psi = \lim_{m\to\infty}(e^{-\beta H_0/m}e^{-\beta W/m})^m\psi$$

is valid, Corollary 3.1.31. But by successive use of

$$e^{-\beta H_0/m}\varphi(x) = \int_{\mathbb{R}^\nu} dy\, p\left(x, y; \frac{\beta}{m}\right)\varphi(y)$$

and

$$(e^{-\beta W/m}\varphi)(x) = e^{-\beta W(x)/m}\varphi(x)$$

[9]Strictly speaking the expression

$$\int_0^\beta dt\,[U(\omega(t)) + V(\omega(t))]$$

does not make sense for a general $\omega \in \Omega_\beta$. Since, however, the Wiener measures are supported by Hölder continuous paths, the expression can be defined for almost every $\omega \in \Omega_\beta$ and the integrals in the formulas should be interpreted as integrals over Ω^α_β where $0 < \alpha < \frac{1}{2}$

one obtains

$$
\begin{aligned}
((e^{-\beta H_0/m}e^{-\beta W/m})^m\psi)(x) &= \int dx_1 \cdots \int dx_m\, p\left(x, x_m; \frac{\beta}{m}\right) \\
&\quad \times p\left(x_m, x_{m-1}; \frac{\beta}{m}\right) \cdots p\left(x_2, x_1; \frac{\beta}{m}\right) \exp\left\{-\sum_{j=1}^{m} \frac{\beta W(x_j)}{m}\right\}\psi(x_1) \\
&= \int_{\Omega^x} d\mu_x(\omega) \exp\left\{-\frac{\beta}{m}\sum_{j=1}^{m} W\left(\omega\left(\frac{\beta j}{m}\right)\right)\right\}\psi(\omega(\beta)) \,.
\end{aligned}
$$

Now by passing to a subsequence one may assume that the left-hand side converges almost everywhere to $\exp\{-\beta H\}\psi$. Moreover, if ω is a continuous path

$$
\lim_{m\to\infty} \frac{\beta}{m}\sum_{j=1}^{m} W\left(\omega\left(\frac{\beta j}{m}\right)\right) = \int_0^\beta dt\, W(\omega(t)) \,.
$$

But for each x almost all (with respect to μ_x) paths are continuous by Theorem 6.3.6 and hence

$$
\lim_{m\to\infty} \exp\left\{-\frac{\beta}{m}\sum_{j=1}^{m} W\left(\frac{\beta j}{m}\right)\right\}\psi(\omega(\beta)) = \exp\left\{-\int_0^\beta dt\, W(\omega(t))\right\}\psi(\omega(\beta))
$$

pointwise almost everywhere on Ω^x. Furthermore,

$$
\begin{aligned}
&\int_{\Omega^x} d\mu_x(\omega)\left|\exp\left\{-\frac{\beta}{m}\sum_{j=1}^{m} W\left(\frac{\beta j}{m}\right)\right\}\psi(\omega(\beta))\right| \\
&\quad \le e^{\beta\|W\|_\infty}\int d\mu_x(\omega)|\psi(\omega(\beta))| \\
&\quad = e^{\beta\|W\|_\infty}(e^{-\beta H_0}|\psi|)(x) \\
&\quad = e^{\beta\|W\|_\infty}(4\pi\beta)^{-\nu/2}\int dy\, e^{-(x-y)^2/4\beta}|\psi(y)| \\
&\quad \le e^{\beta\|W\|_\infty}(4\pi\beta)^{-\nu/2}\left(\int dy\, e^{-(x-y)^2/2\beta}\right)^{1/2}\|\psi\| \\
&\quad = e^{\beta\|W\|_\infty}2^{-\nu/2}\|\psi\| < +\infty
\end{aligned}
$$

for all x. Therefore,

$$
\begin{aligned}
&\lim_{m\to\infty}\int d\mu_x(\omega)\exp\left\{-\frac{\beta}{m}\sum_{j=1}^{m} W\left(\frac{\beta j}{m}\right)\right\}\psi(\omega(\beta)) \\
&\quad = \int d\mu_x(\omega)\exp\left\{-\int_0^\beta W(\omega(t))\right\}\psi(\omega(\beta))
\end{aligned}
$$

by the Lebesgue-dominated convergence theorem and the proof is finished for the special case of a bounded continuous interaction.

Next we remove the continuity assumption.

Suppose $W \in L^\infty(\mathbb{R}^\nu)$ and that W_n is a sequence of continuous functions such that $|W_n(x)| \le \|W\|_\infty$ and $W_n(x) \to W(x)$ pointwise almost everywhere. Then $W_n \to W$ in the strong operator topology by the Lebesgue-dominated convergence theorem. Thus, $H_0 + W$ is the graph limit of the sequence of operators $H_0 + W_n$ and it follows

from Theorem 3.1.28 that the C_0-semigroups $\beta > 0 \mapsto \exp\{-\beta(H_0 + W_n)\}$ converge strongly to $\beta > 0 \to \exp\{-\beta(H_0 + W)\}$. Hence by passing to a subsequence one may assume that $(\exp\{-\beta(H_0 + W_n)\}\psi)(x)$ converges pointwise almost everywhere to $(\exp\{-\beta(H_0 + W)\}\psi)(x)$. But by the previous argument the Feynman–Kac formula is valid for the $H_0 + W_n$ and, as $W_n(x) \to W(x)$ pointwise almost everywhere it follows for almost all $\omega \in \Omega^\alpha$ that $W_n(\omega(t)) \to W(\omega(t))$ pointwise almost everywhere in t. Therefore, since the W_n and W are uniformly bounded, one may apply the previous argument based on the Lebesgue-dominated convergence theorem to deduce that

$$\begin{aligned}\lim_{n\to\infty} \int_\Omega d\mu_x(\omega) \exp\left\{-\int_0^\beta dt\ W_n(\omega(t))\right\}\psi(\omega(\beta)) \\ = \int_\Omega d\mu_x(\omega) \exp\left\{-\int_0^\beta dt\ W(\omega(t))\right\}\psi(\omega(\beta)))\end{aligned}$$

and the proof is complete for $W \in L^\infty(\mathbb{R}^\nu)$.

Now each H_0-bounded U is locally square integrable because for each $\Lambda \subset \mathbb{R}^\nu$ one may find a $\psi \in C_0^\infty(\mathbb{R}^\nu)$ such that $\psi(x) = 1$ for $x \in \Lambda$ and hence

$$\left(\int_\Lambda dx\, |U(x)|^2\right)^{1/2} \leq \|U\psi\| \leq a\|\psi\| + b\|H_0\psi\| \ .$$

Therefore one may introduce a double sequence of approximants $U_{n,m} \in L^\infty(\mathbb{R}^\nu)$ by

$$\begin{aligned}U_{n,m}(x) &= \min(U(x), n) \qquad \text{if } U(x) \geq 0 \ , \\ &= \max(U(x), -m) \quad \text{if } U(x) \leq 0 \ .\end{aligned}$$

It immediately follows that $\|U_{n,m}\psi - U\psi\| \to 0$ for all $\psi \in C_0^\infty(\mathbb{R}^\nu)$. But $C_0^\infty(\mathbb{R}^\nu)$ is a core of H_0 and hence by the relative boundedness of U it is a core for $H_0 + U + W$ where $W \in L^\infty(\mathbb{R}^\nu)$. Consequently $H_0 + U_{n,m} + W$ converges in the graph limit to $H_0 + U + W$ and the convergence of the corresponding semigroups follows from Theorem 3.1.28. But the Feynman–Kac formula is valid for the potentials $U_{n,m} + W$ and the right-hand side of this formula converges to the appropriate expression with $U + W$ by the previous arguments concerning the continuous paths in Ω^α. Here one uses the Lebesgue-dominated convergence theorem to control the limit $n \to \infty$ and the monotone convergence theorem to control the limit $m \to \infty$.

Thus by the previous argument one has the desired result for $U + W$.

Now since $V \in L^1_{\text{loc}}(\mathbb{R}^\nu)$ and V is lower semi-bounded, there exists a sequence $W_n \in L^\infty(\mathbb{R}^\nu)$ such that W_n is monotonically increasing and $W_n(x) \to V(x)$ almost everywhere. But it then follows from Lemmas 5.2.13 and 5.2.25 that the C_0-semigroups $\beta > 0 \mapsto \exp\{-\beta(H_0 + U + W_n)\}$ converge strongly to the C_0-semigroup $\beta > 0 \mapsto \exp\{-\beta(H_0 + U) \dot{+} V)\}$. Thus the general Feynman–Kac formula follows by repetition of the previous arguments.

So far, we have developed the theory of the Wiener measure and the Feynman–Kac formula only for the infinite-volume Laplacian $-\nabla^2$. In order to apply the theory to finite-volume Gibbs states and their thermodynamic limits, one has to develop the corresponding concepts for the finite volume Laplacians $T^{(n)}_{\sigma,\Lambda}$. The theory for $T^{(n)}_{\sigma,\Lambda}$ follows from the theory for $T^{(1)}_{\sigma,\Lambda}$ and the tensor product structure. Thus we concentrate on $T^{(1)}_{\sigma,\Lambda}$.

Consider the diffusion equation

$$\frac{\partial \rho}{\partial t} = \nabla^2 \rho, \quad t > 0,\ x \in \Lambda\ ,$$

with boundary condition

$$\frac{\partial \rho}{\partial n}(x,t) = \sigma(x)\rho(x,t), \quad t > 0,\ x \in \partial\Lambda$$

(which is interpreted as $\rho(x,t) = 0$ in the case $\sigma = \infty$) and with initial condition

$$\rho(x,0) = f(x)$$

where, for example, $f \in L^2(\Lambda)$. This equation has the unique solution

$$\rho(x,t) = (e^{-tT^{(1)}_{\sigma,\Lambda}} f)(x) = \int_\Lambda p_{\sigma,\Lambda}(x,y;t) f(y) dy\ .$$

The function $p_{\sigma,\Lambda}$ is the kernel of the semigroup $t \mapsto \exp\{-t\, T^{(1)}_{\sigma,\Lambda}\}$ and it is usually called the *Green function* for the problem. It has the following properties

(1) Positivity conservation:

$$p_{\sigma,\Lambda}(x,y;t) \geq 0$$

for $t > 0$, x, $y \in \Lambda$.

(2) Semigroup property:

$$\int_\Lambda p_{\sigma,\Lambda}(x,y;t) p_{\sigma,\Lambda}(y,z;s) dy = p_{\sigma,\Lambda}(x,z;t+s)\ .$$

(3) Contraction property:

$$\int_\Lambda p_{\sigma,\Lambda}(x,y;t) dy \leq 1$$

for $x \in \Lambda, t > 0$, with equality if and only if $\sigma = 0$ (Neumann boundary conditions).

(4) Monotonicity in boundary conditions:
If $\sigma_1(x) \leq \sigma_2(x)$ for all $x \in \partial\Lambda$, then

$$p_{\sigma_1,\Lambda}(x,y;t) \geq p_{\sigma_2,\Lambda}(x,y;t)$$

for all $x, y \in \Lambda, t > 0$.

Now once again let

$$p(x,y;t) = (4\pi t)^{-\nu/2} e^{-|x-y|^2/4t}$$

be the Green's function for the whole space and define the *compensating Green function* $z_{\sigma,\Lambda}$ by

$$z_{\sigma,\Lambda}(x,y;t) = p(x,y;t) - p_{\sigma,\Lambda}(x,y;t)$$

for $x, y \in \Lambda, t > 0$. This difference $z_{\sigma,\Lambda}$ describes how the free diffusion process is affected by the introduction of boundary conditions. One would expect $z_{\sigma,\Lambda}(x,y;t)$ to be small when x and y are far from the boundary $\partial\Lambda$ and this is corroborated by the following result.

Theorem 6.3.8. *For each $\beta > 0$ there exist constants $C, c', c'' > 0$ such that*

$$|z_{\sigma,\Lambda}(x,y;t)| \leq Cp(x,y;t/c')\exp\left\{-c''d(y,\partial\Lambda)^2/4t\right\}$$

for all $x, y \in \Lambda$, $0 < t \leq \beta$, where $d(y,\partial\Lambda)$ is the distance from y to $\partial\Lambda$. Furthermore, the constants C, c' and c'' can be chosen to be independent of the function $\sigma \geq 0$, and they are independent of Λ in the sense that if $R > 0$, then there exist constants $\lambda \geq 0, C > 0, c > 0$ such that for every bounded convex domain $\Lambda \subset \mathbb{R}^\nu$, whose boundary $\partial\Lambda$ is a C^3-surface of mean curvature less than $1/R$, the following inequality holds

$$|z_{\sigma,\Lambda}(x,y;t)| \leq Ce^{\lambda t}t^{-\nu/2}\exp\left\{-(c(d(x,d\Lambda)^2 + d(y,\partial\Lambda)^2)/4t\right\} .$$

Proof. We will only prove this result in the simple case of Dirichlet boundary conditions, i.e., $\sigma = \infty$. In this case, if $y \in \Lambda$ is fixed, $x, t \mapsto z_{\infty,\Lambda}(x,y;t) = z(x,t)$ is nothing but the solution of the diffusion equation

$$\frac{\partial z}{\partial t} = \nabla^2 z, \quad x \in \Lambda, t > 0,$$

with initial condition

$$z(x,0) = 0, \quad x \in \Lambda$$

and boundary condition

$$z(x,t) = p(x,y;t), \quad x \in \partial\Lambda, t > 0 .$$

Hence, by the maximum principle,

$$0 \leq z(x,t) \leq \sup_{\substack{0 \leq \tau \leq t \\ x' \in \partial\Lambda}} p(x',y;\tau) \leq \sup_{0 \leq \tau \leq t} (4\pi\tau)^{-\nu/2}e^{-d(y,\partial\Lambda)^2/4\tau} .$$

But the function

$$\tau \mapsto (4\pi\tau)^{-\nu/2}e^{-d^2/4\tau}$$

is increasing with τ when $0 < \tau \leq d^2/2\nu$ and hence

$$0 \leq z_{\infty,\Lambda}(x,y;t) \leq (4\pi t)^{-\nu/2}e^{-d(y,\partial\Lambda)^2/4t}$$

for $0 \leq t \leq d^2/2\nu$. If, however, $t > d^2/2\nu$, we can use the positivity of $p_{\infty,\Lambda}$ to conclude that

$$\begin{aligned} 0 &\leq z_{\infty,\Lambda}(x,y;t) \leq p(x,y;t) \\ &\leq (4\pi t)^{-\nu/2} \leq (4\pi t)^{-\nu/2}e^{-d(y,\partial\Lambda)^2/4t}e^{\nu/2} . \end{aligned}$$

Hence, in all cases

$$0 \leq z_{\infty,\Lambda}(x,y;t) \leq e^{\nu/2}(4\pi t)^{-\nu/2}e^{-d(y,\partial\Lambda)^2/4t} .$$

The last estimate in the theorem now follows because

$$z_{\infty,\Lambda}(x,y;t) = z_{\infty,\Lambda}(y,x;t) \quad \text{for all } x, y \in \Lambda .$$

One can construct functional measures corresponding to the transition probabilities $p_{\sigma,\Lambda}$ in almost exactly the same manner as the Wiener measures were constructed from p.

The trajectory space will be

$$\Omega_{\Lambda,\beta} = \bigtimes_{0 \leq \tau \leq \beta} \overline{\Lambda} = (\overline{\Lambda})^{[0,\beta]} ,$$

where $\overline{\Lambda}$ is the closure of Λ. Again $\Omega_{\Lambda,\beta}$ is compact in the product topology. One next defines a positive Radon measure $\mu_{x,y}^{\sigma,\Lambda,\beta}$ on $C(\Omega_{\Lambda,\beta})$ by first defining it on functions φ of the form

$$\varphi(\omega) = F(\omega(t_1), \omega(t_2), \ldots, \omega(t_m)) ,$$

where $F : (\overline{\Lambda})^m \mapsto \mathbb{C}$ is continuous and $0 \leq t_1 < t_2 < \cdots < t_m \leq \beta$ by

$$\begin{aligned}\mu_{x,y}^{\sigma,\Lambda,\beta}(\varphi) = \int_\Lambda \cdots \int_\Lambda & F(x_1, \ldots, x_m)\, p_{\sigma,\Lambda}(x, x_1; t_1) \\ & \times p_{\sigma,\Lambda}(x_1, x_2; t_2 - t_1) \cdots p_{\sigma,\Lambda}(x_{m-1}, x_m; t_m - t_{m-1}) \\ & \times p_{\sigma,\Lambda}(x_m, y; \beta - t_m) dx_1 \ldots dx_m .\end{aligned}$$

The Riesz theorem then assures the existence of a unique regular Borel measure $\mu_{x,y}^{\sigma,\Lambda,\beta}$ on $\Omega_{\Lambda,\beta}$ such that

$$\mu_{x,y}^{\sigma,\Lambda,\beta}(\varphi) = \int_{\Omega_{\Lambda,\beta}} \varphi(\omega) d\mu_{x,y}^{\sigma,\Lambda,\beta}(\omega) .$$

It follows from the monotonicity of $p_{\sigma,\Lambda}$ in σ (property (4)) and the definition of $\mu_{x,y}^{\sigma,\Lambda,\beta}$ that the functional measures are monotonic in the boundary conditions, i.e.,

$$0 \leq \sigma_1 \leq \sigma_2 \leq +\infty$$

implies that

$$\mu_{x,y}^{\infty,\Lambda,\beta}(B) \leq \mu_{x,y}^{\sigma_2,\Lambda,\beta}(B) \leq \mu_{x,y}^{\sigma_1,\Lambda,\beta}(B) \leq \mu_{x,y}^{0,\Lambda,\beta}(B)$$

for all Borel sets $B \subseteq \Omega_{\Lambda,\beta}$.

One can prove the analogue of Theorem 6.3.6 for the measures $\mu_{x,y}^{\sigma,\Lambda,\beta}$, i.e., these measures are supported by the set of Hölder continuous paths of order α if $0 < \alpha < \frac{1}{2}$ and the set of Hölder continuous paths of order α has measure zero if $\frac{1}{2} \leq \alpha \leq 1$.

We next discuss the physical interpretation of the various boundary conditions and how they influence the functional measures. Dirichlet boundary

conditions, $\sigma = \infty$, give rise to solutions ρ of the diffusion equation with $\rho(x,t) = 0$ for x in the boundary $\partial\Lambda$. In the context of Brownian motion this means that a particle which hits the boundary is immediately absorbed or annihilated. This interpretation will be corroborated in a precise mathematical way in Corollary 6.3.10. In the context of heat flow, Dirichlet boundary conditions mean that the medium outside Λ is at temperature zero and absorbs all heat reaching the boundary. Therefore, $\sigma = \infty$ corresponds to *completely absorptive boundary conditions*. This is also reflected in the fact that the solution $\rho(x,t)$ tends to zero, uniformly in x, as $t \to \infty$.

Neumann boundary conditions, $\sigma = 0$, give rise to solutions ρ of the diffusion equation with $\partial\rho/\partial n = 0$ at the boundary $\partial\Lambda$. In the context of Brownian motion this can be interpreted as stating that any particle which hits the boundary is reflected into Λ again, with the result that the gradient of the particle density normal to the boundary is zero. For heat flow this corresponds to a *completely reflecting boundary condition*. The intermediary cases $0 < \sigma < \infty$ correspond to semi-reflecting, semi-absorbing boundary conditions, i.e., more and more particles are absorbed at the boundary with increasing σ.

In the context of quantum mechanics, Dirichlet boundary conditions have a completely different interpretation, while the interpretation of Neumann boundary conditions is the same. The diffusion equation is replaced by the Schrödinger equation

$$i\frac{\partial\psi}{\partial t} = -\nabla^2\psi$$

on $L^2(\Lambda)$, with the appropriate boundary condition, and this equation describes the motion of a noninteracting quantum-mechanical particle confined to Λ. If $\psi(x,0) = f(x)$ the equation has the unique solution

$$\psi(x,t) = (e^{-itT^{(1)}_{\sigma,\Lambda}} f)(x)$$

and if $\|f\| = \|\psi\| = 1$, the measure $x \in \Lambda \mapsto |\psi(x,t)|^2 dx$ describes the probability that the particle is in the volume element dx, located at the point x, at time t. In particular, the eigenfunctions of $T^{(1)}_{\sigma,\Lambda}$ describe the stationary stable states of the particle, i.e., $|\psi(x,t)|^2 = |f(x)|^2$. But for Dirichlet boundary conditions these latter states attribute a relatively small probability of finding the particle near the boundary of Λ, while the total probability of finding the particle somewhere in Λ remains constant, i.e., the boundary is repulsive. If on the other hand one has Neumann boundary conditions, then there is no effect of exclusion near the boundaries. In fact, the state corresponding to the lowest eigenvalue (lowest energy) has a constant eigenfunction and there is equiprobability for finding the particle near any given point, i.e., the boundaries are perfectly elastic. This interpretation is corroborated by examination of the boundary conditions $\partial\psi/\partial n = \sigma\psi$. The parameter σ is related to the elasticity of the boundaries with positive values corresponding to repulsion and negative values corresponding to attraction. For example, if σ is sufficiently negative,

then $T^{(1)}_{\sigma,\Lambda}$ has eigenfunctions with negative eigenvalues (negative energies) which describe bound states in which the particle is close to the boundary with large probability.

If these interpretations of the boundary condition are correct, then they really are conditions at the boundary, i.e., a Brownian particle moving inside Λ without hitting $\partial\Lambda$ should not "feel" the effect of the boundary conditions. The following theorem gives a precise mathematical statement of this fact.

Define a function α_Λ on $\Omega_{\Lambda,\beta}$ by

$$\alpha_\Lambda(\omega) = \begin{cases} 1 & \text{if } \omega(t) \in \Lambda \text{ for all } t \in [0,\beta] \\ 0 & \text{otherwise .} \end{cases}$$

Since the Wiener measure $\mu^\beta_{x,y}$ and the finite-volume Wiener measures $\mu^{\sigma,\Lambda,\beta}_{x,y}$ are all supported by continuous trajectories, it follows that the function α_Λ is measurable with respect to these measures (although not a Borel function). We emphasize that α_Λ is different from $\alpha_{\overline{\Lambda}}$.

Theorem 6.3.9. *The identity*

$$\int_B \alpha_\Lambda(\omega) d\mu^{\sigma,\Lambda,\beta}_{x,y}(\omega) = \int_B \alpha_\Lambda(\omega) d\mu^\beta_{x,y}(\omega)$$

is valid for all Borel sets $B \subseteq \Omega_{\Lambda,\beta}$.

Proof. Consider first the case $B = \Omega_{\Lambda,\beta}$. Let $K_n \subset \Lambda$ be a sequence of compact sets such that K_n is contained in the interior of K_{n+1} for $n = 1, 2, \ldots$ and $\bigcup_n K_n = \Lambda$. Define functions $\alpha_{K_n}\colon \Omega_\beta \mapsto \{0,1\}$ by

$$\alpha_{K_n}(\omega) = \begin{cases} 1 & \text{if } \omega(t) \in K_n \text{ for all } t \in [0,\beta] \\ 0 & \text{otherwise.} \end{cases}$$

If ω is a continuous trajectory which does not touch $\partial\Lambda$, then $\omega([0,\beta])$ is a compact subset of Λ, and hence contained in some K_n. It follows that

$$\lim_{n\to\infty} \alpha_{K_n}(\omega) = \alpha_\Lambda(\omega)$$

for $\mu^\beta_{x,y}$- and $\mu^{\sigma,\Lambda,\beta}_{x,y}$-almost all $\omega \in \Omega_{\Lambda,\beta}$. In view of the Lebesgue-dominated convergence theorem it is therefore sufficient to show that

$$\int_{\Omega_{\Lambda,\beta}} \alpha_K(\omega) d\mu^{\sigma,\Lambda,\beta}_{x,y}(\omega) = \int_{\Omega_\beta} \alpha_K(\omega) d\mu^\beta_{x,y}(\omega)$$

for all compact $K \subset \Lambda$. Let d be the distance between K and $\partial\Lambda$; $d > 0$ by compactness. Let $n \geq 1$ and

$$t_k = \frac{k\beta}{n+1} \ , \qquad k = 0, 1, \ldots, n+1 \ .$$

Define

$$\alpha_n(\omega) = \begin{cases} 1 & \text{if } \omega(t_k) \in K \text{ for all } k = 0, 1, \ldots, n+1 \\ 0 & \text{otherwise.} \end{cases}$$

Then $\lim \alpha_n(\omega) = \alpha_K(\omega)$ for almost all ω, with respect to the functional measures. We compute

$$\begin{aligned}\int_{\Omega_{\Lambda,\beta}} \alpha_n(\omega) d\mu_{x,y}^{\sigma,\Lambda,\beta}(\omega) &= \int_{K^n} dx_1 \cdots dx_n \prod_{k=0}^{n} p_{\sigma,\Lambda}\left(x_{k+1}, x_k; \frac{\beta}{n+1}\right) \\ &= \int_{K^n} dx_1 \cdots dx_n \prod_{k=0}^{n} \left(p\left(x_{k+1}, x_k; \frac{\beta}{n+1}\right) \right. \\ &\quad \left. - z_{\sigma,\Lambda}\left(x_{k+1}, x_k; \frac{\beta}{n+1}\right)\right) \\ &= \int_{K^n} dx_1 \cdots dx_n \prod_{k=0}^{n} p\left(x_{k+1}, x_k; \frac{\beta}{n+1}\right) + R_n \\ &= \int_{\Omega_\beta} \alpha_n(\omega) d\mu_{x,y}^{\beta}(\omega) + R_n \ ,\end{aligned}$$

where $x_0 = x$, $x_{n+1} = y$, and we must show that $\lim R_n = 0$.

But R_n is a sum of $2^{n+1} - 1$ terms of the form

$$\pm \int_{K^n} dx_1 \cdots dx_n \, Q \ ,$$

where Q is a product of $k+1$ factors $z_{\sigma,\Lambda}$ and $n-k$ factors p, and $k \in \{0, 1, 2, \ldots, n\}$. Taking moduli of the factors in Q, extending to $\mathbb{R}^\nu$ all integrals which do not involve $z_{\sigma,\Lambda}$-factors and using the semigroup property of p, this term will be majorized by an integral containing $k+1$ factors $|z_{\sigma,\Lambda}|$ and at most $k+2$ factors p. By the first inequality in Theorem 6.3.8 the $|z_{\sigma,\Lambda}|$ factors are dominated by expressions of the form

$$Cp\left(x_{i+1}, x_i; \frac{\beta}{c'(n+1)}\right) \exp\left\{-c'' \frac{d^2(n+1)}{4\beta}\right\} \ .$$

Hence using the estimate

$$p(x, y; t) \leq c'^{-\nu/2} p\left(x, y; \frac{t}{c'}\right)$$

which is valid for $0 < c' \leq 1$, extending the integrals to all of $\mathbb{R}^\nu$, using the semigroup property of p, and counting terms one obtains

$$\begin{aligned}|R_n| &\leq c'^{-\nu/2} p\left(y, x; \frac{\beta}{c'}\right) \sum_{k=0}^{n} \frac{(n+1)!}{(k+1)!\,(n-k)!} \left[Cc'^{-\nu/2} \exp\left\{-c'' \frac{d^2(n+1)}{4\beta}\right\}\right]^{k+1} \\ &= c'^{-\nu/2} p\left(y, x; \frac{\beta}{c'}\right) \left(\left[1 + Cc'^{-\nu/2} \exp\left\{-c'' \frac{d^2(n+1)}{4\beta}\right\}\right]^{n+1} - 1\right) \underset{n=\infty}{\longrightarrow} 0 \ .\end{aligned}$$

This ends the proof in the case $B = \Omega_{\Lambda,\beta}$.

If $B \subset \Omega_{\Lambda,\beta}$ is an arbitrary Borel set, there is a sequence of functions in $C_{\text{fin}}(\Omega_{\Lambda,\beta})$ converging to the characteristic function of B, and it is sufficient to prove

$$\int_{\Omega_{\Lambda,\beta}} \varphi(\omega)\alpha_\Lambda(\omega) d\mu_{x,y}^{\sigma,\Lambda,\beta}(\omega) = \int_{\Omega_\beta} \varphi(\omega)\alpha_\Lambda(\omega) d\mu_{x,y}^{\beta}(\omega)$$

for $\varphi \in C_{\text{fin}}(\Omega_{\Lambda,\beta})$. But φ has the form

$$\varphi(\omega) = F(\omega(t_1), \ldots, \omega(t_m)) \ ,$$

where $F : (\dot{\mathbb{R}}^\nu)^m \mapsto \mathbb{C}$ is continuous, and $0 \le t_1 < t_2 \cdots < t_m \le \beta$. It follows from the first part of the proof that

$$\begin{aligned}
&\int_{\Omega_{\Lambda,\beta}} \varphi(\omega)\alpha_\Lambda(\omega)d\mu_{x,y}^{\sigma,\Lambda,\beta}(\omega) \\
&\quad = \int_{\Lambda^m} dx_1 \ldots dx_m F(x_1,\ldots,x_m) \int_{\Omega_{\Lambda,t_1}} \alpha_\Lambda(\omega_1)d\mu_{x,x_1}^{\sigma,\Lambda,t_1}(\omega_1) \\
&\qquad \times \int_{\Omega_{\Lambda,t_2-t_1}} \alpha_\Lambda(\omega_2)d\mu_{x_1,x_2}^{\sigma,\Lambda,t_2-t_1}(\omega_2)\cdots \int_{\Omega_{\Lambda,\beta-t_m}} \alpha_\Lambda(\omega_{m+1})d\mu_{x_m,y}^{\sigma,\Lambda,\beta-t_m}(\omega_{m+1}) \\
&\quad = \int_{\Lambda^m} dx_1 \ldots dx_m F(x_1,\ldots,x_m) \int_{\Omega_{t_1}} \alpha_\Lambda(\omega_1)d\mu_{x,x_1}^{t_1}(\omega_1) \\
&\qquad \times \int_{\Omega_{\Lambda,t_2-t_1}} \alpha_\Lambda(\omega_2)d\mu_{x_1,x_2}^{t_2-t_1}(\omega_2)\cdots \int_{\Omega_{\Lambda,\beta-t_m}} \alpha_\Lambda(\omega_{m+1})d\mu_{x_m,y}^{\beta-t_m}(\omega_{m+1}) \\
&\quad = \int_{\Omega_\beta} \varphi(\omega)\alpha_\Lambda(\omega)d\mu_{x,y}^{\beta}(\omega) \ .
\end{aligned}$$

One implication of Theorem 6.3.9 is that the Wiener measure $\mu_{x,y}^{\infty,\Lambda,\beta}$ corresponding to Dirichlet boundary conditions is obtained from the free measure $\mu_{x,y}^{\beta}$ by multiplication with the characteristic function α_Λ of Λ. This confirms the physical interpretation of Dirichlet boundary conditions as completely absorbtive.

Corollary 6.3.10. *For every Borel subset $B \subseteq \Omega_{\Lambda,\beta}$ and all $x, y \in \Lambda$ one has*

$$\mu_{x,y}^{\infty,\Lambda,\beta}(B) = \int_B \alpha_\Lambda(\omega)d\mu_{x,y}^{\beta}(\omega) = \mu_{x,y}^{\beta}(B \cap \{\omega\,;\ \alpha_\Lambda(\omega) = 1\}) \ .$$

PROOF. Because of Theorem 6.3.9., it is enough to show that the set A of trajectories inside $\overline{\Lambda}$ which touch $\partial\Lambda$ for some $t \in [0,\beta]$ has $\mu_{x,y}^{\infty,\Lambda,\beta}$ measure zero. But in the proof of Theorem 6.3.8 we demonstrated that $z_{\infty,\Lambda}(x,y\,;t) \ge 0$ for all $x, y \in \Lambda, t > 0$ and hence

$$0 \le p_{\infty,\Lambda}(x,y\,;t) \ \le \ p(x,y\,;t) \ .$$

Using the definitions of Wiener measures this leads to the estimate

$$\mu_{x,y}^{\infty,\Lambda,\beta}(B) \ \le \ \mu_{x,y}^{\beta}(B)$$

for all measurable sets $B \subseteq \Omega_{\Lambda,\beta}$. Hence, it is enough to show that

$$\mu_{x,y}^{\beta}(A) = 0 \ .$$

This is a well-known general property of the Wiener process which can roughly be expressed by stating that if a point lies near a smooth $(\nu-1)$-dimensional surface, then it is very improbable that a trajectory starting at the point will not cross the surface in the near future (see Notes and Remarks).

EXAMPLE 6.3.11. If Λ is a parallelepiped, the Green's functions corresponding to Dirichlet and Neumann boundary conditions can be explicitly calculated. It suffices to consider the case $\nu = 1$ since the Green's functions in higher dimensions are simply

products of the functions in one dimension. Now for $x, y \in \langle -L/2, L/2\rangle$ and $t > 0$ one has

$$p_{0,\Lambda}(x, y; t) = \sum_{n=-\infty}^{\infty} p(x, y + 2nL; t) + \sum_{n=-\infty}^{\infty} p(x, (2n+1)L - y; t) ,$$

$$p_{\infty,\Lambda}(x, y; t) = \sum_{n=-\infty}^{\infty} p(x, y + 2nL; t) - \sum_{n=-\infty}^{\infty} p(x, (2n+1)L - y; t) .$$

This again illustrates the nature of the boundary conditions.

It is often technically convenient when Λ is a parallelepiped to work with *periodic boundary conditions,* i.e.,

$$\rho(L/2, t) = \rho(-L/2, t) , \quad \frac{\partial \rho}{\partial x}(L/2, t) = \frac{\partial \rho}{\partial x}(-L/2, t) .$$

The corresponding Green's function is then given by

$$p_{\mathrm{per},\Lambda}(x, y; t) = \sum_{n=-\infty}^{\infty} p(x, y + nL; t) .$$

If we define $\varepsilon : \mathbb{R} \mapsto [-L/2, L/2]$ by

$$\varepsilon(x) = \begin{cases} x - 2nL & \text{if } (2n - \frac{1}{2})L \le x \le (2n + \frac{1}{2})L \\ (2n+1)L - x & \text{if } (2n + \frac{1}{2})L \le x \le (2n + \frac{3}{2})L \end{cases}$$

$$n = 0, \pm 1, \pm 2, \ldots$$

and $\varepsilon'; \Omega_\beta \mapsto \Omega_{[-L/2, L/2], \beta}$ by

$$[\varepsilon'(\omega)](t) = \varepsilon(\omega(t)) ,$$

then the relation between the Green's functions $p_{0,\Lambda}$ and p is reflected in the following relations between the functional measures:

$$\mu_{x,y}^{0,\Lambda,\beta}(B) = \sum_{z \in \varepsilon^{-1}(y)} \mu_{x,z}^{\beta}(\varepsilon'^{-1}(B))$$

for all Borel subsets $B \subseteq \Omega_{[-L/2, L/2], \beta}$. A similar relation can be derived for periodic boundary conditions.

To conclude this section we state the finite-volume version of the Feynman–Kac formula which will be needed in the sequel and show that it immediately implies a monotonicity property used in Chapter 5.

Theorem 6.3.12. *Let U, V be operators of multiplication by real functions on $L^2(\mathbb{R}^\nu)$. Assume that U is $T_{\sigma,\Lambda}^{(1)}$-bounded with relative bound less than one and that $V \in L^1_{\mathrm{loc}}(\mathbb{R}^\nu)$ is bounded below. If*

$$H_{\sigma,\Lambda}^{(1)} = (T_{\sigma,\Lambda}^{(1)} + U) \dot{+} V$$

and $\beta > 0$, it follows that $\exp\{-\beta H^{(1)}_{\sigma,\Lambda}\}$ *is an integral operator on* $L^2(\bar{\Lambda})$ *with kernel*

$$e^{-\beta H^{(1)}_{\sigma,\Lambda}}(x, y) = \int_{\Omega_{\Lambda,\beta}} d\mu^{\sigma,\Lambda,\beta}_{x,y}(\omega) \exp\left\{-\int_0^\beta dt(U(\omega(t)) + V(\omega(t)))\right\} .$$

In the case of Dirichlet conditions, $\sigma = \infty$, this kernel has the simpler representation

$$e^{-\beta H^{(1)}_{\infty,\Lambda}}(x, y) = \int_{\Omega_\beta} d\mu^{\beta}_{x,y}(\omega)\alpha_\Lambda(\omega) \exp\left\{-\int_0^\beta dt(U(\omega(t)) + V(\omega(t)))\right\} .$$

But $\mu^{\beta}_{x,y}$ is positive and the integrand is monotonic in Λ. Therefore, one has the following.

Corollary 6.3.13. *Under the hypotheses of Theorem* 6.3.12 *it follows that the mapping*

$$\Lambda \to e^{-\beta H^{(1)}_{\infty,\Lambda}}(x, y)$$

is positive and monotone increasing.

This property was used in the noninteracting case to prove Proposition 5.2.31.

One can also use the Feynman–Kac technique to obtain an integral relation for the kernels of n-particle semigroups $\exp\{-\beta H^{(n)}_{\sigma,\Lambda}\}$ but the symmetry, or anti-symmetry, of the wave functions arising from quantum statistics causes some additional combinatorial complications. This will be examined in more detail in the next section.

6.3.3. The Thermodynamic Limit. I. The Reduced Density Matrices

In Section 6.3.1 we defined a class of selfadjoint interacting Hamiltonians $H_{\sigma,\Lambda}$ on Fock space and subsequently showed that if the interaction is stable, then $\exp\{-\beta(H_{\sigma,\Lambda} - \mu N_\Lambda)\}$ is of trace-class for $\beta > 0$ and μ sufficiently negative. Therefore, one may introduce the finite-volume Gibbs states $\omega^{\beta,\mu}_{\sigma,\Lambda}$,

$$\omega^{\beta,\mu}_{\sigma,\Lambda}(A) = \frac{\mathrm{Tr}_{\mathfrak{F}_\pm(\Lambda)}(e^{-\beta(H_{\sigma,\Lambda}-\mu N_\Lambda)}A)}{\mathrm{Tr}_{\mathfrak{F}_\pm(\Lambda)}(e^{-\beta(H_{\sigma,\Lambda}-\mu N_\Lambda)})} ,$$

where $A \in \mathfrak{A}_\pm(\Lambda)$. In this section we begin the study of the thermodynamic limits

$$\omega^{\beta,\mu}_{\sigma}(A) = \lim_{\Lambda\to\infty} \omega^{\beta,\mu}_{\sigma,\Lambda}(A) .$$

Since β, μ, and σ are usually held fixed, we will often omit the suffices. Thus, we write $\omega_\Lambda = \omega^{\beta,\mu}_{\sigma,\Lambda}, \omega = \omega^{\beta,\mu}_{\sigma}$, etc. The analysis of these limits is based upon

examination of a family of functions $\tilde{\rho}_\Lambda$ on $\mathbb{R}^{\nu m} \times \mathbb{R}^{\nu m}, m = 1, 2, \ldots$, which are defined such that

$$\begin{aligned}\omega_\Lambda(a^*(f_1)\cdots a^*(f_m)a(g_m)\cdots a(g_1)) \\ = \int dx_1 \ldots dx_m\, dy_1 \ldots dy_m\, \overline{g_1(y_1)} \ldots \overline{g_m(y_m)} f_1(x_1) \ldots f_m(x_m) \\ \times \tilde{\rho}_\Lambda(y_1, \ldots, y_m\,; x_1, \ldots, x_m)\ .\end{aligned}$$

These functions are called the *reduced density matrices*. It is of course not clear *a priori* that the $\tilde{\rho}_\Lambda$ exist as functions but this will subsequently be established for a variety of interactions and values of β and μ. Formally one may write

$$\tilde{\rho}_\Lambda(y_1, \ldots, y_m\,; x_1, \ldots, x_m) = \omega_\Lambda(a^*_{\omega_\Lambda}(x_1)\cdots a^*_{\omega_\Lambda}(x_m)a_{\omega_\Lambda}(y_m)\cdots a_{\omega_\Lambda}(y_1))$$

and we will show the thermodynamic limit of the states exists by first proving that the $\tilde{\rho}_\Lambda$ have an infinite volume limit for sufficiently small values of the activity $z = \exp\{\beta\mu\}$. The strategy of the proof is to find a convenient functional integral representation of the $\tilde{\rho}_\Lambda$ in terms of a sequence of functions ρ_Λ which are analogues of *correlation functions* of classical statistical mechanics. The ρ_Λ are functions over trajectories joining the points x, y, occurring in the $\tilde{\rho}_\Lambda$, and correspond physically to the probability densities for finding the different trajectories.

The second crucial observation is that the ρ_Λ can be interpreted as the solution of an inhomogeneous linear integral equation of the type already encountered in the discussion of spin systems in Section 6.2.5. Therefore, one may derive an analogue of Proposition 6.2.45 which in the present context corresponds to a uniqueness statement for the thermodynamic limit of the ρ_Λ, and hence the $\tilde{\rho}_\Lambda$, at small activity.

The existence of the thermodynamic limit for the Gibbs states ω_Λ of a system of fermions follows immediately from the existence property for the $\tilde{\rho}_\Lambda$. In the case of bosons it is also possible to relate the two properties by use of the theory of analytic states discussed in Section 5.2.3. The $\tilde{\rho}_\Lambda$ directly determine the derivatives of the functions $t \mapsto \omega_\Lambda(W(tf))$ and to relate the two limits it suffices to obtain suitable *a priori* bounds on the $\tilde{\rho}_\Lambda$ which control the growth of $\tilde{\rho}_\Lambda(y_1, \ldots, y_m\,; x_1, \ldots, x_m)$ with m. At small activities these bounds follow from the integral equations but for positive interactions they may be directly deduced from the functional integration representation of the $\tilde{\rho}_\Lambda$. Thus, in the latter case one may obtain some tentative global information on the Gibbs states ω. We leave the discussion of the limits of the states ω_Λ to the next subsection and now concentrate on the $\tilde{\rho}_\Lambda$.

Although the above strategy for establishing the thermodynamic limit may seem strangely indirect, it is quite natural to introduce and study the reduced density matrices $\tilde{\rho}_\Lambda$ since it may be argued that their values are directly related to physically measurable correlation effects. One then sees that the Wiener integral plays a purely technical role in this context and it seems worthwhile to pursue a more pure operator-theoretic approach. In fact the seemingly most significant information openly exhibited by the Wiener integral is the pointwise

positivity of the semigroup kernels. This, for example, implies pointwise positivity for the $\tilde{\rho}_\Lambda$ with Bose statistics. This type of positivity is less accessible from the pure operator approach but apparently has many important consequences.

We now enter into more detail of the program outlined above. First, we introduce some notation. We denote m-tuples $(x_1, \ldots, x_m)$ of points in Λ by x^m, and m-tuples $(\omega_1, \ldots, \omega_m)$ of paths in $\Omega_{\Lambda,\beta}$ by ω^m. The symbol $\bar{\rho}_\Lambda$ will be used alternatively to denote the operator

$$(\mathrm{Tr}_{\mathfrak{F}_\pm(\Lambda)}(e^{-\beta(H_{\sigma,\Lambda}-\mu N_\Lambda)}))^{-1} e^{-\beta(H_{\sigma,\Lambda}-\mu N_\Lambda)}$$

and the integral kernel of this operator. The m-particle part of this operator and the associated kernel will be denoted by $\bar{\rho}_{\Lambda,m}$. Thus, we have the decomposition

$$\bar{\rho}_\Lambda = \bigoplus_{m=0}^{\infty} \bar{\rho}_{\Lambda,m}$$

corresponding to the decomposition

$$\mathfrak{F}_\pm(\Lambda) = \bigoplus_{m=0}^{\infty} L^2(\Lambda)^m_\pm$$

of Fock space. The operator $\bar{\rho}_\Lambda$ is called the *density matrix* for the problem.

The *reduced density matrices* $\tilde{\rho}_{\Lambda,m}$ may now be defined by

$$\tilde{\rho}_{\Lambda,m} = \sum_{n=0}^{\infty} \frac{(m+n)!}{n!} \mathrm{Tr}_n(\bar{\rho}_{\Lambda,\,m+n}) \ ,$$

where Tr_n is the partial trace over n particles. This is unambiguously defined because of the symmetry of $\bar{\rho}_{\Lambda,m+n}$ in the $m+n$ particles. The integral kernels of $\tilde{\rho}_{\Lambda,m}$ will also be denoted by $\tilde{\rho}_{\Lambda,m}$ or simply $\tilde{\rho}_\Lambda$. One can then prove the relation

$$\omega_\Lambda(a^*_{\omega_\Lambda}(x_1)\cdots a^*_{\omega_\Lambda}(x_m) a_{\omega_\Lambda}(y_m)\cdots a_{\omega_\Lambda}(y_1)) = \tilde{\rho}_\Lambda(y^m; x^m)$$

mentioned earlier.

We are principally interested in deriving integral representations of $\bar{\rho}_\Lambda$ and $\tilde{\rho}_\Lambda$ in the case of Bose or Fermi statistics, but this involves combinatorial problems which can be avoided in the case of *Boltzmann statistics*, so we first consider this latter case. The appropriate Hilbert space $\mathfrak{F}(\Lambda)$, density matrix $\bar{\rho}_\Lambda$, and partition function Z_Λ for Boltzmann statistics are

$$\mathfrak{F}(\Lambda) = \bigoplus_{n\geq 0} L^2(\Lambda)^n \ ,$$

where $L^2(\Lambda)^n$ is the n-fold tensor product of $L^2(\Lambda)$ without any symmetrization,

$$\bar{\rho}_\Lambda = Z_\Lambda^{-1} \bigoplus_{n\geq 0} \frac{1}{n!} \exp\{-\beta(H^{(n)}_{\sigma,\Lambda} - \mu n \mathbb{1})\}$$

and

$$Z_\Lambda = \sum_{n\geq 0} \frac{1}{n!} \mathrm{Tr}_{L^2(\Lambda)^n}(\exp\{-\beta(H^{(n)}_{\sigma,\Lambda} - \mu n \mathbb{1})\}) \ .$$

Let $\omega^m = (\omega_1, \ldots, \omega_m)$ and $\tilde{\omega}^m = (\tilde{\omega}_1, \ldots, \tilde{\omega}_m)$ be two families of trajectories in $\Omega_{\Lambda,\beta}$ with starting points x^m and u^n and end points y^m and v^n, respectively. Define the *interaction* $U(\omega^m)$ of the family ω^m by

$$U(\omega^m) = \int_0^\beta dt\ U^{(m)}(\omega_1(t), \ldots, \omega_m(t))$$

and similarly $U(\omega^m, \tilde{\omega}^n)$ is the interaction of the family $\omega^m \cup \tilde{\omega}^n$. With these notations, the Feynman–Kac formula, Theorem 6.3.7, can be written as

$$\begin{aligned}&\exp(-\beta H_{\sigma,\Lambda}^{(m+n)})(x^m u^n, y^m v^n)\\ &\quad = \int_{\Omega_{\Lambda^{n+m},\beta}} \exp\{-U(\omega^m, \tilde{\omega}^n)\} d\mu_{x^m u^n, y^m v^n}^{\sigma,\Lambda,\beta}(\omega^m, \tilde{\omega}^n)\ ,\end{aligned}$$

where we use the notation

$$d\mu_{x^m u^n, y^m v^n}^{\sigma,\Lambda,\beta}(\omega^m, \tilde{\omega}^n) = \left(\prod_{k=1}^m d\mu_{x_k, y_k}^{\sigma,\Lambda,\beta}(\omega_k)\right)\left(\prod_{l=1}^n d\mu_{u_l, v_l}^{\sigma,\Lambda,\beta}(\tilde{\omega}_l)\right)\ .$$

We now take the partial trace over the last n particles. This amounts to putting $u^n = v^n$ in the expression above, and then integrating over u_l in Λ for $l = 1, 2, \ldots, n$. We then substitute the result into the definition of $\tilde{\rho}_\Lambda$ and decompose the integration over the $m+n$ trajectories ω^m and $\tilde{\omega}^n$ in two steps. The second step is an integration over the m open trajectories in ω^m of an intermediate functional $\rho_\Lambda(\omega^m)$ of these trajectories. The function $\rho_\Lambda(\omega^m)$ is obtained in the first step by integrating over the closed trajectories in $\tilde{\omega}^n$ and then summing over n. The result is

$$\tilde{\rho}_\Lambda(x^m; y^m) = \int_{\Omega_{\Lambda^m,\beta}} \rho_\Lambda(\omega^m) d\mu_{x^m, y^m}^{\sigma,\Lambda,\beta}(\omega^m)\ ,$$

where

$$\rho_\Lambda(\omega^m) = Z_\Lambda^{-1} \sum_{n \geq 0} \frac{1}{n!} \int_{\Omega_{\Lambda^n,\beta}} d\tilde{\omega}_1 \ldots d\tilde{\omega}_n\, z^{m+n} \exp\{-U(\omega^m, \tilde{\omega}^n)\}\ ,$$

$z = \exp\{\beta\mu\}$ is the activity, and

$$d\tilde{\omega}_k = \int_\Lambda d\mu_{u,u}^{\sigma,\Lambda,\beta}(\tilde{\omega}_k) du\ .$$

This is the desired integral representation of $\tilde{\rho}_\Lambda$ in the case of Boltzmann statistics. The partition function Z_Λ can be represented as

$$Z_\Lambda = \sum_{n \geq 0} \frac{z^n}{n!} \int_{\Omega_{\Lambda^n,\beta}} d\tilde{\omega}_1 \ldots d\tilde{\omega}_n \exp\{-U(\tilde{\omega}^n)\}\ .$$

In analogy with classical statistical mechanics we call ρ_Λ the *correlation functionals*.

We next turn to the case of Bose and Fermi statistics. The density matrix is now given by

$$\bar{\rho}_\Lambda = Z_{\Lambda,\varepsilon}^{-1} P_\varepsilon \bigoplus_{n\geq 0} \exp\{-\beta(H_{\sigma,\Lambda}^{(n)} - \mu n \mathbb{1})\} \ ,$$

where P_ε is the projection onto the even or odd subspace of $L^2(\Lambda)^n$ according to whether $\varepsilon = +1$ or $\varepsilon = -1$. The partial trace formulas for the reduced density matrices now become

$$\tilde{\rho}_\Lambda(x^m; y^m) = Z_{\Lambda,\varepsilon}^{-1} \sum_{n=0}^{\infty} \frac{z^{m+n}}{n!} \int du^n \sum_\pi \varepsilon^\pi e^{-\beta H_{\sigma,\Lambda}^{(n)}}(x^m u^n, \pi(y^m u^n)) \ ,$$

where π is a permutation of $m+n$ variables, and

$$Z_{\Lambda,\varepsilon} = \sum_{n=0}^{\infty} \frac{z^n}{n!} \int du^n \sum_\pi \varepsilon^\pi e^{-\beta H_{\sigma,\Lambda}^{(n)}}(u^n, \pi(u^n)) \ ,$$

where π is a permutation of n variables. The π-sum is over the full symmetric group in both expressions, and $\varepsilon^\pi = +1$ for bosons, but ε^π is the signature of the permutation π for fermions.

We proceed as previously by putting the Feynman–Kac formula for the kernel of $\exp\{-\beta H_{\sigma,\Lambda}^{(n)}\}$ into the above formula for the reduced density matrices. Now, however, complications arise from the permutations π of the endpoints $y^m u^n$ of the $m+n$ trajectories in the path space integration. The path starting at a point x_k does not necessarily go to the point y_k along ω_k as previously. Instead one may go to one of the integration points u_i, then to another one u_j, etc., and finally end up in a point y_l which might differ from y_k. This has the effect that several *elementary trajectories,* by which we mean trajectories with time interval β, may be inserted between x_k and the corresponding y_l to build a *composite trajectory* with time interval $j_k\beta$ for some positive integer j_k. Similarly, the elementary trajectories that are not used to build composite trajectories connecting some x_k with some y_l combine together to form composite closed loops with time intervals which are integer multiples of β. We rearrange the sum defining $\tilde{\rho}_\Lambda$, which is a sum over n and over the permutations of $m+n$ elements, so as to separate the integrations over the composite open trajectories and over the composite closed loops. We will omit the ensuing combinatorial argument, and only cite the end result.

Theorem 6.3.14. *The m-particle reduced density matrices of an interacting Bose or Fermi gas enclosed in a finite region Λ with boundary conditions σ can be written as follows:*

$$\tilde{\rho}_\Lambda(x^m; y^m) = \sum_\pi \varepsilon^\pi \prod_{i=1}^{m} \left\{ \sum_{j_i=1}^{\infty} \varepsilon^{j_i - 1} \int d\mu_{x_i,\pi(y_i)}^{\sigma,\Lambda,j_i\beta}(\omega_i) \right\} \rho_\Lambda(\omega^m) \ ,$$

where $\omega^m = (\omega_1, \ldots, \omega_m)$ is a family of m composite trajectories with time intervals $j_1\beta, j_2\beta, \ldots, j_m\beta$, respectively. The first sum runs over all permutations of the m points $y_1, \ldots, y_m$ and $\varepsilon^\pi = 1$ for bosons, but ε^π is the signature of π for fermions. Also, $\varepsilon = 1$ for bosons and $\varepsilon = -1$ for fermions. The correlation functional $\rho_\Lambda(\omega^m)$ is defined by the formula

$$\rho_\Lambda(\omega^m) = Z_{\Lambda,\varepsilon}^{-1} \sum_{n=0}^{\infty} \frac{1}{n!} \int d\tilde{\omega}_1 \ldots d\tilde{\omega}_n z^{q+r} \exp\{-U(\omega^m, \tilde{\omega}^n)\} \ ,$$

where $\tilde{\omega}^n = (\tilde{\omega}_1, \ldots, \tilde{\omega}_n)$ *is a family of* n *composite closed loops,* q *and* r *are the number of elementary trajectories that constitute* ω^m *and* $\tilde{\omega}^n$*, respectively,* $Z_{\Lambda,\varepsilon}$ *is the appropriate partition function, and* $z = \exp\{\beta\mu\}$ *the activity. Moreover,* $U(\omega^m, \tilde{\omega}^n)$ *is the integral from* 0 to β *of the potential energy of the* $q + r$ *points on the* $m + n$ *trajectories* $\omega^m, \tilde{\omega}^n$ *at time* t *modulo* β*. Finally, the integrals* $d\tilde{\omega}$ *are defined by*

$$d\tilde{\omega} = \sum_{j=1}^{\infty} \frac{\varepsilon^{j-1}}{j} \int_\Lambda d\mu_{u,u}^{\sigma,\Lambda,j\beta}(\tilde{\omega}) du$$

and the partition function is given by

$$Z_{\Lambda,\varepsilon} = \sum_{n=0}^{\infty} \frac{1}{n!} \int d\tilde{\omega}_1 \ldots d\tilde{\omega}_n z^r \exp\{-U(\tilde{\omega}^n)\} \ .$$

EXAMPLE 6.3.15. The formulas in Theorem 6.3.14 can be simplified in the case of Dirichlet boundary conditions, $\sigma = \infty$. This simplication occurs because the finite-volume Wiener measure with Dirichlet boundary conditions is obtained from the infinite-volume measure by multiplication with the characteristic function α_Λ of Λ, see Corollary 6.3.10. Thus, in this case it is convenient to define ρ_Λ slightly differently than above. The formulas then become

$$\tilde{\rho}_\Lambda(x^m; y^m) = \sum_\pi \varepsilon^\pi \prod_{i=1}^{m} \left\{ \sum_{j_i=1}^{\infty} \varepsilon^{j_i-1} \int d\mu_{x_i,\pi(y_i)}^{j_i,\beta}(\omega_i) \right\} \rho_\Lambda(\omega^m) \ ,$$

where

$$\rho_\Lambda(\omega^m) = Z_{\Lambda,\varepsilon}^{-1} \sum_{n\geq 0} \frac{1}{n!} \int d\tilde{\omega}_1 \ldots d\tilde{\omega}_n z^{q+r} \alpha_\Lambda(\omega^m, \tilde{\omega}^n) \exp\{-U(\omega^m, \tilde{\omega}^n)\} \ ,$$

$$d\tilde{\omega} = \sum_{j=1}^{\infty} \frac{\varepsilon^{j-1}}{j} \int d\mu_{u,u}^{j\beta}(\tilde{\omega}) du \ ,$$

$$Z_{\Lambda,\varepsilon} = \sum_{n=0}^{\infty} \frac{1}{n!} \int d\tilde{\omega}_1 \ldots d\tilde{\omega}_n z^r \alpha_\Lambda(\tilde{\omega}_n) \exp\{-U(\tilde{\omega}^n)\} \ ,$$

$d\mu_{x,y}^t$ is the infinite-volume Wiener measure, and

$$\alpha_\Lambda(\omega^m, \tilde{\omega}^n) = \begin{cases} 1 & \text{if all the trajectories } \omega_1, \ldots, \omega_m, \tilde{\omega}_1, \ldots, \tilde{\omega}_n, \text{ remain inside } \Lambda, \\ 0 & \text{otherwise.} \end{cases}$$

In the case of Boltzmann statistics the formulas become

$$\tilde{\rho}_\Lambda(x^m; y^m) = \int d\mu_{x^m,y^m}^{\beta}(\omega^m) \rho_\Lambda(\omega^m) \ ,$$

where

$$\rho_\Lambda(\omega^m) = Z_\Lambda^{-1} \sum_{n=0}^{\infty} \frac{1}{n!} \int d\tilde{\omega}_1 \ldots d\tilde{\omega}_n z^{m+n} \alpha_\Lambda(\omega^m, \tilde{\omega}^n) \exp\{-U(\omega^m, \tilde{\omega}^n)\}$$

and

$$d\tilde{\omega} = \int d\mu^\beta_{u,u}(\omega) du \ ,$$

$$Z_\Lambda = \sum_{n=0}^{\infty} \frac{z^n}{n!} \int d\tilde{\omega}_1 \ldots d\tilde{\omega}_n \, \alpha_\Lambda(\tilde{\omega}^m) \exp\{-U(\tilde{\omega}^n)\} \ .$$

In these cases the measures defining the reduced density matrices $\tilde{\rho}_\Lambda$ from the correlation functions ρ_Λ contain no information about the detailed properties of the system, i.e., properties of the interaction U, the chemical potential μ, and the region Λ. All this information is contained in the functionals ρ_Λ.

EXAMPLE 6.3.16. In the case of the ideal Bose or Fermi gas, $U = 0$, and with Dirichlet boundary conditions, $\sigma = \infty$, the expression for the partition function obtained in Example 6.3.15 takes the form

$$Z_{\Lambda,\varepsilon} = \exp\left\{ \sum_{j=1}^{\infty} \frac{\varepsilon^{j-1} z^j}{j} \int_\Lambda \int d\mu^{j\beta}_{x,x}(\tilde{\omega}) dx \ \alpha_\Lambda(\tilde{\omega}) \right\}$$

and hence the infinite-volume limit of the pressure

$$P = \lim_{\Lambda \to \infty} \frac{1}{\beta|\Lambda|} \log \ Z_{\Lambda,\varepsilon}$$

exists and can be computed as

$$\begin{aligned} P &= \lim_{\Lambda \to \infty} \frac{1}{\beta|\Lambda|} \sum_{j=1}^{\infty} \frac{\varepsilon^{j-1} z^j}{j} \int_\Lambda \int d\mu^{j\beta}_{x,x}(\tilde{\omega}) dx \ \alpha_\Lambda(\tilde{\omega}) \\ &= \lim_{\Lambda \to \infty} \frac{1}{\beta|\Lambda|} \sum_{j=1}^{\infty} \frac{\varepsilon^{j-1} z^j}{j} \int_\Lambda dx \, (4\pi j\beta)^{-\nu/2} = \frac{1}{\beta} \frac{1}{(4\pi\beta)^{\nu/2}} \sum_{j=1}^{\infty} \frac{\varepsilon^{j-1} z^j}{j^{1+\nu/2}} \ . \end{aligned}$$

Since both the finite- and infinite-volume states are quasi-free (see Propositions 5.2.28 and 5.2.29), we have the following expansion of the $\tilde{\rho}_\Lambda(x^m; y^m)$ reduced density matrices in terms of the $\tilde{\rho}_\Lambda(x; y)$ reduced density matrices:

$$\tilde{\rho}_\Lambda(x^m; y^m) = \sum_\pi \varepsilon^\pi \prod_{j=1}^{m} \tilde{\rho}_\Lambda(x_j; \pi(y_j)) \ .$$

Here the sum extends over all $m!$ permutations of $\{y_1, y_2, \ldots, y_m\}$ and the two-point reduced density matrix is given by

$$\tilde{\rho}_\Lambda(x; y) = \sum_{j=1}^{\infty} \varepsilon^{j-1} z^j \int d\mu^{j\beta}_{x,y}(\omega) \alpha_\Lambda(\omega) \ .$$

Thus for Bose statistics $\Lambda \mapsto \tilde{\rho}_\Lambda$ is a positive monotonically increasing function. Moreover the infinite-volume reduced density matrices $\tilde{\rho}(x^m; y^m)$ exist for both statistics and

$$\tilde{\rho}(x^m; y^m) = \sum_\pi \varepsilon^\pi \prod_{j=1}^{m} \tilde{\rho}(x_j; \pi(y_j)) \ ,$$

where

$$\tilde{\rho}(x;y) = \lim_{\Lambda\to\infty} \tilde{\rho}_\Lambda(x;y) = (4\pi\beta)^{-\nu/2} \sum_{j=1}^{\infty} \frac{\varepsilon^{j-1} z^j}{j^{\nu/2}} \exp\left\{-\frac{(x-y)^2}{4j\beta}\right\} .$$

To illustrate the utility of the integral representation for the reduced density matrices we first prove that for a Bose gas with positive interaction potentials these matrices are bounded by the corresponding matrices without interaction. This form of *a priori* estimate is particularly useful for linking the existence of the thermodynamic limits of the states and the reduced density matrices.

Note that if the interaction potentials are positive then

$$U^{(m+n)}(x^m, y^n) \geq U^{(m)}(x^m) + U^{(n)}(y^n) .$$

This follows by remarking that the difference between the two expressions is the interaction energy between the particles at the points x and the particles at the points y, i.e., it is a sum of positive potentials.

Theorem 6.3.17. *Consider an interacting Bose gas for which all the potentials $\Phi^{(k)}$ are positive and $\Phi^{(k)} \in L^1_{\mathrm{loc}}(\mathbb{R}^{\nu k})$. Let $\tilde{\rho}^U_{\sigma,\Lambda}$ and $\tilde{\rho}^0_{\sigma,\Lambda}$ denote the finite volume reduced density matrices with interaction U and without interaction.*

It follows that

$$0 \leq \tilde{\rho}^U_{\sigma,\Lambda}(x^m; y^m) \leq \tilde{\rho}^0_{\sigma,\Lambda}(x^m; y^m) \leq \tilde{\rho}^0_{0,\Lambda}(x^m; y^m) .$$

for all $x^m, y^m \in \Lambda^m$, all $\beta > 0$, $\mu < 0$ and $\sigma \geq 0$.

Proof. It follows from the integral representation in Theorem 6.3.14 and the choice of Bose statistics that each term in the representation is positive. Thus, $\rho^U_{0,\Lambda} \geq 0$ and for the first upper bound it suffices to prove

$$0 \leq \rho^U_{\sigma,\Lambda}(\omega^m) \leq \rho^0_{\sigma,\Lambda}(\omega^m) .$$

But

$$\rho^U_{\sigma,\Lambda}(\omega^m) = Z^{-1}_{\sigma,\Lambda} \sum_{n=0}^{\infty} \frac{1}{n!} \int d\tilde{\omega}_1 \ldots d\tilde{\omega}_n z^{q+r} \exp\{-U(\omega^m, \tilde{\omega}^n)\}$$

and because we assume the potentials to be positive one has

$$\exp\{-U(\omega^m, \tilde{\omega}^n)\} \leq \exp\{-U(\omega^m)\} \exp\{-U(\tilde{\omega}^n)\} .$$

Therefore

$$\begin{aligned}\rho^U_{\sigma,\Lambda}(\omega^m) &\leq z^q \exp\{-U(\omega^m)\} Z^{-1}_{\sigma,\Lambda} \sum_{n=0}^{\infty} \frac{1}{n!} \int d\tilde{\omega}_1 \ldots d\tilde{\omega}_n z^r \exp\{-U(\tilde{\omega}^n)\} \\ &= z^q \exp\{-U(\omega^m)\} \leq z^q .\end{aligned}$$

But the same computation for $U = 0$ gives

$$\rho^0_{\sigma,\Lambda}(\omega^m) = z^q$$

and this completes the proof of the upper bound. Finally, the Green's functions are monotonically decreasing functions of the boundary condition function σ and hence the largest value for $\tilde{\rho}^0_{\sigma,\Lambda}$ occurs for the smallest value of σ, i.e., the Neumann condition $\sigma = 0$.

If one considers Dirichlet boundary conditions, then one may utilize the monotonicity in Λ of the noninteracting reduced density matrices (see example 6.3.16) to obtain a bound which is uniform in Λ and is even valid for $\mu = 0$.

Corollary 6.3.18. *Adopt the general assumptions of Theorem* 6.3.17 *but with Dirichlet boundary conditions.*

It follows that

$$0 \leq \tilde{\rho}^U_\Lambda(x^m; y^m) \leq \tilde{\rho}^0_\Lambda(x^m; y^m) \leq \lim_{\Lambda \to \infty} \tilde{\rho}^0_\Lambda(x^m; y^m) \ ,$$

where $\tilde{\rho}^U_\Lambda (= \tilde{\rho}^U_{\infty,\Lambda})$ *denotes the Dirichlet reduced density matrices and* $\beta > 0$ *and* $\mu \leq 0$ *Consequently,*

$$0 \leq \tilde{\rho}^U_\Lambda(x^m; y^m) \leq z^m \sum_\pi \prod_{i=1}^m \rho(x_i - \pi(y_i)) \ ,$$

where

$$\rho(x) = (2\pi)^{-\nu} \int d^\nu p \, e^{ipx} e^{-\beta p^2} (1 - z e^{-\beta p^2})^{-1} \ .$$

Thus, for positive interactions and arbitrary Λ the Dirichlet reduced density matrices are positive bounded functions.

Next we discuss the reduced density matrices for small values of the activity. In order to proceed it is necessary to impose conditions on the interactions U_Λ. In fact, as pointed out in Section 6.3.1, we need a stability condition

$$U_\Lambda \geq -BN_\Lambda$$

(or possibly a weaker condition on the total Hamiltonian) in order that the finite-volume partition function should exist. Moreover, the path space expressions we have derived for the reduced density matrices will certainly diverge without some condition of this sort. Typically, this condition implies the estimate

$$U(\omega^m, \tilde{\omega}^n) \geq -(m+n)B\beta$$

and hence

$$0 \leq \exp\{-U(\omega^m, \tilde{\omega}^n)\} \leq e^{B\beta(m+n)} \ .$$

Thus $\exp\{-U(\omega^m, \tilde{\omega}^n)\}$ is integrable, and this certainly ensures that all the path space formulas we have considered in this section converge when the activity z is sufficiently small, i.e., $z \exp\{B\beta\} < 1$.

Next, for simplicity, we assume that U_Λ is defined by a translationally invariant two-body potential, i.e.,

$$U^{(m)}(x_1, \ldots, x_m) = \sum_{1 \le i < j \le m} \Phi(x_i - x_j) \ .$$

We place several auxiliary conditions on Φ. First, we impose a continuity condition which is needed for technical reasons in subsequent proofs but which would probably prove to be redundant by a finer analysis

(A) $x \mapsto \Phi(x)$ is an even real function which is continuous except possibly at the origin.

The next condition is the stability condition which ensures the existence of finite-volume Gibbs states.

(B) The interaction is stable, i.e., there exists a constant $B \ge 0$ such that

$$\sum_{1 \le i < j \le m} \Phi(x_i - x_j) \ge -mB$$

for any finite family $\{x_1, x_2, \ldots, x_m\}$ of points in $\mathbb{R}^\nu$.

Finally, in order that the thermodynamic limit shall exist, we need a condition of decrease of Φ at infinity.

(C) There exists a constant $c \ge 0$ such that Φ is integrable for $|x| \ge c$, i.e.,

$$\int_{|x| \ge c} dx \, |\Phi(x)| < +\infty \ .$$

Now with all these conditions on Φ, and with Dirichlet boundary conditions, it is possible to establish the existence of the thermodynamic limit for small activity by the indirect method discussed at the beginning of the section.

Theorem 6.3.19 (Ginibre). *Let Φ be a two-body potential satisfying conditions (A), (B), and (C). Then there exists a Banach space $\mathscr{E}$ of sequences of functions of $m = 1, 2, \ldots$ trajectories (elementary trajectories for Boltzmann statistics, composite trajectories for quantum statistics), bounded linear operators K_Λ, K on $\mathscr{E}$, vectors ζ_Λ, ζ in $\mathscr{E}$ such that K_Λ, K, ζ_Λ, ζ depend linearly on the activity z, and a constant $R > 0$ such that the following are satisfied.*

(i) *For all complex z with $|z| < R$ one has $\|K_\Lambda\| < 1$, and hence the equation*

$$\rho_\Lambda = \zeta_\Lambda + K_\Lambda \rho_\Lambda$$

has a unique solution ρ_Λ in $\mathscr{E}$. This solution is given by

$$\rho_\Lambda = \sum_{n \ge 0} K_\Lambda^n \zeta_\Lambda$$

and hence is a norm-analytic function of z for $|z| < R$. In the case that $0 \le z < R$, the solution is given by

$$\rho_\Lambda(\omega^m) = Z_{\varepsilon,\Lambda}^{-1} \sum_{n \geq 0} \frac{1}{n!} \times \int d\tilde{\omega}_1 \cdots d\tilde{\omega}_n \, z^{q+r} \alpha_\Lambda(\omega^m, \tilde{\omega}^n) \exp\{-U(\omega^m, \tilde{\omega}^n)\}$$

in the case of Bose or Fermi statistics, and by

$$\rho_\Lambda(\omega^m) = Z_\Lambda^{-1} \sum_{n \geq 0} \frac{1}{n!} \int d\tilde{\omega}_1 \cdots d\tilde{\omega}_n \, z^{m+n} \alpha_\Lambda(\omega^m, \tilde{\omega}^n) \times \exp\{-U(\omega^m, \tilde{\omega}^n)\}$$

in the case of Boltzmann statistics, with the appropriate definitions of $d\tilde{\omega}$ *in each case* (*see Example* 6.3.15).

(ii) *For all complex* z *with* $|z| < R$, *one has* $\|K\| < 1$, *and hence the equation*

$$\rho = \zeta + K\rho$$

has the unique solution

$$\rho = \sum_{n \geq 0} K^n \zeta$$

in $\mathscr{E}$. *This solution* ρ *depends norm-analytically on* z *for* $|z| < R$.

(iii) *When the boundary of* Λ *recedes to infinity,* $\rho_\Lambda(\omega^m)$ *converges to* $\rho(\omega^m)$. *The convergence is uniform in* z *for* $|z| \leq R' < R$ *and uniform in* ω^m *when all the* m *trajectories in* ω^m *remain in a fixed bounded region.*

We will not give the rather complicated technical details of the proof of this theorem (see Notes and Remarks), but remark simply that one obtains the equation

$$\rho_\Lambda = \zeta_\Lambda + K_\Lambda \rho_\Lambda$$

by an expansion about the case $U_\Lambda = 0$. A very similar expansion about the case $\beta\Phi = 0$ was used in the proof of Proposition 6.2.45. In fact in the present context the expansion is really about the case $\exp\{-\beta U_\Lambda\} = 1$. Typically, one sets

$$e^{-\beta\Phi(x)} = 1 + f_\beta(x)$$

and obtains results when the f_β have appropriate small bounds.

One may now define the reduced density matrices $\tilde{\rho}_\Lambda(x^m; y^m)$ from the correlation functions ρ_Λ as in Example 6.3.15, and one may use exactly the same formulas to *define* $\tilde{\rho}$ from ρ. Theorem 6.3.19 has the immediate corollary.

Corollary 6.3.20. *The reduced density matrices $\tilde{\rho}_\Lambda(x^m; y^m)$ and $\tilde{\rho}(x^m; y^m)$ are bounded continuous functions of x^m, y^m and analytic functions of z for $|z| < R$. Moreover, $\tilde{\rho}(x^m; y^m)$ is translationally invariant. When $\Lambda \to \infty$ in the sense that the boundary recedes to infinity, $\tilde{\rho}_\Lambda(x^m; y^m)$ tends to $\tilde{\rho}(x^m; y^m)$ uniformly in z for $|z| \leq R' < R$ and uniformly in (x^m, y^m) when all the points in x^m, y^m remain in a fixed bounded region. Finally, there exists $\zeta \in \langle 0, 1\rangle$ such that*

$$|\tilde{\rho}_\Lambda(x^m; y^m)| \leq (|z|/\zeta)(1 - |z|/R)^{-1}\ \tilde{\rho}_\Lambda^{0,\zeta}(x^m; y^m)$$

for all $|z| < R$, where $\tilde{\rho}_\Lambda^{0,\zeta}$ denotes the reduced density matrices of the non-interacting Bose system at activity ζ. Moreover, for Bose and Boltzmann statistics one has

$$\tilde{\rho}_\Lambda(x^m; y^m) \geq 0 \ .$$

By the same methods used to prove convergence of the reduced density matrices, one can also show that truncations of these matrices have good clustering properties in space. Recall that the matrices are related to the state ω by the expression

$$\tilde{\rho}_\Lambda(x_1, \ldots, x_m\,; y_1, \ldots, y_m) = \omega(a_\omega^*(y_1) \ldots a_\omega^*(y_m) a_\omega(x_m) \ldots a_\omega(x_1)) \ ,$$

where the right-hand side should be interpreted in the distributional sense. If we form the truncated expectation of ω as in Section 5.2.3, all truncations with an unequal number of $a_\omega^*(y)$ and $a_\omega(x)$ disappear because of gauge invariance. It is therefore natural to define truncated expectation values of $\tilde{\rho}$ such that

$$\begin{aligned} \tilde{\rho}(x\,; y) &= \tilde{\rho}_T(x\,; y) \ , \\ \tilde{\rho}(x_1, x_2\,; y_1, y_2) &= \tilde{\rho}_T(x_1, x_2\,; y_1, y_2) + \tilde{\rho}_T(x_1; y_1)\tilde{\rho}_T(x_2; y_2) \\ &\quad + \varepsilon\tilde{\rho}_T(x_1\,; y_2)\tilde{\rho}_T(x_2\,; y_1) \ , \end{aligned}$$

etc., where $\varepsilon = 1$ for bosons and $\varepsilon = -1$ for fermions. Here ε has to be set equal to zero for Boltzmann statistics. The cluster property then takes the form.

Theorem 6.3.21. *Let Φ be a translational-invariant two-body interaction satisfying (A), (B), and (C), and let $|z| < R$, where R is defined in Theorem 6.3.19. Then the infinite-volume truncated reduced density matrices $\tilde{\rho}_T$ are absolutely integrable functions of the difference of their arguments, i.e.,*

$$\int dx_1 \ldots dx_m\, dy_1 \ldots dy_{m-1} |\, \tilde{\rho}_T(x^m; y^m)\, | < +\infty \ .$$

So far we have not discussed the influence of boundary conditions on the thermodynamic limit, but only worked with the tractable Dirichlet conditions. Combining the path space representation of the reduced density matrices, derived in Theorem 6.3.14, with the fact that the influence of the boundary on the path space measures disappears when the boundary recedes to infinity, Theorem 6.3.8, one would expect the infinite-volume small activity reduced

density matrices to exist for all classical boundary conditions and to be equal to those obtained with Dirichlet boundary conditions. This result, although feasible, has not been proven. Some tentative results have, however, been obtained for the pressure. If

$$Z_{\sigma,\Lambda}(\beta,\mu) = \mathrm{Tr}(e^{-\beta(H_{\sigma,\Lambda}-\mu N_\Lambda)})$$

is the partition function, then the *local pressure* is defined by

$$P_{\sigma,\Lambda}(\beta,\mu) = (\beta|\Lambda|)^{-1}\log Z_{\sigma,\Lambda}(\beta,\mu) \ .$$

Now if $\sigma_1 \geq \sigma_2$, then

$$H_{\sigma_1,\Lambda} \geq H_{\sigma_2,\Lambda}$$

in the sense of quadratic forms. Thus, it follows from the minimax theorem that

$$Z_{\infty,\Lambda}(\beta,\mu) \leq Z_{\sigma,\Lambda}(\beta,\mu) \leq Z_{0,\Lambda}(\beta,\mu)$$

for $\sigma \geq 0$. Thus, to show that the thermodynamic limit exists for all positive boundary conditions but that it is independent of the particular choice it suffices to show

$$\lim_{\Lambda\to\infty} |\Lambda|^{-1}\log\frac{Z_{\infty,\Lambda}}{Z_{0,\Lambda}} = 0$$

and *either*

$$P_\infty = \lim_{\Lambda\to\infty}(\beta|\Lambda|)^{-1}\log Z_{\infty,\Lambda}$$

exists *or*

$$P_0 = \lim_{\Lambda\to\infty}(\beta|\Lambda|)^{-1}\log Z_{0,\Lambda}$$

exists. The latter questions of existence have been handled by operator-theoretic methods in a relatively satisfactory manner.

For the Dirichlet boundary conditions it suffices to assume that the interaction is stable and

$$U^{(n+m)}(x^n, y^m) \leq U^{(n)}(x^n) + U^{(m)}(y^m) \ .$$

when the distance between the sets x^n and y^m is larger than some fixed value R. This condition corresponds to potentials which are attractive at distances greater than R. It can in fact be relaxed to deal with positive interactions which decrease sufficiently fast at infinity. The utility of the condition is that it implies

$$Z_{\infty,\Lambda} \geq Z_{\infty,\Lambda_1\cup\Lambda_2} \geq Z_{\infty,\Lambda_1}Z_{\infty,\Lambda_2}$$

whenever $\Lambda_1\cup\Lambda_2 \subset \Lambda$ and the distance between Λ_1 and Λ_2 is greater than R. This and similar inequalities discussed below are all straightforward applications of the minimax theorems. The existence of P_∞ then follows for translation invariant interactions by the same type of argument as in Proposition 6.2.38.

The case of Neumann boundary conditions is quite different. If there is no interaction, one finds that the partition function satisfies

$$Z_{0,\Lambda_1 \cup \Lambda_2} \leq Z_{0,\Lambda_1} Z_{0,\Lambda_2} \tag{*}$$

for all Λ_1 and Λ_2 such that $\Lambda_1 \cap \Lambda_2 = \varnothing$. These inequalities are in the opposite sense to the corresponding ones with Dirichlet conditions. Thus if one hopes that they should remain valid in the presence of an interaction then it appears necesary to impose conditions on $U^{(n)}$ which are in the opposite sense to the above. The situation is particularly simple with positive potentials because one then has

$$U^{(n+m)}(x^n, y^m) \geq U^{(n)}(x^n) + U^{(m)}(y^m)$$

for all sets x^n and y^m and this once more allows the deduction of the submultiplicative property (*). Then the existence of P_0 can again be established for translationally invariant interactions by arguments of the type used to prove Proposition 6.2.38. But the restriction to positive potentials makes the Neumann case much less satisfactory than the Dirichlet case.

Now let us consider the comparison of $Z_{0,\Lambda}$ and $Z_{\infty,\Lambda}$. There have been two basic methods used for this purpose and they both have severe drawbacks. The first method is operator-theoretic and has the advantage that it works for all forms of statistics, Bose, Fermi, or Boltzmann, and for many-body interactions. Nevertheless, it has two severe disadvantages. It works only for positive decreasing interactions and for parallelepipeds. Basically, one proves that if Λ_L is a cube of side length L, then

$$P_{0,\Lambda_{L-a}}(\beta, \mu - 8\nu/a^2) \leq P_{\infty,\Lambda_L}(\beta,\mu) \leq P_{0,\Lambda_L}(\beta,\mu) \ .$$

Subsequently, one uses the existence of $P_0(\beta,\mu)$ and its continuity in μ to obtain the existence of $P_\infty(\beta,\mu)$ and the identity $P_\infty = P_0$. Hard cores can be incorporated into these results if Dirichlet conditions are used on the boundaries of the hard cores. This is accomplished by approximating the cores by an increasing sequence of positive bounded potentials and then using Lemma 5.2.13 and a dominated convergence argument to prove the above inequalities between P_0 and P_∞.

The second method for comparing $Z_{0,\Lambda}$ and $Z_{\infty,\Lambda}$ uses functional integration and has the advantage that for particles with hard cores one may incorporate an interparticle attraction, if it is mediated by a suitable two-body potential. If there is no hard core, then the corresponding estimates have only been carried through for positive translationally invariant two-body potentials Φ of finite range, i.e., $\Phi(X) = 0$ for $|X| > R$ for some $R > 0$. This second method has other disadvantages. It requires that the surface of Λ is smooth and it only works for Bose or Boltzmann statistics. Basically, the idea of this method is to write down the functional integral representation of $Z_{0,\Lambda}$ and then split the functional integrals into two parts, the integral over trajectories which touch the surface $\partial\Lambda$ of Λ and trajectories which do not touch the surface. The latter trajectories give the total contribution to the Dirichlet partition function and hence if U is positive one readily obtains

$$P_{0,\Lambda}(\beta,\mu) - P_{\infty,\Lambda}(\beta,\mu) \leq \frac{1}{\beta|\Lambda|}\sum_{j=1}^{\infty}\frac{e^{\beta\mu j}}{j}\int_{\Lambda}dx\int_{\Omega_{\Lambda,j\beta}}d\mu_{x,x}^{0,\Lambda,j\beta}(\tilde{\omega})[1-\alpha_{\Lambda}(\tilde{\omega})] \ .$$

But

$$\begin{aligned}\int_{\Omega_{\Lambda,j\beta}}d\mu_{x,x}^{0,\Lambda,j\beta}(\tilde{\omega})[1 - \alpha_{\Lambda}(\tilde{\omega})] &= z_{\infty,\Lambda}(x,x;j\beta) - z_{0,\Lambda}(x,x;j\beta)\\ &\leq z_{\infty,\Lambda}(x,x;j\beta) + |z_{0,\Lambda}(x,x;j\beta)| \ ,\end{aligned}$$

where $z_{\sigma,\Lambda}$ is the compensating Green's function introduced prior to Theorem 6.3.8. Now combining the estimates on $|z_{\sigma,\Lambda}|$ given by this latter theorem together with some regularity assumptions on the surface of Λ one again deduces that $P_{0,\Lambda} - P_{\infty,\Lambda} \to 0$ (for references and further details on these methods see Notes and Remarks).

6.3.4. The Thermodynamic Limit. II. States and Green's Functions

In the previous subsection we studied the thermodynamic limit $\tilde{\rho}$ of the reduced density matrices $\tilde{\rho}_{\Lambda}$ associated with a Gibbs state $\omega_{\sigma,\Lambda}^{\beta,\mu}$. In this subsection we exploit some of the information concerning convergence of the $\tilde{\rho}_{\Lambda}$ to obtain results on convergence of the states, viewed as states on the CAR or CCR algebra.

The CAR case is simple. One has

$$\begin{aligned}&\omega_{\sigma,\Lambda}^{\beta,\mu}(a^*(f_1)\ldots a^*(f_m)a(g_m)\ldots a(g_1))\\ &\quad = \int dx_1\ldots dx_m\,dy_1\ldots dy_m\,\overline{g_1(y_1)}\cdots\overline{g_m(y_m)}f_1(x_1)\cdots f_m(x_m)\tilde{\rho}_{\Lambda}(y^m;x^m)\end{aligned}$$

and

$$\|a(f)\| = \|a^*(f)\| = \|f\|$$

for $f \in L^2(\mathbb{R}^{\nu})$. Thus, if the $\tilde{\rho}_{\Lambda}$ converge uniformly on compacts, then the states converge. But this is the case, for example, in the small activity region by Corollary 6.3.20.

The CCR case is more difficult. One can obtain convergence of the states from convergence of the reduced density matrices if all the states involved are analytic states in the sense of Section 5.2.3 and if the corresponding reduced density matrices are suitably bounded. There is one example which is particularly amenable to this kind of treatment, the Bose gas with positive potentials. We will consider states ω on the CCR algebra $\mathfrak{A}$ over $\bigcup_{\Lambda} L^2(\Lambda)$ which are obtained as limit points of the Gibbs states ω_{Λ} with Dirichlet boundary conditions. The bounds for the reduced density matrices, $0 \leq \tilde{\rho}_{\Lambda}^{U} \leq \tilde{\rho}_{\Lambda}^{0}$ obtained in Corollary 6.3.18 will play an important role. Other boundary conditions could also be handled by appealing to similar bounds in Theorem 6.3.17.

These bounds imply that the limit points ω are locally normal states over the quasi-local algebra $(\mathfrak{A}, \bigcup_\Lambda \mathfrak{A}_+(\Lambda))$. In fact, all the states ω describe a finite number of particles per unit volume. To see this we first remark that

$$\begin{aligned}\omega_\Lambda(a^*_{\omega_\Lambda}(f)a_{\omega_\Lambda}(f)) &= \int dx\,dy\ \tilde{\rho}^U_\Lambda(x;y)f(x)\bar{f}(y)\\ &\le \int dx\,dy\ \tilde{\rho}^0_\Lambda(x;y)|f(x)|\,|f(y)|\\ &\le \int dx\,dy\ \tilde{\rho}(x;y)|f(x)|\,|f(y)|\ ,\end{aligned}$$

where $\tilde{\rho}(x;y)$ is the reduced density matrix of the infinite-volume Gibbs states ω^0 of the ideal gas (see Example 6.3.16). In particular, the left-hand side is well defined. Thus, we can define the number functional for ω_Λ restricted to any $\mathfrak{A}_+(\Lambda_0)$ with $\Lambda_0 \subset \Lambda$,

$$\hat{N}_{\Lambda_0}(\omega_\Lambda) = \sup_{\mathfrak{F}} \sum_{f\in\mathfrak{F}} \omega_\Lambda(a^*_{\omega_\Lambda}(f)a_{\omega_\Lambda}(f))\ ,$$

where the supremum is over all finite orthonormal subsets of $L^2(\Lambda_0)$. Therefore, calculating with the above bounds

$$0 \le \hat{N}_{\Lambda_0}(\omega_\Lambda) = \int_{\Lambda_0} dx\,\tilde{\rho}^U_\Lambda(x;x) \le \int_{\Lambda_0} dx\,\tilde{\rho}(x;x) = \hat{N}_{\Lambda_0}(\omega^0)\ .$$

Now we can estimate the number functional of ω restricted to $\mathfrak{A}_+(\Lambda_0)$. In Section 5.2.3 we pointed out that the number functional is lower semi-continuous and hence

$$\begin{aligned}0 \le \hat{N}_{\Lambda_0}(\omega) &= \hat{N}_{\Lambda_0}\Big(\lim_\alpha \omega_{\Lambda_\alpha}\Big)\\ &\le \lim_\alpha \hat{N}_{\Lambda_0}(\omega_{\Lambda_\alpha}) \le N_{\Lambda_0}(\omega^0)\ .\end{aligned}$$

This shows that the number of particles in Λ_0 in each such state ω is finite and hence we have established the last statement of the following theorem for positive interactions.

Theorem 6.3.22. *Consider an interacting Bose gas for which all the k-body potentials $\Phi^{(k)}$ are positive and $\Phi^{(k)} \in L^1_{\mathrm{loc}}(\mathbb{R}^\nu)$. Let ω_Λ denote the finite volume Gibbs states for some $\beta > 0, \mu < 0$, and Dirichlet boundary conditions. Further let $\{\omega_{\Lambda_\alpha}\}$ be a subnet such that the limits*

$$\omega(A) = \lim_\alpha \omega_{\Lambda_\alpha}(A)$$

exist for all $A \in \bigcup_\Lambda \mathfrak{A}_+(\Lambda)$.

It follows that ω defines an entire analytic state over the CCR algebra $\mathfrak{A} = \overline{\bigcup_\Lambda \mathfrak{A}_+(\Lambda)}$ and

$$\lim_\alpha \omega_{\Lambda_\alpha}(\Phi_{\omega_{\Lambda_\alpha}}(g_1)\cdots\Phi_{\omega_{\Lambda_\alpha}}(g_n)) = \omega(\Phi_\omega(g_1)\cdots\Phi_\omega(g_n))$$

for all $g_1, \cdots, g_n \in L^2(\mathbb{R}^\nu)$ *with compact support and all* $n \geq 1$. *The state* ω *has finite local particle density and hence is locally normal.*

Remark. The assumption that the potentials are positive can be relaxed somewhat by the introduction of a suitable notion of superstability (see Example 6.3.2). Assume the interaction $U^{(m)}$ is defined by a translationally invariant, real, even, two-body interaction potential $\Phi \in L^1_{\text{loc}}(\mathbb{R}^\nu)$,

$$U^{(m)}(x_1, \ldots, x_m) = \sum_{1 \leq i,j \leq m} \Phi(x_i - x_j) \ .$$

Suppose that $U^{(m)}$ is superstable in the sense that

$$U^{(m)}(X) \ \geq \ C \sum_{r \in \mathbb{Z}^\nu} n(X,r)^2 - Bm$$

for $X = (x_1, \ldots, x_m)$ where $B \geq 0, C > 0$ and $n(X,r)$ is the number of points of X contained in the half-open cube centred at r. Assume also that Φ is strongly regular, i.e., there exists a positive decreasing function ψ on $\langle 0, \infty \rangle$ such that

$$\int_0^\infty dt\, \psi(t) t^{\nu+\mu-1} < \infty$$

for some $\mu > 1/2$ and

$$\Phi(x) \ \geq \ -\psi(|x|)$$

for all $x \in \mathbb{R}^\nu$. If $\nu \leq 3$, or if Φ is positive, one can prove an estimate

$$\omega_\Lambda(\exp\{aN_X\}) \ \leq \ c(\text{diam}(\text{X}), \text{a})$$

for any $a > 0$, any bounded region Λ and all $X \subset \Lambda$, where N_X is the local number operator for X. From this one can deduce the conclusions of Theorem 6.3.22. One can also deduce the modularity of the limiting states as in Theorem 6.3.31. (See Notes and Remarks.)

A principal ingredient in the proof is the following straightforward result of real analysis.

Lemma 6.3.23. *Let* $\{f_\alpha\}$ *be a net of* $n \geq 1$ *times continuously differentiable functions from* $\mathbb{R}$ *into* $\mathbb{C}$, *and assume that* f_α *converges pointwise to a function* f. *Assume that the derivatives of* f_α *up to order* n *are bounded on compacts, uniformly in* α, *i.e.,*

$$\sup_\alpha \sup_{t \in [-k,\, k]} |f_\alpha^{(m)}(t)| < +\infty$$

for $m = 1, 2, \ldots, n$, *and all* $k > 0$. *It follows that* f *is* $n-1$ *times continuously differentiable, and*

$$f_\alpha^{(m)} \to f^{(m)}$$

for $m = 0, 1, \ldots, n-1$, *where the convergence is uniform on compacts.*

PROOF. If $n = 1$, it suffices to establish uniformity on compact intervals I for the convergence of f_α to f. Let $\varepsilon > 0$. Choose points $t_1, \ldots, t_m \in I$ and an $h > 0$ such that

$$\bigcup_{i=1}^{m} [t_i - h, t_i + h] = I$$

and

$$h \sup_{t \in I} |f'_\alpha(t)| < \varepsilon/4.$$

But for $|s| < h$ one has

$$\begin{aligned} |f_\alpha(t_i + s) - f_\beta(t_i + s)| &\leq |f_\alpha(t_i + s) - f_\alpha(t_i)| + |f_\alpha(t_i) - f_\beta(t_i)| \\ &\quad + |f_\beta(t_i) - f_\beta(t_i + s)| \\ &\leq h \sup_{t \in I} |f'_\alpha(t)| + h \sup_{t \in I} |f'_\beta(t)| \\ &\quad + |f_\alpha(t_i) - f_\beta(t_i)| \\ &< \varepsilon/2 + |f_\alpha(t_i) - f_\beta(t_i)| \ . \end{aligned}$$

Consequently,

$$|f_\alpha(t_i + s) - f(t_i + s)| < \varepsilon/2 + |f_\alpha(t_i) - f(t_i)|$$

and uniform convergence on I follows from pointwise convergence.

Now the proof proceeds by induction and it suffices to consider the case $n = 2$ because higher cases are obtained by replacing f by one of its derivatives.

Given $t \in \mathbb{R}$ choose $M \geq 0$ such that

$$|f''_\alpha(t + h)| \leq M$$

for all α and all $|h| < 1$. By Taylor's theorem

$$f_\alpha(t + h) = f_\alpha(t) + f'_\alpha(t)h + R(t + h) \ ,$$

where

$$|R(t + h)| \leq Mh^2/2$$

and hence

$$|f'_\alpha(t) - f'_\beta(t)| \leq |f_\alpha(t + h) - f_\beta(t + h)|/|h| + |f_\alpha(t) - f_\beta(t)|/|h| + M|h|$$

for $|h| < 1$. It follows that $f'_\alpha(t)$ has a limit as $\alpha \to \infty$. But another application of Taylor's theorem gives

$$\left|(f_\alpha(t + h) - f_\alpha(t))/|h| - f'_\alpha(t)\right| \leq Mh/2$$

Thus f is differentiable, and

$$f'_\alpha(t) \to f'(t) \ .$$

The uniform convergence on compacts follows from the pointwise convergence by the same reasoning as in the case $n = 1$.

The proof of Theorem 6.3.22 follows from bounds of Corollary 6.3.18 and the entire analyticity of the infinite-volume Gibbs state ω^0 of the non-interacting Bose gas,

$$\omega^0(W(f)) = \exp\left\{ -\omega^0(\Phi_{\omega^0}(f)^2)/2 \right\}$$
$$= \exp\left\{ -(f, (\mathbb{1} + ze^{\beta\nabla^2})(\mathbb{1} - ze^{\beta\nabla^2})^{-1} f)/4 \right\}$$

(see Proposition 5.2.29).

Proof of Theorem 6.3.22. First, choose $g \in L^2(\Lambda)$. Next, note that the states ω_Λ and ω^0 are all gauge invariant and hence

$$\omega_\Lambda(\Phi_{\omega_\Lambda}(g)^n) = 0 = \omega^0(\Phi_{\omega^0}(g)^n)$$

when n is odd. If, however, $n = 2m$ is even

$$\omega_\Lambda(\Phi_{\omega_\Lambda}(g)^{2m}) = \omega_\Lambda((a^*_{\omega_\Lambda}(g) + a_{\omega_\Lambda}(g))^{2m})/2^m$$
$$= \omega_\Lambda(a^*_{\omega_\Lambda}(g)^{2m} + a^*_{\omega_\Lambda}(g)^{2m-1} a_{\omega_\Lambda}(g) + \cdots)/2^m$$

But in the last expansion ω_Λ vanishes on all terms which contain an unequal number of creation operators $a^*_{\omega_\Lambda}(g)$ and annihilation operators $a_{\omega_\Lambda}(g)$. This is again a consequence of gauge invariance, i.e., conservation of particle number. Thus, by use of the commutation relations

$$a_{\omega_\Lambda}(g) a^*_{\omega_\Lambda}(g) = a^*_{\omega_\Lambda}(g) a_{\omega_\Lambda}(g) + \|g\|^2 \ ,$$

one obtains a representation

$$\omega_\Lambda(\Phi_{\omega_\Lambda}(g)^{2m}) = \sum_{k=0}^{m} C_k^m \omega_\Lambda(a^*_{\omega_\Lambda}(g)^k a_{\omega_\Lambda}(g)^k)$$
$$= \sum_{k=0}^{m} C_k^m \int dx^k dy^k \, \tilde{\rho}^U_\Lambda(x^k; y^k) \prod_{i=1}^{k} g(x_i)\overline{g(y_i)} \ ,$$

where the coefficients are positive polynomials in $\|g\|^2$. (We have used $\tilde{\rho}^U_\Lambda$ to denote the reduced density matrices corresponding to ω_Λ.) But by Corollary 6.3.18

$$0 \le \tilde{\rho}^U_\Lambda(x^k; y^k) \le \tilde{\rho}^0(x^k; y^k) \ ,$$

where $\tilde{\rho}^0$ are the reduced density matrices associated with the infinite-volume non-interacting equilibrium state ω^0. Thus since $C_k^m \ge 0$ one has

$$0 \le \omega_\Lambda(\Phi_{\omega_\Lambda}(g)^{2m}) \le \sum_{k=0}^{m} C_k^m \int dx^k dy^k \, \tilde{\rho}^0(x^k; y^k) \prod_{i=1}^{n} |g(x_i)| \, |\overline{g(y_i)}|$$
$$= \omega^0(\Phi_{\omega^0}(|g|)^{2m}) \ .$$

The last evaluation follows from the gauge invariance of ω^0 and the definition of the C_k^m.

Next introduce the family of functions $f_\alpha; \mathbb{R} \mapsto \mathbb{C}$

$$f_\alpha(t) = \omega_{\Lambda_\alpha}(W(tg)) \ .$$

These functions converge pointwise to the function $f; \mathbb{R} \mapsto \mathbb{C}$ defined by

$$f(t) = \omega(W(tg)) \ .$$

Furthermore, they satisfy the hypotheses of Lemma 6.3.23 for all n. For example

$$|f_\alpha^{(m)}(t)|^2 = |i^m \omega_{\Lambda_\alpha}(\Phi_{\omega_{\Lambda_\alpha}}(g)^m W(tf))|^2$$
$$\leq |\omega_{\Lambda_\alpha}(\Phi_{\omega_{\Lambda_\alpha}}(g)^{2m})| \leq \omega^0(\Phi_{\omega^0}(|g|)^{2m}) \ .$$

Hence $f \in C^\infty(\mathbb{R})$ and $f_\alpha^{(m)} \to f^{(m)}$ uniformly on compacts. But if $F_0; \mathbb{R} \to \mathbb{C}$ is defined by

$$F_0(t) = \omega^0(W(t|g|)) \ ,$$

then F_0 is entire analytic and

$$|f^{(m)}(0)| = \lim_\alpha |f_\alpha^{(m)}(0)| \leq \omega^0(\Phi_{\omega^0}(|g|)^m) = |F_0^{(m)}(0)| \ .$$

Thus, f is an entire analytic function. Therefore,

$$t \mapsto \omega(W(tg))$$

is an entire analytic function for all $g \in L^2(\mathbb{R}^\nu)$ with compact support and hence ω is an entire analytic state.

Next from convergence of the derivatives one has

$$\omega_{\Lambda_\alpha}(\Phi_{\omega_{\Lambda_\alpha}}(g)^n) = i^{-n} f_\alpha^{(n)}(0) \to i^{-n} f^{(n)}(0) = \omega(\Phi_\omega(g)^n) \ .$$

The more general statement of the theorem with n different functions $g_1, \ldots, g_n$ is obtained in a similar manner by examining derivatives of a function $f_\alpha(t_1, \ldots, t_n) = \omega_{\Lambda_\alpha}(W(t_1 g_1 + t_2 g_2 + \cdots + t_n g_n))$ of several variables. We omit the details.

There is a partial converse of Theorem 6.3.22.

Corollary 6.3.24. *Adopt the assumptions of Theorem* 6.3.22 *but further assume that the reduced density matrices $\tilde{\rho}_\Lambda$ associated with the Gibbs states ω_Λ are pointwise convergent. It follows that the states are weakly* convergent.*

PROOF. It follows from the bounds

$$0 \leq \tilde{\rho}_\Lambda(x^m; y^m) \leq \tilde{\rho}^0(x^m; y^m)$$

and the Lebesgue-dominated convergence theorem that $\omega_\Lambda(\Phi_{\omega_\Lambda}(g)^{2m})$ converges for all $g \in L^2(\mathbb{R}^\nu)$ with compact support. Moreover, the estimates

$$0 \leq \omega_\Lambda(\Phi_{\omega_\Lambda}(g)^{2m}) \leq \omega^0(\Phi_{\omega^0}(|g|)^{2m})$$

imply that one can define numbers

$$\omega(W(g)) = \sum_{m=0}^{\infty} \frac{(-1)^m}{(2m)!} \lim_{\Lambda \to \infty} \omega_\Lambda(\Phi_{\omega_\Lambda}(g)^{2m})$$

for each such g. It is then readily verified that these numbers uniquely determine an entire analytic state ω over the CCR algebra and $\omega_\Lambda \to \omega$.

Remark. We have shown that the local particle density of the interacting state ω is bounded by the corresponding density of the noninteracting state ω^0. It is not surprising that such a bound exists since for β, μ fixed the introduction of a positive interaction, i.e., an interparticle repulsion, should

reduce the density. In fact, the bound is just one implication of the bounds $0 \leq \tilde{\rho}^U \leq \tilde{\rho}^0$ on the reduced density with and without interaction. This follows because

$$\hat{N}_\Lambda(\omega) = \int_\Lambda dx\ \tilde{\rho}^U(x;x) \leq \int_\Lambda dx\ \tilde{\rho}^0(x;x) = \hat{N}_\Lambda(\omega^0)\ .$$

But the noninteracting Gibbs states ω^0 can be extended to all powers of the number operator and the inequalities

$$0 \leq \int_{\Lambda^k} dx^k\ \tilde{\rho}^U(x^k;x^k) \leq \int_{\Lambda^k} dx^k\ \tilde{\rho}^0(x^k;x^k)$$

correspond to bounds

$$0 \leq \omega(N_\Lambda(N_\Lambda - 1)\cdots(N_\Lambda - k + 1)) \leq \omega^0(N_\Lambda(N_\Lambda - 1)\cdots(N_\Lambda - k + 1))\ .$$

Finally, a combinatorial calculation establishes that there are positive coefficients[10] S_k^m such that

$$\rho^m = \sum_{k=1}^m S_k^m \rho(\rho - 1)\cdots(\rho - k + 1)$$

for all $\rho \in \mathbb{R}$. Therefore

$$\begin{aligned} 0 \leq \omega(N_\Lambda^m) &= \sum_{k=1}^m S_k^m \omega(N_\Lambda(N_\Lambda - 1)\cdots(N_\Lambda - k + 1)) \\ &\leq \sum_{k=1}^m S_k^m \omega^0(N_\Lambda(N_\Lambda - 1)\cdots(N_\Lambda - k + 1)) = \omega^0(N_\Lambda^m)\ . \end{aligned}$$

Theorem 6.3.22 states properties of the thermodynamic limit with $\beta > 0$ and $\mu < 0$ fixed. It is also possible to consider the thermodynamic limit with $\beta > 0$ and the overall particle density fixed. Recall that this latter form of limit was essential for the discussion of Bose–Einstein condensation of the ideal Bose gas in Section 5.2.5. The basic difficulty for the ideal gas with Dirichlet boundary conditions was that the formalism was only defined for $z = \exp\{\beta\mu\} \leq 1$ and for z fixed in this range the local particle densities $\rho_\Lambda(\beta, z)$ were uniformly bounded, whenever $\nu \geq 3$, by the density of the infinite ideal gas at $z = 1$, i.e.,

$$\rho_\Lambda(\beta, z) \leq \rho_c(\beta) = (2\pi)^{-\nu} \int d^\nu p (e^{\beta p^2} - 1)^{-1}\ .$$

(This was discussed prior to Theorem 5.2.30). Now it follows from the bound $\hat{N}_\Lambda(\omega) \leq \hat{N}_\Lambda(\omega^0)$ that the density of the interacting gas is also uniformly bounded by $\rho_c(\beta)$ if $z \leq 1$. This seeming paradox was resolved for the ideal gas by remarking that if $\rho_\Lambda(\beta, z) > \rho_c(\beta)$, one must have $z_\Lambda > 1$ for each finite Λ

[10]The S_k^m are known as Stirling numbers of the second kind. Their positivity follows from the recurrence relation $S_k^{m+1} = S_{k-1}^m + kS_m^m = 1$ and $S_1^m = 1$.

and in the thermodynamic limit at fixed density this leads to a range of choices z_Λ such that $z_\Lambda \to 1$. The discussion of the interacting system at fixed density is less tractable and it is not evident that the corresponding z_Λ would converge to a critical finite value. Nevertheless, the above method of bounds could be used to discuss properties of any limit for which $z_\Lambda \to 1$.

One may also obtain results for the small activity region for interactions which are not necessarily positive.

Theorem 6.3.25. *Consider an interacting Bose gas satisfying all the assumptions of Theorem* 6.3.19. *For* $0 \le z < R$, *it follows that the limits of the local Gibbs states* $\omega_\Lambda (= \omega^{\beta,\mu}_{\sigma,\Lambda})$ *exist,*

$$\omega(A) = \lim_{\Lambda \to \infty} \omega_\Lambda(A)$$

for all $A \in \bigcup_\Lambda \mathfrak{A}_+(\Lambda)$, *and determine a unique state over the CCR algebra. This state is entire analytic, locally normal, and*

$$\lim_{\Lambda \to \infty} \omega_\Lambda(\Phi_{\omega_\Lambda}(f_1) \cdots \Phi_{\omega_\Lambda}(f_n)) = \omega(\Phi_\omega(f_1) \cdots \Phi_\omega(f_n))$$

for all $f_1, \ldots, f_n \in L^2(\mathbb{R}^\nu)$ *with compact support.*

Proof. The proof is almost identical to the proofs of Theorem 6.3.22 and Corollary 6.3.24. It relies on bounds on $\omega_\Lambda(\Phi_{\omega_\Lambda}(g)^n)$ which are obtained as follows. First, by gauge invariance these quantities are zero if n is odd. But if $n = 2m$,

$$\omega_\Lambda(\Phi_{\omega_\Lambda}(g)^{2m}) = \sum_{k=0}^{m} C_k^m \omega_\Lambda(a^*_{\omega_\Lambda}(g)^k a_{\omega_\Lambda}(g)^k)$$

with $C_k^m \ge 0$, and for $g \in L^2(\Lambda_g)$ one has

$$\begin{aligned}\omega_\Lambda(a^*_{\omega_\Lambda}(g)^k a_{\omega_\Lambda}(g)^k) &= \int_{\Lambda_g^k} dx^k \int_{\Lambda_g^k} dy^k\, \tilde{\rho}_\Lambda(x^k; y^k) \prod_{i=1}^{k} \overline{g(x_i)} g(y_i) \\ &\le (z/\zeta)(1 - z/R)^{-1} \int_{\Lambda_g^k} dx^k \int_{\Lambda_g^k} dy^k\, \tilde{\rho}^{0,\zeta}_\Lambda(x^k; y^k) \prod_{i=1}^{n} |g(x_i)|\, |g(y_i)| \ ,\end{aligned}$$

where we have used the bounds of Corollary 6.3.20. Now, since we are using Dirichlet boundary conditions, $\Lambda \to \rho^{0,\zeta}_\Lambda(x; y)$ is a pointwise increasing function, Example 6.3.16, and hence we may replace $\rho^{0,\zeta}_\Lambda$ by its thermodynamic limit $\rho^{0,\zeta}$. Thus,

$$\omega_\Lambda(a^*_{\omega_\Lambda}(g)^k a_{\omega_\Lambda}(g)^k) \le (z/\zeta)(1 - z/R)^{-1} \omega^{0,\zeta}(a^*_{\omega^{0,\zeta}}(|g|)^k a_{\omega^{0,\zeta}}(|g|)^k) \ ,$$

where $\omega^{0,\zeta}$ is the Gibbs state of the noninteracting Bose gas at activity ζ. Therefore,

$$0 \le \omega_\Lambda(\Phi_{\omega_\Lambda}(g)^{2m}) \le (z/\zeta)(1 - z/R)^{-1} \omega^{0,\zeta}(\Phi_{\omega^{0,\zeta}}(|g|)^{2m})$$

and the proof now proceeds as previously.

Under slightly more stringent conditions on the interaction it is also possible to prove convergence of the *time-dependent Green functions*

$$G_\Lambda(A_0, \ldots, A_n; t_1, \ldots, t_n) = \omega_\Lambda(A_0\, \tau^\Lambda_{t_1}(A_1) \cdots \tau^\Lambda_{t_n}(A_n)) \ ,$$

where

$$\tau_t^\Lambda(A) = e^{it(H_\Lambda - \mu N_\Lambda)} A e^{-it(H_\Lambda - \mu N_\Lambda)}$$

but this is substantially more difficult to prove.

Theorem 6.3.26. *Consider a Bose or Fermi gas interacting through a two-body potential Φ which satisfies the requirements*

(A) *Φ is even ($\Phi(x) = \Phi(-x)$) and continuous for $x \neq 0$,*
(B) *the interaction is stable,*
(C) $\Phi \in L^1(\mathbb{R}^\nu) \cap L^2(\mathbb{R}^\nu)$.

Assume Dirichlet boundary conditions and define local Green's functions

$$G_\Lambda(A^m; \zeta^m) = Z_\Lambda^{-1} \mathrm{Tr}_{\mathfrak{F}_\pm(\Lambda)}(A_1 e^{-(\zeta_2 - \zeta_1)K_\Lambda} \times A_2 e^{-(\zeta_3 - \zeta_2)K_\Lambda} \dots e^{(\zeta_m - \zeta_{m-1})K_\Lambda} A_m e^{-(\beta + \zeta_1 - \zeta_m)K_\Lambda}),$$

where

$$Z_\Lambda = \mathrm{Tr}_{\mathfrak{F}_\pm(\Lambda)}(e^{-\beta K_\Lambda}) \qquad \text{and} \qquad K_\Lambda = H_{\infty,\Lambda} - \mu N_\Lambda \ .$$

Here $A^m = (A_1, \dots, A_m)$ denotes an m-tuple of operators with

$$\begin{aligned} A_i &= A(f_i) \text{ or } a^*(f_i) && \text{in the Fermi case} \\ &= W(f_i) && \text{in the Bose case} \ , \end{aligned}$$

and $\zeta^m = (\zeta_1, \dots, \zeta_m)$ denotes an m-tuple of complex numbers with $\zeta^m \in \bar{\mathfrak{D}}$ where

$$\mathfrak{D} = \{\zeta^m; \mathrm{Re}\,\zeta_1 < \mathrm{Re}\,\zeta_2 < \dots < \mathrm{Re}\,\zeta_m < \mathrm{Re}\,\zeta_1 + \beta\} \ .$$

It follows for sufficiently small values of the activity $z = \exp\{\beta\mu\}$ that there exist functions $G(A^m; \zeta^m)$ analytic for $\zeta^m \in \mathfrak{D}$ and continuous for $\zeta^m \in \bar{\mathfrak{D}}$ such that

$$G(A^m; \zeta^m) = \lim_{\Lambda \to \infty} G_\Lambda(A^m; \zeta^m) \ ,$$

where the convergence is uniform on compacts in $\mathfrak{D}$.

We will not attempt to prove this result although some of the necessary estimates will be derived in the subsequent discussion of quantum gases (see also Notes and Remarks).

Although the Green's functions

$$G_\Lambda(A, B; t) = \omega_\Lambda(A e^{itK_\Lambda} B e^{-itK_\Lambda})$$

converge in the small activity region one would not expect this result in general. For example, if phase transitions occur, one would expect the G_Λ to have several distinct limit points each giving information about the distinct phases. In fact, the bounds

$$|G_\Lambda(A, B; t)| \leq \|A\| \|B\|$$

imply that there always exist subnets Λ_α such that the limits

$$G(A,B;t) = \lim_\alpha G_{\Lambda_\alpha}(A,B;t)$$

exist for all observables A, B, and all $t \in \mathbb{R}$. This is a consequence of Tychonoff's theorem. Thus, it is of interest to have an interpretation of the functions G. Clearly, the values

$$\omega(A) = G(A, \mathbb{1}; 0)$$

determine a state ω over the observable algebra and ideally one would like to have an automorphism group τ of $\mathfrak{A}$, or of $\pi_\omega(\mathfrak{A})''$, such that

$$G(A,B;t) = \omega(A\tau_t(B)) \ .$$

It is however too optimistic to expect to find this structure under all circumstances. Nevertheless, one can derive weaker forms of this result. But before doing this we single out some relevant properties of the $G_\Lambda(A,B;t)$ which are mostly preserved in the limits.

The definition

$$G_\Lambda(A,B;t) = \omega_\Lambda(A\tau_t^\Lambda(B)) \ .$$

immediately implies that

(1) $A \mapsto G_\Lambda(A,B;t)$ is linear,
(2) $B \mapsto G_\Lambda(A,B;t)$ is linear,
(3) $t \to G_\Lambda(A,B;t)$ is continuous,
(4) $G_\Lambda(A,CB;0) = \omega_\Lambda(ACB) = G_\Lambda(AC,B;0)$,
(5) $G_\Lambda(\mathbb{1},\mathbb{1};0) = \omega_\Lambda(\mathbb{1}) = 1$.

If $\{A_i\}_{1\le i\le n} \subseteq \mathfrak{A}$ and $\{t_i\}_{1\le i\le n} \subset \mathbb{R}$ are finite sequences, one has

$$\begin{aligned}
&\sum_{i,j=1}^n G_\Lambda(A_i^*, A_j;\ t_j - t_i) \\
&\quad = \sum_{i,j=1}^n (U_{\omega_\Lambda}(t_i)\pi_{\omega_\Lambda}(A_i)\Omega_{\omega_\Lambda}, U_{\omega_\Lambda}(t_j)\pi_{\omega_\Lambda}(A_j)\Omega_{\omega_\Lambda}) \\
&\quad = \left\| \sum_{i=1}^n U_{\omega_\Lambda}(t_i)\pi_{\omega_\Lambda}(A_i)\Omega_{\omega_\Lambda} \right\|^2
\end{aligned}$$

and hence

(6) $$\sum_{i,j=1}^n G_\Lambda(A_i^*, A_j; t_j - t_i) \ge 0.$$

From the fact that ω_Λ is a τ^Λ-KMS state at value β one also has

(7) There exists a $\beta \in \mathbb{R}$ such that

$$\int_{-\infty}^{\infty} dt\, f(t) G_\Lambda(A,B;t) = \int_{-\infty}^{\infty} dt\, f(t+i\beta) G_\Lambda(B,A;-t)$$

for all $A, B, \in \mathfrak{A}$ and all f with $\hat{f} \in \mathscr{D}$. (See Proposition 5.3.12.) Of these properties, (1), (2), (4), (5), and (6) are clearly preserved under weak limits. This is not necessarily the case of the continuity property of condition (3) but it would follow if one had bounds on the derivatives $|dG_\Lambda(A, B; t)/dt|$ which are uniform both in Λ and t. This would also imply uniformity in t of the convergence $G_\Lambda(A, B; t) \to G(A, B; t)$ and hence the weak KMS condition (7) would follow in the limit. We will discuss these bounds later, after first investigating the general structure of a function G satisfying (1)–(7).

Theorem 6.3.27. *Let $\mathfrak{A}$ be a C^*-algebra with identity $\mathbb{1}$, and let $G; \mathfrak{A} \times \mathfrak{A} \times \mathbb{R} \mapsto \mathbb{C}$ be a function such that*

(1) *$A \mapsto G(A, B; t)$ is linear for all B in $\mathfrak{A}$ and t in $\mathbb{R}$,*
(2) *$B \mapsto G(A, B; t)$ is linear for all $A \in \mathfrak{A}$ and $t \in \mathbb{R}$,*
(3) *$t \mapsto G(A, B; t)$ is continuous for all $A, B \in \mathfrak{A}$,*
(4) *$G(A, CB; 0) = G(AC, B; 0)$ for all $A, B, C, \in \mathfrak{A}$,*
(5) *$G(\mathbb{1}, \mathbb{1}; 0) = 1$,*
(6) *$\sum_{i,j=1}^n G(A_i^*, A_j; t_j - t_i) \geq 0$ for all finite sequences $\{A_i\}_{1 \leq i \leq n} \subseteq \mathfrak{A}$, and $\{t_i\}_{1 \leq i \leq n} \subset \mathbb{R}$.*

It follows that

$$A \mapsto \omega(A) = G(\mathbb{1}, A; 0)$$

is a state on $\mathfrak{A}$. Let $(\mathfrak{H}_\omega, \pi_\omega, \Omega_\omega)$ be the corresponding cyclic representation. There exists a Hilbert space $\mathfrak{K}$ containing $\mathfrak{H}_\omega$, and a strongly continuous unitary representation U of $\mathbb{R}$ on $\mathfrak{K}$ such that

(i) $\mathfrak{K} = \bigvee_{t \in \mathbb{R}} U(t)\mathfrak{H}_\omega$
(ii) $G(A, B; t) = (\pi_\omega(A^*)\Omega_\omega, U(t)\pi_\omega(B)\Omega_\omega)$

for all $A, B, \in \mathfrak{A}, t \in \mathbb{R}$. Furthermore, properties (i) *and* (ii) *determine $(\mathfrak{K}, U)$ up to unitary equivalence in the sense that if $(\mathfrak{K}', U')$ is another pair satisfying* (i) *and* (ii), *then there exists a unitary operator $W : \mathfrak{K} \mapsto \mathfrak{K}'$ such that*

$$W|_{\mathfrak{H}_\omega} = \mathbb{1}_{\mathfrak{H}_\omega}$$

and

$$U(t) = W^* U'(t) W$$

for all $t \in \mathbb{R}$.

Proof. Condition (6) applied on the trivial sequences $\{A\}$ and $\{0\}$ implies that

$$G(A^*, A; 0) \geq 0$$

and hence (4) implies

$$\omega(A^*A) = G(\mathbb{1}, A^*A; 0) = G(A^*, A; 0) \geq 0 \ .$$

Since $\omega(\mathbb{1}) = G(\mathbb{1}, \mathbb{1}; 0) = 1$, it follows as a corollary of Proposition 2.3.11 that ω is a state. Let $(\mathfrak{H}_\omega, \pi_\omega, \Omega_\omega)$ be the associated representation of $\mathfrak{A}$.

Condition (6), applied to the sequences $\{\bar{c}_1 A^*, c_2 B\}$ and $\{t, 0\}$, where $c_1, c_2 \in \mathbb{C}$, implies that the matrix

$$\begin{pmatrix} G(A,\ A^*;0) & G(A,\ B;t) \\ G(B^*,\ A^*;-t) & G(B^*,\ B;0) \end{pmatrix}$$

is positive. It follows that

$$G(B^*, A^*; -t) = \overline{G(A, B; t)}$$

and

$$|G(A, B; t)|^2 \leq \omega(AA^*)\omega(B^*B) = \|\pi_\omega(A^*)\Omega_\omega\|^2 \ \|\pi_\omega(B)\Omega_\omega\|^2 \ .$$

Hence the function G defines a one-parameter family of bounded sesquilinear forms on $\pi_\omega(\mathfrak{A})\Omega_\omega \times \pi_\omega(\mathfrak{A})\Omega_w$. The closures of these forms define a one-parameter family $t \mapsto X_t$ of bounded operators on $\mathfrak{H}_\omega$, i.e.,

$$G(A, B; t) = (\pi_\omega(A^*)\Omega_\omega, X_t\ \pi_\omega(B)\Omega_\omega)$$

and the bound on G implies

$$\|X_t\| \leq 1 \ .$$

The definition of ω implies

$$X_0 = 1$$

and condition (6) has as a consequence that

$$\sum_{i,j=1}^{n} (\psi_i, X_{t_j - t_i}\psi_j) \geq 0$$

for all finite sequences$\{\psi_i\}_{1 \leq i \leq n}$ *in* $\mathfrak{H}_\omega$.

Now let $\tilde{\mathfrak{K}}$ be the vector space of all mappings φ from $\mathbb{R}$ into $\mathfrak{H}_\omega$ such that the set $\{t; t \in \mathbb{R}, \varphi(t) \neq 0\}$ is finite, and convert $\tilde{\mathfrak{K}}$ into a pre-Hilbert space by defining

$$\langle \varphi_1, \varphi_2 \rangle = \sum_{s,t} (\varphi_1(t), X_{s-t}\varphi_2(s)) \ .$$

This is really a positive semi-definite inner product by the inequality derived in the last paragraph. In analogy with the procedure employed in the beginning of Subsection 2.3.3, the GNS construction, we define

$$\mathfrak{J} = \{\varphi \in \tilde{\mathfrak{K}}; \langle \varphi, \varphi \rangle = 0\}$$

and $\mathfrak{K}$ as the Hilbert space completion of $\tilde{\mathfrak{K}}/\mathfrak{J}$ in the induced inner product. If $\psi \in \mathfrak{H}_\omega$ is identified with the element $\varphi \in \tilde{\mathfrak{K}}$ defined by

$$\varphi(t) = \begin{cases} \psi & \text{if } t = 0, \\ 0 & \text{otherwise,} \end{cases}$$

it follows that

$$\langle \varphi, \varphi \rangle = (\psi, \psi)$$

and this identifies $\mathfrak{H}_\omega$ as a subspace of $\mathfrak{K}$.

If $t \in \mathbb{R}$, define a map $\hat{U}(t)$ of $\tilde{\mathfrak{K}}$ by

$$(\hat{U}(t)\varphi)(s) = \varphi(s-t) \ .$$

Then $\hat{U}(t)\hat{U}(-t) = \hat{U}(-t)\hat{U}(t) = \mathbb{1}$, and

$$\begin{aligned}\langle \varphi_1, \hat{U}(t)\varphi_2\rangle &= \sum_{s,u}(\varphi_1(s), X_{u-s}\,\varphi_2(u-t)) \\ &= \sum_{s',u'}(\varphi_1(s'+t), X_{u'+1-(s'+t)}\varphi_2(u')) \\ &= \sum_{s,u}(\varphi_1(s+t), X_{u-s}\,\varphi_2(u)) = \langle \hat{U}(-t)\varphi_1, \varphi_2\rangle \ .\end{aligned}$$

It follows that $\hat{U}(t)$ lifts to a unitary operator $U(t)$ on $\mathfrak{K}$, and $t \mapsto U(t)$ becomes a homomorphism of $\mathbb{R}$ into the unitary group on $\mathfrak{K}$. This homomorphism is weakly continuous since $t \mapsto X_t$ is weakly continuous by assumption (3), and

$$\begin{aligned}\langle \varphi_1, \hat{U}(t)\varphi_2\rangle &= \sum_{s,u}(\varphi_1(s), X_{u-s}\,\varphi_2(u-t)) \\ &= \sum_{s,u}(\varphi_1(s), X_{u+t-s}\,\varphi_2(u)) \ .\end{aligned}$$

Hence $t \mapsto U_t$ is a strongly continuous unitary representation of $\mathbb{R}$ (weak and strong continuity are equivalent by Corollary 3.1.8).

The identification of $\mathfrak{H}_\omega$ as a subspace of $\mathfrak{K}$ immediately implies

(i) $$\mathfrak{K} = \bigvee_{t\in\mathbb{R}} U_t\mathfrak{H}_\omega$$

and, furthermore,

$$G(A,B;t) = (\pi_\omega(A^*)\Omega_\omega, X_t\pi_\omega(B)\Omega_\omega) = \langle \varphi_1, \varphi_2\rangle \ ,$$

where $\varphi_1, \varphi_2 \in \tilde{\mathfrak{K}}$ are defined by

$$\varphi_1(s) = \begin{cases} \pi_\omega(A^*)\Omega_\omega & \text{if } s = 0 \ , \\ 0 & \text{if } s \neq 0 \end{cases}$$

and

$$\varphi_2(s) = \begin{cases} \pi_\omega(B)\Omega_\omega & \text{if } s = t \ , \\ 0 & \text{if } s \neq t \ . \end{cases}$$

But then $\varphi_2 = \hat{U}(t)\varphi_3$, where

$$\varphi_3(s) = \begin{cases} \pi_\omega(B)\Omega_\omega & \text{if } s = 0 \ , \\ 0 & \text{if } s \neq 0 \ . \end{cases}$$

Hence

$$G(A,B;t) = \langle \varphi_1, \hat{U}(t)\varphi_2\rangle = (\pi_\omega(A^*)\Omega_\omega, U(t)\pi_\omega(B)\Omega_\omega) \ ,$$

where the last step uses the identification of $\mathfrak{H}_\omega$ as a subspace of $\mathfrak{K}$.

It remains to prove that $(\mathfrak{K}, U)$ is unique up to unitary equivalence. Let $(\mathfrak{K}', U')$ be another pair satisfying (i) and (ii), and define a map $W : \mathfrak{K} \mapsto \mathfrak{K}'$ by

$$W\Big(\sum_i U(t_i)\pi_\omega(A_i)\Big)\Omega_\omega = \sum_i U'(t_i)\pi_\omega(A_i)\Omega_\omega \ .$$

This map is well defined and isometric because

$$\begin{aligned}(U'(t)\pi_\omega(A)\Omega_\omega, U'(s)\pi_\omega(B)\Omega_\omega) &= (\pi_\omega(A)\Omega_\omega, U'(s-t)\pi_\omega(B)\Omega_\omega)\\ &= G(A^*, B; s-t)\\ &= (U(t)\pi_\omega(A)\Omega_\omega, U(s)\pi_\omega(B)\Omega_\omega)\end{aligned}$$

and W extends by closure to an isometry on $\mathfrak{K}$. But W is onto since

$$\bigvee_{t\in\mathbb{R}} U'(t)\mathfrak{H}_\omega = \mathfrak{K}'$$

and one has that

$$W|_{\mathfrak{H}_\omega} = \mathbb{1}_{\mathfrak{H}_\omega} \ .$$

One then verifies as in the proof of Theorem 2.3.16 that

$$U(t) = W^* U'(t) W \ .$$

Theroem 6.3.28. *Let $\mathfrak{A}$ be a C^*-algebra with identity $\mathbb{1}$, and let $G : \mathfrak{A}\times\mathfrak{A}\times\mathbb{R}\mapsto\mathbb{C}$ be a function satisfying assumptions* (1)–(6) *of Theorem* 6.3.27 *together with the following weak KMS condition:*

(7) *There exists a $\beta\in\mathbb{R}$ such that*

$$\int_{-\infty}^{\infty} dt f(t) G(A,B;t) = \int_{-\infty}^{\infty} dt\, f(t+i\beta) G(B,A;-t)$$

for all $A, B\in\mathfrak{A}$ and all f with $\hat{f}\in\mathscr{D}$.

Let $(\mathfrak{H}_\omega, \pi_\omega, \Omega_\omega, \mathfrak{R}, U)$ be the representatives associated with G by Theorem 6.3.27.

It follows that Ω_ω is separating for $\pi_\omega(\mathfrak{A})''$. Furthermore, the positive selfadjoint operator $U(i\beta)$ is a form extension of the modular operator Δ associated with the pair $(\pi_\omega(\mathfrak{A})'', \Omega_\omega)$, i.e.,

$$\|U(i\beta)^{1/2}\psi\| = \|\Delta^{1/2}\psi\|$$

for all $\psi\in D(\Delta^{1/2})$.

Warning. Even if $\mathfrak{K} = \mathfrak{H}_\omega$, i.e., if U is a unitary group on $\mathfrak{H}_\omega$ such that

$$G(A,B;t) = (\Omega_\omega, \pi_\omega(A)U(t)\pi_\omega(B)\Omega_\omega)$$

it does not follow that $U(i\beta)$ and Δ are equal. A counterexample can be constructed as follows: Let $\mathfrak{M}_1$ and $\mathfrak{M}_2$ be von Neumann algebras on a Hilbert space $\mathfrak{H}$ with a common separating and cyclic vector Ω such that $\mathfrak{M}_1 \subsetneq \mathfrak{M}_2$ (such pairs are common in relativistic quantum field theory, see Notes and Remarks), and let Δ_1 and Δ_2 be the associated modular operators. If $A\in\mathfrak{M}_1$, we have

$$\|\Delta_1^{1/2} A\Omega\| = \|A^*\Omega\| = \|\Delta_2^{1/2} A\Omega\|$$

and as $\mathfrak{M}_1$ is a core for $\Delta_1^{1/2}$ it follows that Δ_2 is a form extension of Δ_1. But $\Delta_2 \neq \Delta_1$ by the following reasoning: If $\Delta_2 = \Delta_1$ and J_1, J_2 are the modular conjugations associated with $\mathfrak{M}_1$ and $\mathfrak{M}_2$, then $J_2\Delta_2^{1/2}$ is an extension of $J_1\Delta_1^{1/2}$ and hence $J_2 = J_1$. But then we have

$$\mathfrak{M}_1 = J_1\mathfrak{M}_1'J_1 \supsetneqq J_1\mathfrak{M}_2'J_1 = J_2\mathfrak{M}_2'J_2 = \mathfrak{M}_2$$

and this contradicts $\mathfrak{M}_1 \subsetneqq \mathfrak{M}_2$. But in this case

$$G(A, B; t) = (\Omega,\ A\Delta_2^{-it/\beta}B\Omega)$$

with $\mathfrak{A} = \mathfrak{M}_1$ satisfies the axioms (1)–(7), and one has the identifications

$$\mathfrak{H}_\omega = \mathfrak{K} = \mathfrak{H}, \quad \Omega_\omega = \Omega, \quad U(t) = \Delta_2^{-it/\beta} \ .$$

Proof. The first part of the theorem is proved exactly as in Example 5.3.13. Next let

$$U(t) = \int dE(p)e^{-ipt}$$

be the spectral decomposition of U. Then assumption (7) implies that

$$\int d(A\Omega_\omega, E(p)A\Omega_\omega)\hat{f}(p) = \int d(A^*\Omega_\omega, E(p)A^*\Omega_\omega)\hat{f}(p)e^{\beta p}$$

for $A \in \pi_\omega(\mathfrak{A})''$ and one concludes that

$$\|A\Omega_\omega\|^2 = (A\Omega_\omega, A\Omega_\omega) = \int d(A^*\Omega_\omega, E(p)A^*\Omega_\omega)e^{\beta p} = \|U(i\beta)^{1/2}A^*\Omega_\omega\|^2 \ ,$$

i.e.,

$$\|\Delta^{1/2}A^*\Omega_\omega\|^2 = \|U(i\beta)^{1/2}A^*\Omega_\omega\|^2 \ .$$

The last conclusion of the theorem now follows because $\pi_\omega(\mathfrak{A})''\Omega_\omega$ is a core for $\Delta^{1/2}$.

We next examine criteria for the limit Green's functions to satisfy properties (1)–(7) of the proceeding theorems. As we remarked it is only the continuity in t, property (3), which poses a problem. We will work in a semi-abstract setting which is devised to cover typical models in statistical mechanics. Subsequently we discuss some applications.

Let $(\mathfrak{A}, \{\mathfrak{A}_\Lambda\})$ be a quasi-local C^*-algebra, and assume that each $\mathfrak{A}_\Lambda$ acts as an irreducible algebra on some Hilbert space $\mathfrak{H}_\Lambda$. We say that a family $\mathfrak{C}_\Lambda \subseteq \mathfrak{A}_\Lambda$ of *-algebras is an *isotonic family* if

(1) each $\mathfrak{C}_\Lambda$ is an irreducible subalgebra of $\mathscr{L}(\mathfrak{H}_\Lambda)$ containing the identity,

(2) if $\Lambda_1 \subseteq \Lambda_2$, then $\mathfrak{C}_{\Lambda_1} \subseteq \mathfrak{C}_{\Lambda_2}$.

In order to define Gibbs states we introduce a family of Hamiltonians H_Λ. Each H_Λ is a lower-semi-bounded[11] selfadjoint operator on $\mathfrak{H}_\Lambda$, with the property that

$$Z_\Lambda = \mathrm{Tr}_{\mathfrak{H}_\Lambda}(e^{-\beta H_\Lambda}) < +\infty$$

[11] Note that we have now implicitly assumed that the chemical potential term μN_Λ is incorporated in H_Λ and hence lower semi-boundedness corresponds to stability.

for all $\beta > 0$. The family of Gibbs states ω_Λ associated with the system are then introduced by

$$\omega_\Lambda(A) = \mathrm{Tr}_{\mathfrak{H}_\Lambda}(e^{-\beta H_\Lambda} A)/Z_\Lambda$$

where $A \in \mathfrak{A}_\Lambda$. The finite-volume Green's functions G_Λ are defined by

$$G_\Lambda(A,\ B; t) = \mathrm{Tr}_{\mathfrak{H}_\Lambda}(e^{-\beta H_\Lambda} A e^{itH_\Lambda} B e^{itH_\Lambda})/Z_\Lambda \ ,$$

where $A, B \in \mathfrak{A}_\Lambda$ and $t \in \mathbb{R}$. Note that each pointwise limit point of ω_Λ (respectively G_Λ) as $\Lambda \to \infty$ can be extended by continuity to a state (respectively Green's function) on $\mathfrak{A} = \overline{\bigcup_\Lambda \mathfrak{A}_\Lambda}$, and by a slight abuse of language we refer to such limits as weak* limits of ω_Λ (respectively, G_Λ). (See the discussion in the beginning of Section 6.2.2.)

In the following we will encounter commutator expressions of the form $[H_\Lambda, A]$ and the additional assumptions we now introduce are designed to ensure that these expressions have a well-defined meaning for a large enough set of A. We assume

(H) There exists an isotonic family $\mathfrak{D}_\Lambda \subseteq \mathfrak{A}_\Lambda$ such that

(1) if $A \in \mathfrak{D}_\Lambda$, then $AD(H_\Lambda) \subseteq D(H_\Lambda)$;

(2) the closures of the operators

$$[H_\Lambda, A]e^{-\beta H_\Lambda}$$

exist and are of trace-class for all $A \in \mathfrak{D}_\Lambda$ and all $\beta > 0$;

(3) $$\omega_\Lambda([H_\Lambda, A]^*[H_\Lambda, A]) < C_A < +\infty \ ,$$

where C_A is independent of Λ and the bound is valid for all $A \in \mathfrak{D}_\Lambda$ and all Λ.

Note that condition (1) implies that the operator of condition (2) is defined on $D(H_\Lambda)$. In condition (3) the definition of ω_Λ is extended to unbounded operators for which the appropriate operators are of trace-class.

Proposition 6.3.29. *Let $\{G_\Lambda\}$ denote the Green's functions associated with the family of Hamiltonians $\{H_\Lambda\}$, and let G be any weak*-limit point of the G_Λ. Assume that there exists an isotonic family $\{\mathfrak{D}_\Lambda\}$ of *-algebras satisfying* (H), *and assume that $\pi_\omega(\bigcup_\Lambda \mathfrak{D}_\Lambda)$ is weakly dense in $\pi_\omega(\mathfrak{A})''$ where $\omega(A) = G(A, \mathbb{1}; 0)$ is the state associated with G.*

It follows that G satisfies:

(1),(2) *$A, B \mapsto G(A, B; t)$ is bilinear for all $t \in \mathbb{R}$;*

(3) *$t \mapsto G(A, B; t)$ is continuous for all $A, B \in \mathfrak{A}$;*

(4) *$G(A, CB; 0) = G(AC, B; 0)$ for all $A, B, C \in \mathfrak{A}$;*

(5) *$G(\mathbb{1}, \mathbb{1}; 0) = 1$;*

(6) *$\sum_{i,j=1}^n G(A_i^*, A_j; t_j - t_i) \geq 0$ for all finite sequences $\{A_i\}_{1 \leq i \leq n} \subset \mathfrak{A}$, and $\{t_i\}_{1 \leq i \leq n} \subset \mathbb{R}$;*

(7) *$\int_{-\infty}^{\infty} dt f(t) G(A, B; t) = \int_{-\infty}^{\infty} dt f(t + i\beta) G(B, A; -t)$ for all $A, B \in \mathfrak{A}$ and all $\hat{f} \in \mathscr{D}$.*

Before proving the proposition we state an immediate corollary.

Corollary 6.3.30. *Let $\{\omega_\Lambda\}$ denote the Gibbs states associated with the family of Hamiltonians $\{H_\Lambda\}$ and let ω denote a limit point of the ω_Λ in the weak* topology. Assume there exists an isotonic family $\{\mathfrak{D}_\Lambda\}$ of *-algebras satisfying* (H), *such that $\pi_\omega(\bigcup_\Lambda \mathfrak{D}_\Lambda)$ is weakly dense in $\pi_\omega(\mathfrak{A})''$.*

It follows that ω is a modular state over $\mathfrak{A}$, i.e., the cyclic vector Ω_ω associated with ω and π_ω is separating for $\pi_\omega(\mathfrak{A})''$.

Proof of Corollary 6.3.30. Assume that $\omega = \lim_\alpha \omega_{\Lambda_\alpha}$, and let $\Lambda_{\alpha'}$ be a subnet of Λ_α such that $G_{\Lambda_{\alpha'}}$ converges to some function G. The state associated with G is then just ω, and G satisfies properties (1)–(7) of Theorems 6.3.27 and 6.3.28. The corollary is now a consequence of Theorem 6.3.28.

Proof of Proposition 6.3.29. Properties (1), (2), (4), (5), and (6) are obvious consequences of the corresponding properties for G_Λ.

Next let G_{Λ_α} be a net converging to G.

OBSERVATION 1. If $A \in \mathfrak{A}$ and $B \in \bigcup_\Lambda \mathfrak{D}$, then $G_{\Lambda_\alpha}(A,B;t) \to G(A,B;t)$ uniformly for t in compacts.

Proof. Assume that $A \in \mathfrak{A}$ and $B \in \bigcup_\Lambda \mathfrak{D}_\Lambda$. The conditions (H) imply that $G_\Lambda(A,B;t)$ is differentiable in t and

$$\begin{aligned}\left|\frac{d}{dt}G_\Lambda(A,B;t)\right|^2 &= |\omega_\Lambda(Ae^{itH_\Lambda}[iH_\Lambda,B])e^{-itH_\Lambda}|^2\\ &= |\omega_\Lambda(e^{-itH_\Lambda}Ae^{itH_\Lambda}[iH_\Lambda,B])|^2\\ &\le \omega_\Lambda(AA^*)\omega_\Lambda([H_\Lambda,B]^*[H_\Lambda,B]) \le \|A\|^2 C_B\ .\end{aligned}$$

Observation 1 is now a consequence of pointwise convergence and Lemma 6.3.23.

Observation 1 implies that

$$t \mapsto G(A,B;t)$$

is continuous for $A \in \mathfrak{A}$ and $B \in \bigcup_\Lambda \mathfrak{D}_\Lambda$. Now if B is a general element in $\mathfrak{A}$, choose a sequence B_n in $\bigcup_\Lambda \mathfrak{D}_\Lambda$ such that

$$\pi_\omega(B_n)\Omega_\omega \to \pi_\omega(B)\Omega_\omega\ .$$

It follows that

$$\omega((B_n - B)^*(B_n - B)) \to 0$$

and we have

$$\begin{aligned}&|G(A,B;t_1) - G(A,B;t_2)|\\ &\le |G(A,B-B_n;t_1)| + |G(A,B_n;t_1) - G(A,B_n;t_2)|\\ &\quad + |G(A,B_n - B;t_2)|\\ &\le 2\omega(AA^*)^{1/2}\omega((B-B_n)^*(B-B_n))^{1/2} + |G(A,B_n;t_1) - G(A,B_n;t_2)|\end{aligned}$$

for all $A \in \mathfrak{A}$ and $t_1, t_2 \in \mathbb{R}$. The continuity of

$$t \to G(A, B; t)$$

for general $A, B \in \mathfrak{A}$ immediately follows. This completes the proof of (3).

If $\hat{f} \in \mathscr{D} \subset \mathscr{S}$, then $f \in \mathscr{S}$, and it follows from Observation 1 and the KMS property of G_{Λ_α} that

$$\int_{-\infty}^{\infty} dt f(t) G(A, B; t) = \int_{-\infty}^{\infty} dt f(t + i\beta) G(B, A; -t)$$

for $A, B \in \bigcup_\Lambda \mathfrak{D}_\Lambda$. As $\pi_\omega(\bigcup_\Lambda \mathfrak{D}_\Lambda)$ is weakly dense in $\pi_\omega(\mathfrak{A})$, $\pi_\omega(\bigcup_\Lambda \mathfrak{D}_\Lambda)$ is strongly*-dense by Theorem 2.4.11, and hence if $A, B \in \mathfrak{A}$ are given there exist sequences A_n, B_n in $\bigcup_\Lambda \mathfrak{D}_\Lambda$ such that

$$\begin{aligned}
&\omega((A_n - A)^*(A_n - A)) \to 0 \ , \\
&\omega((A_n - A)(A_n - A)^*) \to 0 \ , \\
&\omega((B_n - B)^*(B_n - B)) \to 0 \ , \\
&\omega((B_n - B)(B_n - B)^*) \to 0 \ .
\end{aligned}$$

It then follows from estimates of the type

$$|G(C, D; t)|^2 \leq \omega(CC^*)\omega(D^*D)$$

that

$$G(A_n, B_n; t) \to G(A, B; t)$$

uniformly in t. Hence

$$\int_{-\infty}^{\infty} dt f(t) G(A, B; t) = \int_{-\infty}^{\infty} dt f(t + i\beta) G(B, A; -t)$$

for all $A, B, \in \mathfrak{A}$. This finishes the proof of property (7) and of the proposition.

Remark. If, under the assumptions of Proposition 6.3.29, Λ_α is a net such that G_{Λ_α} converges pointwise to G, and if, furthermore, $\mathfrak{K} = \mathfrak{H}_\omega$ where $\mathfrak{K}$ is defined in Theorem 6.3.27, i.e., there exists a unitary group U on $\mathfrak{H}_\omega$ such that

$$G(A, B; t) = (\Omega_\omega, \pi_\omega(A) U(t) \pi_\omega(B) \Omega_\omega) \ ,$$

then the limits

$$\begin{aligned}
&G(A, B_1, \ldots, B_m; t_1, \ldots, t_m) \\
&= \lim_\alpha \operatorname{Tr}_{\mathfrak{H}_{\Lambda_\alpha}} (e^{-\beta H_{\Lambda_\alpha}} A e^{it_1 H_{\Lambda_\alpha}} B_1 e^{i(t_2 - t_1) H_{\Lambda_\alpha}} B_2 \cdots B_m e^{-it_m H_{\Lambda_\alpha}}) / Z_{\Lambda_\alpha}
\end{aligned}$$

exist for all $A_1, B_1, \ldots, B_m \in \mathfrak{A}$, and one has

$$\begin{aligned}
&G(A, B_1, \ldots, B_m; t_1, \ldots, t_m) \\
&\quad = (\Omega_\omega, \pi_\omega(A) U(t_1) \pi_\omega(B_1) U(t_2 - t_1) \pi_\omega(B_2) \cdots \pi_\omega(B_m) U(-t_m) \Omega_\omega) \ .
\end{aligned}$$

To establish these statements choose a subnet $\Lambda_{\alpha'}$ of Λ_α such that all the limits $G(A, B_1, \ldots, B_m; t_1, \ldots, t_m)$ exist for all m. By an extension of Theorem 6.3.27 one can show that there exists a Hilbert space $\hat{\mathfrak{K}} \supset \mathfrak{H}_\omega$, a representation $\hat{\pi}_\omega$ of $\mathfrak{A}$ and a unitary group $\hat{U}$ on $\hat{\mathfrak{K}}$ such that

$$G(A, B_1, \ldots, B_m; t_1, \ldots, t_m)$$
$$= (\Omega_\omega, \hat{\pi}_\omega(A)\hat{U}(t_1)\hat{\pi}_\omega(B_1)\hat{U}(t_2 - t_1)\hat{\pi}_\omega(B_2) \cdots \hat{\pi}_\omega(B_m)\hat{U}(-t_m)\Omega_\omega) \ .$$

If P is the orthogonal projection from $\hat{\mathfrak{K}}$ onto $\mathfrak{H}_\omega$, one deduces that

$$U(t) = P\hat{U}(t)P$$

and since U is unitary $\hat{U}$ must commute with P. Since

$$\pi_\omega(B) = P\hat{\pi}_\omega(B)P$$

and Ω_ω is cyclic for $(\hat{\pi}, \hat{U})$ it follows that $\hat{\mathfrak{K}} = \mathfrak{H}_\omega$ and hence
$G(A, B_1, \ldots, B_m; t_1, \ldots, t_m)$

$$= (\Omega_\omega, \pi_\omega(A)U(t_1)\pi_\omega(B_1)U(t_2 - t_1)\pi_\omega(B_2) \cdots \pi_\omega(B_m)U(-t_m)\Omega_\omega) \ .$$

This shows that all weak*-limit points of the net are equal, and hence the net itself converges.

We end this section with some applications of the formalism developed on the previous pages to various specific models.

6.3.4.1. Quantum Spin Systems with Long-Range Interactions. We adopt the notation and assumptions from Section 6.2.1 for spin systems, and put $\mathfrak{D}_\Lambda = \mathfrak{A}_\Lambda$ for all finite subsets $\Lambda \subset L$. Let Φ be an interaction such that

$$\sum_{X \in x} \|\Phi(X)\| < +\infty$$

for each $x \in L$. It follows from Proposition 6.2.3 that the derivation

$$\delta(A) = \lim_{\Lambda \to \infty} i[H_\Phi(\Lambda), A]$$

exists for all $A \in \bigcup_\Lambda \mathfrak{A}_\Lambda$, where

$$H_\Phi(\Lambda) = \sum_{X \subseteq \Lambda} \Phi(X) \ .$$

The finite-volume Gibbs states are

$$\omega_\Lambda(A) = \frac{\mathrm{Tr}_{\mathfrak{H}_\Lambda}(e^{-\beta H_\Phi(\Lambda)}A)}{\mathrm{Tr}_{\mathfrak{H}_\Lambda}(e^{-\beta H_\Phi(\Lambda)})}$$

for $A \in \mathfrak{A}_\Lambda$. In this case the commutators

$$[H_\Phi(\Lambda), A]$$

are bounded in norm as $\Lambda \to \infty$ since the limit exists, and assumption (H) is trivially satisfied. In particular, Proposition 6.3.29 and Corollary 6.3.30 apply, and each weak*-limit point ω of the net$\{\omega_\Lambda\}$ is faithful on $\pi_\omega(\mathfrak{A})''$.

In Theorem 6.2.4 it was proved that if the interaction Φ satisfies

$$\sum_{n \geq 0} e^{\lambda n} \left(\sup_{x \in L} \sum_{\substack{X \ni x \\ |X| = n+1}} |\Phi(X)\|\right) < +\infty$$

for some $\lambda > 0$, then the closure of the derivation δ generates a group of automorphisms of $\mathfrak{A} = \overline{\bigcup_\Lambda \mathfrak{A}_\Lambda}$. There exist some interactions Φ which do not satisfy this condition, but nevertheless the weak* limits $\omega_\Lambda \to \omega$ exist, and δ_Φ generates a group of automorphisms of $\pi_\omega(\mathfrak{A})''$. (See Notes and Remarks to Section 6.2.1)

6.3.4.2. Bose Gas with Repulsive Interactions. In Section 6.3.4 we obtained some information about the Bose gas with repulsive interactions by a method of *a priori* estimates on the reduced density matrices. This information can be complemented in certain cases by the exploitation of commutator estimates.

Theorem 6.3.31. *Let $\mathfrak{A} = \overline{\bigcup_\Lambda \mathfrak{A}_-(\Lambda)}$ be the CCR algebra over $\bigcup_\Lambda L^2(\Lambda)$, and consider the finite-volume Dirichlet boundary condition Gibbs states ω_Λ at temperature $\beta > 0$ and chemical potential $\mu < 0$ for a Bose gas interacting through a two-body potential Φ satisfying:*

(1) *Φ is positive, i.e.,*

$$\Phi(x) \geq 0$$

for all $x \in \mathbb{R}^\nu$.

(2) *The estimate*

$$\int d^\nu x\, (1 + |x|^2)^{\nu+\varepsilon} |\Phi(x)|^2 < +\infty$$

is valid for some $\varepsilon > 0$.

Let ω be any weak-limit point of ω_Λ as $\Lambda \to \infty$.*
It follows that

(i) *ω is locally normal,*
(ii) *ω is a modular state, i.e., Ω_ω is separating for $\pi_\omega(\mathfrak{A})''$.*

It has already been proved for more general repulsive interactions that ω is locally normal, see Theorem 6.3.22. In the Remark following that theorem it was established that ω satisfies local number estimates of the form

$$\omega(N_\Lambda^m) < +\infty$$

for all $m \geq 0$ and all finite regions Λ. The strategy behind the proof of the present theorem is to combine these estimates with estimates on

$$\|[T_{\infty,\Lambda}, A]\psi\| \ , \quad \|[U_\Phi, A]\psi\|$$

for suitable $A \in \mathfrak{A}_-(\Lambda)$ in terms of

$$\|N_\Lambda^m \psi\|$$

for suitable $m > 0$. One can then verify the conditions (H) used in Proposition 6.3.29.

We prove the commutator estimates in a series of lemmas. These lemmas are stated both for Bose and Fermi gases with later applications to low density gases in mind, see Section 6.3.4.3. We work on Fock space and ψ always denotes a vector in Fock space which is contained in $D(N_\Lambda^m)$ where Λ and m vary from lemma to lemma.

Lemma 6.3.32. *If $f \in L^2(\Lambda)$, and $\Phi \in L^2(\Lambda')$, then*

$$\begin{aligned}\|[U_\Phi, a(f)]\psi\| &\le \|\Phi\|_2 \|a(f)(N_{\Lambda-\Lambda'} - \mathbb{1})\psi\| \\ &\le \|\Phi\|_2 \|f\|_2 \|N_\Lambda^m (N_{\Lambda-\Lambda'} - \mathbb{1})\psi\| \ ,\end{aligned}$$

where

$$m = 0 \quad \textit{for fermions}$$

$$m = \frac{1}{2} \quad \textit{for bosons}$$

and

$$\Lambda - \Lambda' = \{x \in \mathbb{R}^\nu; x = y - z, y \in \Lambda, z \in \Lambda'\} \ .$$

Proof. Using the action of annihilation operators and of U_Φ,

$$\begin{aligned}(a(f)\psi)^{(n)}(x_1, \ldots, x_n) &= (n+1)^{1/2} \int dx\, \overline{f(x)} \psi^{(n+1)}(x, x_1, \ldots, x_n) \\ (U_\Phi \psi)^{(n)}(x_1, \ldots, x_n) &= \sum_{1 \le i < j \le n} \Phi(x_i - x_j) \psi^{(n)}(x_1, \ldots, x_n) \\ &= \frac{1}{2} \sum_{i \ne j} \Phi(x_i - x_j) \psi^{(n)}(x_1, \ldots, x_n) \ ,\end{aligned}$$

one calculates[12]

$$\begin{aligned}\|[U_\Phi, a(f)]\psi\|^2 = \sum_{n \ge 0} (n+1) \int dx_1 \cdots dx_n \int dx\, dy f(x) \overline{f(y)} \left[\sum_{i=1}^n \Phi(x - x_i)\right] \\ \times \left[\sum_{j=1}^n \Phi(y - y_i)\right] \overline{\psi^{(n+1)}(x, x_1, \ldots, x_n)} \psi^{(n+1)}(y, x_1, \ldots, x_n) \ .\end{aligned}$$

We now sum the right-hand side over a complete orthonormal basis of $L^2(\Lambda')$ which is chosen to contain $\Phi/\|\Phi\|_2$. This gives the inequality

$$\begin{aligned}\|[U_\Phi, a(f)]\psi\|^2 \le \|\Phi\|_2^2 \sum_{n \ge 0} (n+1) \int dx \sum_{i,j} \int_{\substack{x - x_i \in \Lambda' \\ x - x_j \in \Lambda'}} dx_1 \cdots dx_n \\ \times f(x) \overline{f(x - x_i + x_j)}\ \overline{\psi^{(n+1)}(x, x_1, \ldots, x_n)} \psi^{(n+1)}(x - x_i + x_j, x_1, \ldots, x_n) \ .\end{aligned}$$

[12]At this point it is convenient to think in terms of the expression

$$U_\Phi = \frac{1}{2} \int dx\, dy\, \Phi(x - y) a^*(x) a^*(y) a(y) a(x)$$

where $a(x)$ and $a^*(x)$ are defined in Example 5.2.1.

Applying the Cauchy–Schwarz inequality one then finds

$$\begin{aligned}\|[U_\Phi, a(f)]\psi\|^2 &\le \|\Phi\|_2^2 \sum_{n\ge 0}\sum_{i,j}\int_{\substack{x_i\in\Lambda-\Lambda'\\ x_j\in\Lambda-\Lambda'}} dx_1\cdots dx_n |(a(f)\psi)^{(n)}(x_1,\dots,x_n)|^2\\ &= \|\Phi\|_2^2\|N_{\Lambda-\Lambda'}a(f)\psi\|^2\\ &= \|\Phi\|_2^2\|a(f)(N_{\Lambda-\Lambda'}-\mathbb{1})\psi\|^2 \ .\end{aligned}$$

Finally, for fermions one has

$$a^*(f)a(f) \le \|f\|_2^2\ \mathbb{1}\ ,$$

and for bosons

$$a^*(f)a(f) \le \|f\|_2^2\ N_\Lambda\ .$$

Lemma 6.3.33. *If $f \in L^2(\Lambda)$ and $\Phi \in L^2(\Lambda')$ with $0 \in \Lambda'$, then*

$$\begin{aligned}\|[U_\Phi, a^*(f)]\psi\| &\le \|\Phi\|_2\|f\|_2\|N_{\Lambda-\Lambda'}\psi\| && \textit{for fermions}\\ &\le \|\Phi\|_2\|f\|_2\|(N_{\Lambda-\Lambda'}+\mathbb{1})^{1/2}N_{\Lambda-\Lambda'}\psi\| && \textit{for bosons.}\end{aligned}$$

Proof. First note that the Fock space $\mathfrak{F}_\pm(\mathbb{R}^\nu)$ decomposes as

$$\mathfrak{F}_\pm(\Lambda-\Lambda')\otimes\mathfrak{F}_\pm((\Lambda-\Lambda')^c)\ ,$$

where $(\Lambda-\Lambda')^c$ denotes the complement of $\Lambda-\Lambda'$ and $\otimes$ denotes the symmetrized or anti-symmetrized tensor product according to the choice of statistics. As all operators occurring in the statement of the lemma act on $\mathfrak{F}_\pm(\Lambda-\Lambda')$ it is enough to prove the inequalities on this space.

Since $[U_\Phi, a(f)]$ annihilates the zero- and one-particle spaces,

$$[U_\Phi, a(f)](N_{\Lambda-\Lambda'}-\mathbb{1})^{-1}$$

is uniquely defined as an operator on $\mathfrak{F}_\pm(\Lambda-\Lambda')$. By Lemma 6.3.32 one has

$$\|[U_\Phi, a(f)](N_{\Lambda-\Lambda'}-\mathbb{1})^{-1}\| \ \le\ \|f\|_2\|\Phi\|_2$$

in the fermion case. Since $\Lambda\subseteq\Lambda-\Lambda'$, we have $N_\Lambda \le N_{\Lambda-\Lambda'}$ and

$$\|[U_\Phi, a(f)](N_{\Lambda-\Lambda'}-\mathbb{1})^{-1}N_{\Lambda-\Lambda'}^{-1/2}\| \ \le\ \|f\|_2\|\Phi\|_2$$

for bosons. Taking adjoints and using the fact that $[U_\Phi, a^*(f)]$ maps the n-particle space into the $n+1$-particle space we obtain

$$\|[U_\Phi, a^*(f)]N_{\Lambda-\Lambda'}^{-1}\| \ \le\ \|f\|_2\|\Phi\|_2$$

for fermions and

$$\|[U_\Phi, a^*(f)]N_{\Lambda-\Lambda'}^{-1}(N_{\Lambda-\Lambda'}+\mathbb{1})^{1/2}\| \ \le\ \|f\|_2\|\Phi\|_2$$

for bosons. These inequalities are equivalent to those stated in the lemma.

Next for bosons we consider the field operators

$$\Phi(f) = 2^{-1/2}(a(f)+a^*(f))$$

and Weyl operators

$$W(f) = e^{i\Phi(f)}$$

as in Section 5.2.1.

Lemma 6.3.34. *If $f \in L^2(\Lambda)$ and $\Psi \in L^2(\Lambda')$ with $0 \in \Lambda'$, then*

$$\|[U_\Psi, W(f)]\psi\| \leq \|\Psi\|_2 \|f\|_2 (a_0 + a_1 \|f\|_2) \|(N_{\Lambda-\Lambda'} + \mathbb{1})^{3/2}\psi\|$$

where a_0 and a_1 are positive constants independent of f, Ψ, and ψ.

PROOF. One has

$$\begin{aligned} W(f)^*[U_\Psi, W(f)] &= W(f)^* U_\Psi W(f) - U_\Psi \\ &= i \int_0^1 ds\, W(sf)^*[U_\Psi, \Phi(f)] W(sf) \ . \end{aligned}$$

Therefore

$$\|[U_\Psi, W(f)]\psi\| \ \leq \ \int_0^1 ds \|[U_\Psi, \Phi(f)] W(sf)\psi\| \ .$$

We now use $\Phi(f) = (a(f) + a^*(f))/\sqrt{2}$ and Lemmas 6.3.32 and 6.3.33 to obtain

$$\|[U_\Psi, W(f)\psi\| \leq \sqrt{2}\|\Psi\|_2 \|f\|_2 \int_0^1 ds\, \|(N_{\Lambda-\Lambda'} + \mathbb{1})^{3/2} W(sf)\psi\| \ .$$

But if $g \in L^2(\Lambda)$, one has

$$\begin{aligned} W(g)^* N_{\Lambda-\Lambda'} W(g) - N_{\Lambda-\Lambda'} &= i \int_0^1 ds\, W(sg)^*[N_{\Lambda-\Lambda'}, \Phi(g)] W(sg) \\ &= \int_0^1 ds\, W(sg)^* \Phi(ig)] W(sg) \\ &= \int_0^1 ds \{\Phi(ig) - \mathrm{Im}(-sg, ig)\mathbb{1}\} \\ &= \Phi(ig) + \|g\|_2^2 \mathbb{1}/2 \ , \end{aligned}$$

where the next to last step used Proposition 5.2.4. Therefore,

$$W(sf)^*(N_{\Lambda-\Lambda'} + \mathbb{1})^{3/2} W(sf) = \left(N_{\Lambda-\Lambda'} + s\Phi(if) + s^2\|f\|_2^2 \mathbb{1}/2 + \mathbb{1}\right)^{3/2}$$

and thus

$$\begin{aligned} &\|[U_\Psi, W(f)]\psi| \\ &\quad \leq \sqrt{2}\|\Psi\|_2 \|f\|_2 \int_0^1 ds \left\| \left(N_{\Lambda-\Lambda'} + s\Phi(if) + s^2\|f\|_2^2 \mathbb{1}/2 + \mathbb{1}\right)^{3/2} \psi \right\| \ . \end{aligned}$$

Now, we use the commutation relation

$$[N_{\Lambda-\Lambda'}, \Phi(g)] = -i\Phi(ig)$$

valid for $g \in L^2(\Lambda)$ together with the bounds

$$\Phi(g)^2 \leq 2(N_\Lambda + \mathbb{1})\|g\|_2^2 \ ,$$

$$\Phi(g) \leq \sqrt{2}(N_\Lambda + \mathbb{1})^{1/2}|g|_2 \ \leq \ 2^{1/2}(N_{\Lambda-\Lambda'} + \mathbb{1})^{1/2}\|g\|_2$$

to estimate $(N_{\Lambda-\Lambda'} + s\Phi(if) + s^2\|f\|_2^2\mathbb{1}/2 + \mathbb{1})^3$ in terms of $(N_{\Lambda-\Lambda'} + \mathbb{1})^3$. Inserting this estimate in the last estimate for $\|[U_\Psi, W(f)]\psi\|$ the lemma follows.

Lemma 6.3.35. *Let $\psi \in \mathfrak{F}_\pm(L^2(\mathbb{R}^\nu))$ be such that for every $\Lambda \in \mathbb{R}^\nu$ one has $\psi \in D(N_\Lambda^m)$ and*

$$\|(N_\Lambda + \mathbb{1})^m\psi\| \leq (|\Lambda| + 1)^m c_{\psi,m}$$

where $m = 1$ for fermions, $m = \frac{3}{2}$ for bosons, and $c_{\psi,m}$ is independent of Λ. Further let $f \in L^2(\Lambda_f)$ for some Λ_f and take Ψ such that

$$|||\Psi|||_\varepsilon^2 = \int d^\nu x\,(1 + |x|^2)^{\nu+\epsilon}|\Psi(x)|^2 < +\infty$$

for some $\varepsilon > 0$.

It follows that

$$\|[U_\Psi, a^\#(f)]\psi\| \leq d(c_{\psi,m}; \Lambda_f; \varepsilon)|||\Psi|||_\varepsilon\|f\|_2$$

where $a^\#$ denotes either a or a^* and d is a constant. Further, for bosons,

$$\|[U_\Psi, W(f)]\psi\| \leq d(c_{\psi,m}; \Lambda_f; \varepsilon)|||\Psi|||_\varepsilon\|f\|_2(a_0 + a_1\|f\|_2)$$

where a_0 and a_1 are constants.

Proof. Partition $\mathbb{R}^\nu$ into a cubic lattice with unit cells Λ_i, and define $\Psi_i = \chi_{\Lambda_i}\Psi$. One has

$$\begin{aligned}\|[U_\Psi, a^\#(f)]\psi\| &\leq \sum_i \|[U_{\Psi_i}, a^\#(f)]\psi\| \\ &\leq \sum_i \|f\|_2\|\Psi_i\|_2\|(N_{\Lambda_f-\Lambda_i} + \mathbb{1})^m\psi\| \\ &\leq \sum_i \|f\|_2\|\Psi_i\|_2 c_{\psi,m}(|\Lambda_f - \Lambda_i| + 1)^m\end{aligned}$$

where the second step is an application of Lemmas 6.3.32 and 6.3.33. Next note that $|\Lambda_f - \Lambda_i| + 1$ is equal to a constant d_f and

$$|||\Psi|||_\varepsilon^2 \geq a_i\|\Psi_i\|_2^2 \ ,$$

where

$$a_i = \inf_{x \in \Lambda_i}(1 + |x|^2)^{\nu+\varepsilon} \ .$$

Thus

$$\sum_i \|\Psi_i\|_2 \ \leq \ |||\Psi|||_\varepsilon \sum_i a_i^{-1/2} \ .$$

Combining these estimates one has

$$\|[U_\Psi, a^*(f)]\psi\| \le c_{\psi,m} d_f^m \left(\sum_i a_i^{-1/2}\right) \|f\|_2 |||\Psi|||_\varepsilon \ .$$

The second statement of the lemma follows from Lemmas 6.3.32 and 6.3.33 by an identical argument.

Next we turn to estimates involving the kinetic energy operator

$$T = d\Gamma(-\nabla^2) \ .$$

Lemma 6.3.36. *If $f \in L^2(\Lambda)$ is twice continuously differentiable, one has*

$$\|[T, a(f)]\psi\| \le \|\nabla^2 f\|_2 \|N_\Lambda^m \psi\| \ ,$$
$$\|[T, a^*(f)]\psi\| \le \|\nabla^2 f\|_2 \|(N_\Lambda + \mathbb{1})^m \psi\| \ ,$$

where

$$m = 0 \quad \textit{for fermions},$$
$$m = \frac{1}{2} \quad \textit{for bosons}.$$

Proof. One has

$$\begin{aligned}([T, a(f)]\psi)^{(n)}(x_1, \ldots, x_n) &= -\int dx\ f(x) \nabla_x^2 \psi^{(n+1)}(x, x_1, \ldots, x_n) \\ &= -(a(\nabla^2 f)\psi)^{(n)}(x_1, \ldots, x_n)\end{aligned}$$

and hence

$$[T, a(f)] = -a(\nabla^2 f) \ .$$

The first estimate in the lemma follows immediately, and the second is proved from the first as in Lemma 6.3.34.

Lemma 6.3.37. *Let $f \in L^2(\Lambda)$ be twice continuously differentiable. It follows that*

$$\|[T, W(f)]\psi\| \le \|\nabla f\|_2^2 \|\psi\| + 2\|\nabla^2 f\|_2 \|(N_\Lambda + \mathbb{1})^{1/2}\psi\| \ .$$

Proof. One argues as in the proof of Lemma 6.3.34 that

$$\begin{aligned}\|[T, W(f)]\psi\| &\le \int_0^1 ds \|[\Phi(f), T] W(sf)\psi\| \\ &= \int_0^1 ds \|\Phi(i\nabla^2 f) W(sf)\psi\| \\ &= \int_0^1 ds \|\{\Phi(i\nabla^2 f) + s\ \mathrm{Re}(f, \nabla^2 f)\mathbb{1}\}\psi\| \\ &= \int_0^1 ds \|\{\Phi(i\nabla^2 f) + s\|\nabla f\|_2^2 \mathbb{1}\}\psi\| \ ,\end{aligned}$$

where the next to last step uses Proposition 5.2.4. One then uses

$$\Phi(i\nabla^2 f)^2 \leq 2\|\nabla^2 f\|_2^2 (N_\Lambda + \mathbb{1}) \ ,$$

etc.

Proof of Theorem 6.3.31. The limit state is locally normally by Theorem 6.3.22, and by the subsequent Remark one has local number estimates

$$\omega_\Lambda((N_{\Lambda_0} + \mathbb{1})^m) \ \leq \ c_m(|\Lambda_0| + \mathbb{1})^m$$

whenever $\Lambda_0 \subseteq \Lambda$ where c_m is a constant independent of Λ_0 and Λ. We will apply Proposition 6.3.29 and take $\mathfrak{D}_\Lambda$ as the linear span of all $W(f)$ where f is twice continuously differentiable and has compact support inside Λ. We have

$$H_\Lambda \ = \ T_{\infty,\Lambda} + U_\Phi - \mu N_\Lambda \ .$$

Suppose that f is twice continuously differentiable and has support inside some open region Λ_0. Then

$$[T_{\infty,\Lambda}, W(f)] \ = \ [T, W(f)]$$

for all $\Lambda \ \supseteq \ \Lambda_0$, and hence

$$\omega_\Lambda([T_{\infty,\Lambda}, W(f)]^*[T_{\infty,\Lambda}, W(f)]) \ \leq \ b_1(f)\omega_\Lambda((N_{\Lambda_0} + \mathbb{1})) \leq b_1(f)c_1(|\Lambda_0| + \mathbb{1})$$

where $b_1(f)$ is independent of Λ. Similarly from Lemma 6.3.35 one has

$$\omega_\Lambda([U_\Phi, W(f)]^*[U_\Phi, W(f)]) \ \leq \ d(c_3^{1/2}; \Lambda_0; \varepsilon)^2 |||\Phi|||_\varepsilon^2 \|f\|_2^2 (a_0 + a_1\|f\|_2)^2 \ ,$$

where we used

$$\omega_\Lambda((N_{\Lambda_0} + \mathbb{1})^3) \ \leq \ c_3(|\Lambda_0| + 1)^3 \ .$$

Finally one has

$$[N_\Lambda, W(f)] \ = \ W(f)\{\Phi(if) + \tfrac{1}{2}\|f\|_2^2 \mathbb{1}\}$$

by the reasoning used in the proof of Lemma 6.3.34, and hence

$$\begin{aligned}[N_\Lambda, W(f)]^*[N_\Lambda, W(f)] \ &= \ (\Phi(if) + \tfrac{1}{2}\|f\|_2^2 \mathbb{1})^*(\Phi(if) + \tfrac{1}{2}\|f\|_2^2 \mathbb{1}) \\ &\leq \ b_2(f)(N_{\Lambda_0} + \mathbb{1})\end{aligned}$$

and

$$\omega([N_\Lambda, W(f)]^*[N_\Lambda, W(f)]) \ \leq \ b_2(f)c_1(|\Lambda_0| + 1) \ .$$

Combining the estimates of the commutators of $T_{\infty,\Lambda}$, U_Φ, and N_Λ with $W(f)$ we conclude that

$$\omega_\Lambda([H_\Lambda, W(f)]^*[H_\Lambda, W(f)]) \leq b(f) < +\infty \ ,$$

where $b(f)$ is independent of Λ. Hence, condition (H) is satisfied. Since ω is locally normal it follows that $\pi_\omega(\bigcup_\Lambda \mathfrak{D}_\Lambda)$ is weakly dense in $\pi_\omega(\bigcup_\Lambda \mathfrak{A}(\Lambda))''$, and Corollary 6.3.30 implies that ω is a modular state.

6.3.4.3. Dilute Bose and Fermi Gases. Theorem 6.3.26 stated convergence of Dirichlet boundary condition Green's functions in the small activity region, and because of uniformity of the convergence the limit Green's functions are

continuous in time, and one may apply this theorem directly to conclude that the limit state is a modular state without verifying conditions (H). It is however interesting to note that condition (H) is actually used in the proof of the uniformity in Theorem 6.3.26, i.e., one first uses low-activity expansions to establish pointwise convergence of the Green's functions $G_\Lambda(A^m; \zeta^m)$ for $\zeta^m \in \mathfrak{D}$, and then uses estimates on the derivatives of G_Λ with respect to $\zeta_1, \ldots, \zeta_m$, to prove that the convergence is uniform on compacts. These estimates are of the form (H), where $\mathfrak{D}_\Lambda$ is taken to be polynomials in $a(f)$ and $a^*(f)$ with f twice continuously differentiable functions in $L^2(\Lambda)$ in the fermion case. This assures that the commutation with the kinetic energy part of H_Λ is a bounded operator, and the bounds on the commutator with the potential energy part are established by rather straightforward, but long, estimates in which the condition $\Phi \in L^2$ plays an essential part. For bosons one may take $\mathfrak{D}_\Lambda$ to be the linear combinations of $W(f)$ where $f \in L^2(\Lambda)$ is twice continuously differentiable.

6.4. Conclusion

Throughout this volume we have tried to demonstrate the utility of operator algebras and their states in the analysis of quantum statistical mechanics. The most detailed and interesting justification of these techniques is provided by the theory of quantum spin systems discussed in the first half of this chapter. A large class of these models, including all the basic examples such as the Heisenberg and Ising models, can be described by C^*-dynamical systems $(\mathfrak{A}, \tau)$ and states of these systems correspond to the physical states described by the model. A global viewpoint of this type is essential if one desires understanding of such basic questions as the nature of thermodynamic phases, mixture properties of the phases, etc., and this is perhaps the greatest single advantage of the algebraic methods. Traditionally, equilibrium states had been described by a variety of methods, e.g., implicit or explicit thermodynamic limits of the Gibbs ensembles, the principle of maximum entropy, etc., but in all these methods the affine properties of the states were unclear. Phase transitions were partially understood in terms of nondifferentiability of the thermodynamic functions, or through lack of clustering of the states, but no framework really existed for the definition and characterization of pure phases and mixed phases. The realization that the equilibrium states could in fact be identified as states over the appropriate C^*-dynamical systems immediately provided this framework. The equilibrium states at each fixed temperature were seen to form a convex set with the extremal points corresponding to pure phases and the mixed states to mixtures of phases. This immediately motivated much of the analysis of decomposition theory, invariant states, periodic states, almost-periodic states, etc., described in Chapter 4. This point of view was initially somewhat speculative but the theory of spin systems provides a clear vindication of its validity; all the traditional definitions of equilibrium states coincide and they are indeed described by convex subsets of the state space of the spin algebra $\mathfrak{A}$. The global analysis then reveals many properties which were hitherto unclear, e.g., the links between purity and clustering, factoriality, and mixing. Many of these properties are consequences of some form of asymptotic abelianness.

The second striking feature in the algebraic description of equilibrium phenomena is the role played by the KMS condition. Starting from the Gibbs ensemble it is evident that this condition is satisfied but it is completely unclear that this condition alone should characterize equilibrium. Nevertheless, this is

the case for a large class of quantum spin systems, and also for the ideal Fermi gas. This rather surprising result is both of practical and conceptual utility. For example we argued in Section 6.2.5 that under a variety of circumstances there exists a unique KMS state for the infinite spin system. But since the thermodynamic limits of Gibbs states are automatically KMS states, this immediately gives a strong uniqueness statement for the thermodynamic limit, e.g., this limit must be independent of boundary conditions. Moreover, uniqueness implies that the equilibrium state is a factor state and one can immediately deduce spatial clustering properties. On the other hand, we have seen in Chapter 5 that the KMS condition has a variety of characterizations which emphasize different physical features such as stability under perturbations and ergodicity in the form of asymptotic abelianness. This clarifies to a large extent the nature of the equilibrium states even if it does not provide any profound explanation for their definition. Since the spin systems are described by C^*-dynamical systems, one can define the time development of arbitrary states and in principle one could tackle the problems of approach to equilibrium but work in this direction seems difficult and much remains to be done.

Finally, the description of continuous systems is notably incomplete. But this is a feature of all methods which have been applied to their analysis and it is doubtful that any complete understanding of these models will be obtained in the near future.

Notes and Remarks

Sections 6.1 and 6.2.1

The study of spin systems as models of magnetism predates the full development of quantum mechanics. The earliest model of this type was suggested by Lenz [Len 1] in 1920 as a possible microscopic explanation for the phenomenon of magnetization. Lenz argued that atoms in a crystal appeared to have a number of preferred orientations and that the potential energy of an atom with respect to its neighbor should favor their alignment and hence give rise to a spontaneous magnetization. Lenz emphasized the simplest case in which an atom has two possible orientations, the spin-$\frac{1}{2}$ model of Example 6.2.1. The eigenfunctions of σ_3^x with eigenvalue $+1$ are traditionally taken to represent the positive magnetization, spin up, and the eigenfunctions with eigenvalue -1 then correspond to negative magnetization, or spin down. The potential energy, or interaction, suggested by Lenz takes the form $-J\sigma_3^x\sigma_3^y$ for "neighboring" points $x, y \in L$ where $J > 0$. Thus, the energy is negative if, and only if, the atoms at x and y have the same orientation, i.e., the spins are parallel.

In 1925 Ising, a student of Lenz, carried out an exact calculation of the partition function, $\mathrm{Tr}(e^{-\beta H})$, for the one-dimensional $L = \mathbb{Z}$ Lenz model [Isi 1], in his doctoral dissertation. Ising inferred from his calculations that the one-dimensional model failed to exhibit an ordered ferromagnetic state at any temperature but he also argued incorrectly that the same situation would prevail in higher dimensions and backed this argument with various approximate calculations.

Since 1925 the Lenz model has almost universally been referred to as the Ising model (see Example 6.2.2). A full history of this model to 1966 has been given by Brush [Bru 1].

Ising's negative conclusions appear to have been accepted by other authors and in 1928 Heisenberg [Hei 1] proposed a more complex interatomic spin-spin coupling, $-J\sigma^x \cdot \sigma^y$, as the root of ferromagnetism (see Example 6.2.2). While the Lenz–Ising model is basically a classical model, i.e., the Hamiltonian is a function of the mutually commuting third components $\{\sigma_3^x\}_{x \in L}$ of the atomic spin, the more sophisticated Heisenberg model is inherently quantum mechanical and in this sense is the prototype of quantum spin systems as we describe them. Nevertheless, the Heisenberg interaction is not necessary for the understanding of ferromagnetism because in 1935 Peierls [Pei 1] proved that

the Lenz–Ising model exhibits a spontaneous magnetization in two or more dimensions, i.e., with $L = \mathbb{Z}^\nu$ and $\nu \geq 2$. (For a further discussion see the Notes and Remarks to Section 6.2.6)

Spin systems on regular lattices also provide a model of crystalline structure. It was a long-standing notion that crystals were formed in a repeating pattern best described by a periodic structure. This tenet of symmetry then imposed a number of restraints on the possible crystalline forms, e.g., rotational symmetries of order greater than five are impossible for periodic patterns in two or three dimensions (see, for example, [[Sen 1]], Chapter 1). But the 1984 experiments of Schectman, Blech, Gratias and Cahn [Sche 1] revealed a metallic phase of an aluminium-manganese alloy with a six-fold symmetry, the first example of a nonperiodic crystalline structure. These experiments radically affected ideas about crystals, their structure and definition. For example, the definition of a crystal as proposed by a 1992 Commission of the International Union of Crystallography is 'a solid with an essentially discrete diffraction diagram with the symmetry of the crystal that implied by the diffraction pattern'. Thus the traditional definition of a crystal has been replaced by its Fourier transform. The theoretical description has also had to be broadened with a movement away from periodic lattices to aperiodic ones.

The lattice gas interpretation of the spin-$\frac{1}{2}$ system is given explicitly as follows. The eigenfunctions ψ_+ of σ_3^x with eigenvalue $+1$ correspond to states with a particle at x and the eigenfunctions ψ_- with eigenvalue -1 represent states without a particle at x. The spin raising and lowering operators

$$a_x^* = (\sigma_1^x + i\sigma_2^x)/2, \qquad a_x = (\sigma_1^x - i\sigma_2^x)/2 \ ,$$

then act as particle creation and annihilation operators, e.g.,

$$a_x^*(\sigma_3^x + \mathbb{1}) = 0 = (\sigma_3^x - \mathbb{1})a_x^* \ ,$$

$$(\sigma_3^x + \mathbb{1})a_x = 0 = a_x(\sigma_3^x - \mathbb{1}) \ ,$$

and hence

$$\sigma_3^x(a_x\psi_+) \ = \ -(a_x\psi_+), \quad \sigma_3^x(a_x^*\psi_-) \ = \ +(a_x^*\psi_-) \ .$$

The operator $n_x = a_x^* a_x$ measures the number (zero or one) of particles at x and

$$n_\Lambda = \sum_{x \in \Lambda} a_x^* a_x$$

is the number operator for the subsystem Λ.

Now let Ω be a simultaneous eigenfunction of each $\sigma_3^x, x \in \Lambda$, with eigenvalue -1. It follows that $a_x\Omega = 0$ for all $x \in \Lambda$ and the vectors $|X\rangle$ defined by $|\varnothing\rangle = \Omega$ and

$$|X\rangle = \prod_{x \in X} a_x^* |\varnothing\rangle$$

form an orthonormal basis of $\mathfrak{H}_\Lambda$. Thus, a general vector $\Psi \in \mathfrak{H}_\Lambda$ has a decomposition

$$\Psi = \sum_{X \subseteq \Lambda} \Psi(X)|X\rangle$$

with $\Psi(X) \in \mathbb{C}$ and

$$\|\Psi\|^2 = \sum_{X \subseteq \Lambda} |\Psi(X)|^2 \ .$$

This construction is also possible with Λ replaced by L and in the case $L = \mathbb{Z}^\nu$ one obtains a discrete form of the Fock spaces used to describe continuous systems in Chapter 5, i.e., a vector $\Psi \in \mathfrak{H}_{\mathbb{Z}^\nu}$ is a function over the finite subsets $X \subset \mathbb{Z}^\nu$ such that

$$\|\Psi\|^2 = \sum_{X \subset \mathbb{Z}^\nu} |\Psi(X)|^2 < +\infty \ .$$

Note that the creation and annihilation operators satisfy mixed commutation, and anti-commutation, relations, e.g.,

$$[a_x, a_y^*] = 0, \quad \text{if } x \neq y$$

but

$$\{a_x, a_x^*\} = \mathbb{1} \ .$$

Nevertheless, Example 6.2.14 shows that this model is in a certain sense equivalent to a Fermi lattice gas.

In the lattice gas interpretation the phenomenon of magnetization corresponds to a form of liquid-gas phase separation. The regions with the spins up correspond to regions occupied by particles (the liquid phase) and the complementary region with spins down corresponds to zero particles (the gas phase).

The Heisenberg Hamiltonian has an interesting interpretation in the lattice gas language. For simplicity assume that $L = \mathbb{Z}$ and that the interaction is only between nearest neighbors. The total Hamiltonian can be divided into several parts. First there is the X–Y contribution

$$\begin{aligned} H_1 &= -\sum_{x=-n}^{n} J(\sigma_1^x \sigma_1^{x+1} + \sigma_2^x \sigma_2^{x+1})/2 \\ &= -\sum_{x=-n}^{n} J(a_x^* a_{x+1} + a_x a_{x+1}^*) \ . \end{aligned}$$

Therefore, on the one-particle space

$$(H_1\Psi)(\{y\}) = -J(\nabla^2\Psi)(\{y\}) - 2J\Psi(\{y\}) \ ,$$

where ∇^2 is the discrete form of the Laplacian

$$(\nabla^2\Psi)(\{y\}) = \Psi(\{y+1\}) - 2\Psi(\{y\}) + \Psi(\{y-1\}) \ .$$

Thus, H_1 is analogous to the Hamiltonian of the ideal gas and the X–Y model is interpretable as a noninteracting lattice gas. On the other hand the Ising contribution to the Hamiltonian,

$$H_2 = -\sum_{x=-n}^{n} J\sigma_3^x\sigma_3^{x+1}/2 \ ,$$

has a part H_2',

$$H_2' = -2J\sum_{x=-n}^{n} a_x^* a_{x+1}^* a_{x+1} a_x$$

which corresponds to the potential energy arising from a two-body interaction between neighboring particles,

$$(H_2'\,\Psi)(Y) = \left(-J\sum_{x,\,y\in Y}\delta_{x-y,1}\right)\Psi(Y) \ .$$

Thus, the Heisenberg model represents a lattice version of a particle system with two-body interactions.

Most of the early work on spin systems centered on spin-$\frac{1}{2}$ systems with interaction solely between neighboring atoms. The study of higher spin and long-range interactions intensified in the 1950s and 1960s. The general algebraic formalism that we use was introduced by Robinson [Rob 9] in 1967 but it is basically an extension to quantum systems of a framework given for classical systems by Gallavotti, Miracle-Sole, and Ruelle [Gal 2] [Rue 11]. The remark after Proposition 6.2.3 is due to Araki [Ara 13].

The first exact results on time evolution were derived by Streater [Str 2], for the Heisenberg model, and Robinson [Rob 7] for a general class of spin systems. In particular, this latter reference contained a version of Theorem 6.2.4 in which it was assumed that $\Phi(X)$ vanishes for $|X|$ sufficiently large. The extension to the case $\|\Phi\|_\lambda < +\infty$ was subsequently pointed out by Ruelle (see [[Rue 1]]). These results were not stated explicitly in terms of unbounded derivations but, in fact, motivated the development of integration theory for derivations, and the consequent deduction of results such as Theorem 6.2.6. The first statement in this theorem was established by Kishimoto [Kis 1] and the second by Bratteli and Kishimoto [Bra 11].

If Φ is a classical interaction the various $\Phi(X)$, $\Phi(Y), \ldots$ commute and Theorem 6.2.4 can be easily extended to Φ satisfying

$$\|\Phi\|_0 = \sup_{x\in L}\sum_{X\ni x}\|\Phi(X)\| < +\infty$$

because of the estimate

$$\|\delta^n(A)\| = \left\|\sum_{X_1\cap\Lambda\neq\varnothing}\cdots\sum_{X_n\cap\Lambda\neq\varnothing}[\Phi(X_1),[\cdots[\Phi(X_n),A]]]\right\|$$

$$\leq 2^n|\Lambda|(\|\Phi\|_0)^n\|A\|$$

for $A \in \mathfrak{A}_\Lambda$. Bratteli and Kishimoto [Bra 11] have given a generalization to Φ which is "almost classical." If $\|\Phi\|_0 < +\infty$ and

$$\|[H_\Phi(\Lambda), H_\Phi(\Lambda')]\| < M$$

for all $\Lambda, \Lambda' \subset L$, then the first criterion of Proposition 6.2.3 can be verified and hence the dynamics is once again given by a strongly continuous one-parameter group τ^Φ.

Another class of interactions was considered by Matsui [Mat 4] [Mat 5] in 1993. We first discuss these interactions in the spin-$\frac{1}{2}$ case, i.e., $N = 1$. To understand the following formalism note that each element in the local algebra $\mathfrak{A}_\Lambda$ can be uniquely expressed by a sum

$$\sum_{X,Y \subseteq \Lambda} C_{X,Y} \sigma_3(X) \sigma_1(Y)$$

where $C_{X,Y}$ are scalars, $\sigma_i(X) = \Pi_{x \in X} \sigma_i^x$ and $\sigma_i(\emptyset) = \mathbb{1}$. This is an easy consequence of the Pauli spin relations of Example 6.2.14A, or the representation of the matrices in Example 4.2.7. Matsui proves that if the formal Hamiltonian is

$$H = \sum_{x \in \mathbb{Z}^\nu} \tau_x(h)$$

where

$$h = \sum_{X,Y} C_{X,Y}\, \sigma_3(X) \sigma_1(Y)$$

and

$$\sum_{X,Y} |C_{X,Y}|\, |X \cup Y|^2 < \infty$$

then a resolvent estimate in terms of 'oscillation norms' shows that the closure of the corresponding derivation on $\bigcup_\Lambda \mathfrak{A}_\Lambda$ is a generator. The correspondence with our interaction Φ is given by

$$\Phi(X) = \sum_{x,A,B} C_{A,B} \tau_x(\sigma_3(A)\sigma_1(B))$$

where the sum is over all $x \in \mathbb{Z}^\nu$ and $A, B \subset \mathbb{Z}^\nu$ such that $(A + x) \cup (B + x) = X$. Thus one derives the estimate

$$\sum_{X \ni 0} \|\Phi(X)\|\, |X| = \sum_{A,B} |C_{A,B}|\, |A \cup B|^2 \ .$$

For general N one can expand the $(N+1) \times (N+1)$-matrices in powers $U^m V^n, m, n = 0, 1, \ldots, N$ where U and V are the matrices

$$U = \begin{pmatrix} 1 & 0 & \ldots & 0 & 0 \\ 0 & \omega & \ldots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \ldots & \omega^{N-1} & 0 \\ 0 & 0 & \ldots & 0 & \omega^N \end{pmatrix}, \quad V = \begin{pmatrix} 0 & 1 & \ldots & 0 & 0 \\ 0 & 0 & \ldots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \ldots & 0 & 1 \\ 1 & 0 & \ldots & 0 & 0 \end{pmatrix}$$

and $\omega = \exp\{2\pi i/(N+1)\}$ to obtain similar results. Alternatively one can expand h in terms of positive elements $\Psi(X) \in \mathfrak{A}_X$ as $h = \sum_X \Psi(X)$ and then deduce that the closure of the associated derivation on the spin algebra is a generator if

$$\sum_X \|\Psi(X)\| \, |X|^2 < \infty \ .$$

The connection to our formalism is now

$$\Phi(X) = \sum_{x \in \mathbb{Z}^\nu} \tau_x(\Psi(X - x))$$

(see [Mat 6], Theorem 2.9).

The commutator estimates of Proposition 6.2.9 and Corollary 6.2.10 are due to Lieb and Robinson [Lie 1]. Their application to the construction of the dynamics τ^Φ, Theorem 6.2.11, was subsequently given by Robinson [Rob 11].

Despite the early development of the Ising model and the Heisenberg model the pure X–Y model was not studied until 1950 when Nambu [Nam 1] gave a partial analysis. In 1961, Lieb, Schulz, and Mattis [Lie 2] established a preliminary form of the equivalence between the one-dimensional model and the Fermi lattice gas given in Example 6.2.14 and used this to calculate various facets of the model. The transformations used to establish this equivalence date back to the work of Jordan and Wigner [Jor 1] in 1928. The operator T as well as the other results on the dynamics of the X–Y model in Examples 6.2.14A and 6.2.14B are due to Araki in 1984 [Ara 31]. Earlier work in this direction was done by Emch and Radin [Emc 2] and Abraham, Barouch, Gallavotti and Martin-Löf [Abra 1] [Abra 2] in 1971–72 and by Araki and Barouch in 1983 [Ara 32]. The return to equilibrium of the locally perturbed X–Y model is discussed by Hume and Robinson [Hum 1].

Throughout Section 6.2.1 we analyzed the time development of quantum spin systems as a norm limit of the local dynamics. There exist some long-range interactions for which this norm limit cannot be established, but where nevertheless one can prove that the appropriate limits exist in certain representations and define automorphism groups of the weak closure of the spin algebra in these representations. Some such systems were studied by Pulvirenti and Tirozzi in 1973 [Pul 1]. They considered a spin-$\frac{1}{2}$ system on $\mathbb{Z}^\nu$. In terms of the spin raising and lowering operators a_x^* and a_x introduced earlier in the Notes and Remarks, the finite-volume Hamiltonians are defined by

$$H(\Lambda) = \sum_{\substack{x, y \in \Lambda \\ x \neq y}} K(x - y) a_x^* a_y + \sum_{X \subseteq \Lambda} J(X) a^*(X) a(X) \ ,$$

where

$$a^*(X) = \prod_{x \in X} a_x^*, \quad a(X) = \prod_{x \in X} a_x \ .$$

Here K is a real function on $\mathbb{Z}^\nu$ satisfying

$$\sum_{x \neq 0} |K(x)| < +\infty$$

and J is a translationally invariant real function on the finite subsets of $\mathbb{Z}^\nu$ satisfying

$$\sum_{X \ni 0} |J(X)| < +\infty \ .$$

One can now show that the local Gibbs states ω_Λ,

$$\omega_\Lambda(A) = \frac{\mathrm{Tr}_{\mathfrak{H}_\Lambda}(e^{-\beta H(\Lambda)}A)}{\mathrm{Tr}_{\mathfrak{H}_\Lambda}(e^{-\beta H(\Lambda)})}$$

converge in the weak* topology to a state ω if the inverse temperature β and the activity $\exp\{-\beta J(0)\}$ are small enough. In the region of convergence one can derive estimates of the form

$$|\omega([H(\Lambda), A]^{(n)*}[H(\Lambda), A]^{(m)})| \leq K_A(n+1)!(m+1)!c_A^{n+m}$$

for $A \in \bigcup_\Lambda \mathfrak{A}_\Lambda$, where K_A and c_A are constants independent of Λ and the $[H(\Lambda), A]^{(n)}$ are defined inductively by $[H(\Lambda), A]^{(0)} = A$, $[H(\Lambda), A]^{(n)} = [H(\Lambda), [H(\Lambda), A]^{(n-1)}]$ for $n = 1, 2, \ldots$. One next shows that $A \in D(\delta^n)$ for all n, where δ is the closure of the derivation defined on $\bigcup_\Lambda \mathfrak{A}_\Lambda$ in the usual way from the interaction Φ. If H_ω is the symmetric operator defined on $\pi_\omega(D(\delta))\Omega_\omega$ by

$$iH_\omega \pi_\omega(B)\Omega_\omega = \pi_\omega(\delta(B))\Omega_\omega \ ,$$

it follows from the estimates above that $\pi_\omega(\bigcup_\Lambda \mathfrak{A}_\Lambda)\Omega_\omega$ consists of analytic elements for H_ω. Hence, the closure $\overline{H}_\omega$ of H_ω is selfadjoint, and

$$\tau_t(\pi_\omega(\mathfrak{A})'') = e^{it\overline{H}_\omega}\pi_\omega(\mathfrak{A})''e^{-it\overline{H}_\omega} = \pi_\omega(\mathfrak{A})''$$

by Proposition 3.2.58. In this case $t \to \tau_{-\beta t}$ is just the modular automorphism group associated with the pair $(\pi_\omega(\mathfrak{A})'', \Omega_\omega)$, and it follows from the Remark after Corollary 6.3.30 that

$$\lim_{\Lambda \to \infty} \omega_\Lambda(\tau_{t_1}^\Lambda(A_1) \cdots \tau_{t_n}^\Lambda(A_n)) = \omega(\tau_{t_1}(A_1) \cdots \tau_{t_n}(A_n))$$

for all $A_1, \ldots, A_n \in \mathfrak{A}, t_1, \ldots, t_n \in \mathbb{R}$. In the last expression we identified ω with its normal extension to $\pi_\omega(\mathfrak{A})''$ and $\mathfrak{A}$ with $\pi_\omega(\mathfrak{A})$.

Section 6.2.2

The Gibbs ansatz for the equilibrium state of a closed finite system was given by Willard Gibbs in the late nineteenth century. Nevertheless, it is only since the mid-1960s that criteria such as the Gibbs condition of Definition 6.2.16 have been proposed as characteristic for the equilibrium of open systems, i.e., the finite subsystems of an infinite system. The first form of this definition was proposed independently by Dobrushin [Dob 1], [Dob 2] and by Lanford and

Ruelle [Lan 2]. These authors considered classical spin-$\frac{1}{2}$ systems. The general form of Definition 6.2.16 was introduced by Araki and Ion [Ara 24] who also proved a version of Theorem 6.2.18.

The Dobrushin–Lanford–Ruelle version of the Gibbs condition is usually phrased in a measure theoretic manner which is quite different in appearance to the general definition. To illustrate this let us adopt the lattice gas notation given in the notes to Section 6.2.1. The classical C^*-algebra $\mathfrak{C}_\Lambda$ of observables associated with $\Lambda \subset L$ is taken to be the algebra generated by the identity and the number operators $n_x = a_x^* a_x$. This algebra is *-isomorphic to the algebra of complex continuous functions over the finite subsets $X \subset \Lambda$, e.g., the operator

$$f = \sum_{Y \subset \Lambda} f(Y) \left(\prod_{y \in Y} n_y \right) \left(\prod_{z \in \Lambda \setminus Y} (1 - n_z) \right)$$

is a multiplication operator, $f|X\rangle = f(X)|X\rangle$ for all $X \subset \Lambda$. A classical interaction Φ is then an operator of this type,

$$\Phi|X\rangle = \Phi(X)|X\rangle \ ,$$

where the real function $\Phi(X)$ represents the energy of the particles at the points $x \in X$.

Now the Gibbs state ω_Λ is determined by its values on the monomials $n(X) = \prod_{x \in X} n_x$ and

$$\omega_\Lambda(n(X)) = \sum_{\substack{Y \subset \Lambda \\ Y \cap X = \varnothing}} \mu_\Lambda(X \cup Y) \ ,$$

where

$$\mu_\Lambda(X) = \frac{e^{-\Sigma_{S \subset X} \Phi(S)}}{\sum_{T \subset \Lambda} e^{-\Sigma_{S \subset T} \Phi(S)}} \ .$$

Note that μ_Λ is a probability measure on the C^*-algebra $\mathfrak{C}_\Lambda$ because this algebra is *-isomorphic to the complex continuous functions over the finite subsets $X \subset \Lambda$, e.g.,

$$\mu_\Lambda(f) = \sum_{X \subset \Lambda} f(X) \mu_\Lambda(X) \ .$$

Moreover ω_Λ is determined by μ_Λ, and vice versa. This is just an explicit version of the representation theory of abelian C^*-algebras given in Chapter 2. But the μ_Λ satisfy the equations

$$\mu_\Lambda(X \cup Y) = e^{-H(X) - W(X|Y)} \mu_\Lambda(Y) \ ,$$

where

$$H(X) = \sum_{S \subset X} \Phi(S)$$

is the energy of the particles at the points of X and

$$W(X|Y) = \sum_{\substack{S \cap X \neq \emptyset,\ S \cap Y \neq \emptyset \\ S \subset X \cup Y}} \Phi(S)$$

is the energy of interaction of these particles with particles at the points of Y. Thus, if one formally takes the limit $\Lambda \to \infty$, then μ_Λ is replaced by a probability measure μ on the C^*-algebra $\mathfrak{C}$ generated by the $\bigcup_{\Lambda \subset L} \mathfrak{C}_\Lambda$ which satisfies the Dobrushin–Lanford–Ruelle equations

$$\mu(X \cup Y) = e^{-H(X)-W(X|Y)}\mu(Y) \ .$$

Each such measure μ determines a state ω over $\mathfrak{C}$ by

$$\omega(A) = \sum_{X \subset L} A(X)\mu(X) \ .$$

It is readily checked that ω satisfies the Gibbs condition in the sense of Definition 6.2.16 and the Dobrushin–Lanford–Ruelle integral equations are just a reformulation of the Gibbs condition.

Both Dobrushin and Lanford–Ruelle proved special versions of Theorem 6.2.18 in the classical spin-$\frac{1}{2}$ case. The first quantum version was given by Araki and Ion [Ara 24] for one-dimensional systems and multidimensional systems at high temperature. The general version was subsequently established by Araki [Ara 25].

Sections 6.2.3 and 6.2.4

The notions of entropy and conditional entropy have had fruitful applications in a variety of subjects, coding and information theory, ergodic theory, statistical mechanics, etc. This universality is understandable because these quantities determine the asymptotic behavior of the multinomial coefficients and the multinomial distribution. Thus, they play a fundamental role in any application of basic statistics.

Let ${}^nC_{n_1,\ldots,n_m}$ denote the multinomial coefficients

$${}^nC_{n_1,\ldots,n_m} = \frac{n!}{n_1! \cdots n_m!} \ ,$$

where $n_1 + n_2 + \cdots + n_m = n$. These coefficients express the number of ways one can divide n objects into m subsets of $n_1, n_2, \ldots, n_m$ objects, respectively. If n is large it is of interest to examine the number of partitions into m subsets with proportions $p_1 = n_1/n, \ldots, p_m = n_m/n$. Thus, one examines

$$P_n(p) = \frac{n!}{(p_1 n)! \cdots (p_m n)!}$$

with $p_1 + p_2 + \cdots + p_m = 1$. But these coefficients are easily estimated by use of the Stirling-type bounds

$$\sqrt{2\pi n}\ n^n e^{-n} e^{1/(12n+1)} \leq n! \leq \sqrt{2\pi n}\ n^n e^{-n} e^{1/12n}$$

given by Robbins [Robb 1]. If R_n and S are defined by

$$R_n(p) = (2\pi n)^{-(m-1)/2}\left(\prod_{i=1}^{m} p_i\right)^{-1/2}$$

$$S(p) = -\sum_{i=1}^{m} p_i \log p_i \ ,$$

one finds

$$\left|\frac{R_n(p)e^{nS(p)}}{P_n(p)} - 1\right| = O\left(\frac{1}{n}\right), \quad n \to \infty \ .$$

Alternatively

$$|n^{-1} \log P_n(p) - S(p)| = O(n^{-1}\log n)$$

as $n \to \infty$. Thus, the predominant asymptotic feature of the P_n is an exponential increase, $\exp\{nS\}$, where S is the entropy associated with the partition $p_1, \ldots, p_m$.

Next consider n independent repetitions of a trial with m possible outcomes and corresponding probabilities $q_1, q_2, \ldots, q_m$. The probability that the ith event occurs with frequency $p_i, i = 1, 2, \ldots, m$ is given by the multinomial distribution

$$P_n(p|q) = {}^nC_{p_1 n, \ldots, p_m n} q_1^{p_1 n} \cdots q_m^{p_m n} \ .$$

Therefore, the previous estimates allow one to deduce that

$$\left|\frac{R_n(p)e^{nS(p|q)}}{P_n(p|q)} - 1\right| = O\left(\frac{1}{n}\right)$$

as $n \to \infty$, where

$$S(p|q) = -\sum_{i=1}^{m}(p_i \log p_i - p_i \log q_i)$$

is the conditional entropy of the frequencies $\{p_i\}$ with respect to the probabilities $\{q_i\}$. But $S(p\,|\,q) \leq 0$ with equality if, and only if, $p_i = q_i$ for $i = 1, 2, \ldots, m$. Thus, as $n \to \infty$ each of the individual probabilities $p_n(p\,|\,q)$ tends to zero as $n^{-(m-1)/2}$. But if the p_i and q_i are not equal, then there is an exponential decrease $\exp\{nS(p\,|\,q)\}$ governed by the conditional entropy $S(p\,|\,q)$. Therefore, the only results which effectively occur are those for which the frequencies closely approximate the probabilities. Note that this substantially reduces the effective number of results below the theoretical maximum of $m^n = \exp\{n \log m\}$. The effective number is measured by the sum of the $P_n(p)$ in a neighborhood of $p_i = q_i$. Thus, one obtains from the above estimates that

$$\frac{1}{n} \log \text{(effective number)} = S(q) + O\left(\frac{1}{n}\log \frac{1}{n}\right) \ .$$

But if one compares this with the identity

$$\frac{1}{n}\log(\text{total number}) = \log m \ ,$$

one sees that the entropy $S(q)$ replaces $\log m$ as a measure of the number of effective outcomes of each trial.

These estimates explain to a certain extent the quantitative origins of the entropy. To understand its qualitative features it is useful to examine the notion of uncertainty, or unpredictability. Each trial has a certain quality of unpredictability which varies with the probabilities. For example, coin tossing with two equally probable outcomes is much more predictable, or certain, than spinning a roulette wheel for which there are 36, or 37, possible results. This indicates that if one restricts one's attention to trials with equal probabilities $q_1 = \cdots = q_m = m^{-1}$, then the uncertainty F is a positive increasing function of m, i.e.,

$$0 \leq F(m_1) \leq F(m_2)$$

for $m_1 \leq m_2$. But each trial with m_1, m_2 equally probable outcomes can be considered as the composition of two independent trials with m_1 and m_2 outcomes and it is natural to assume that the total uncertainty is the sum of the uncertainties of the subtrials, i.e.,

$$F(m_1 m_2) = F(m_1) + F(m_2) \ .$$

But the only functions which satisfy these two simple properties for all positive integers m_1 and m_2 are given by

$$F(m) = c \log m \ ,$$

where $c \geq 0$. Thus, up to a factor which determines the choice of units, the uncertainty appears to be measured by the logarithm of the number of possible outcomes. This is clearly not the case for trials with unequal probabilities. For example, if one outcome has probability close to one, and all other probabilities are small, then there is almost no uncertainty. The result is predictable because there is only one effective outcome. But in the preceding paragraphs we argued that the entropy measures the effective number of outcomes. Thus, combination of these arguments justifies, to a certain extent, the interpretation of the entropy as a measure of uncertainty. This interpretation appears to date back to Boltzmann's observation, in 1894, that the entropy is related to "missing information" inasmuch as it is related to the number of alternatives which remain possible to a physical system after all the observable information concerning it has been recorded. Thus, any principle of maximum entropy is an expression of maximum uncertainty, or minimal information, or maximal disorder.

As the entropy is of such basic statistical significance it occurs in a wide variety of contexts and it is impossible to describe all such applications in these notes. It is the fundamental concept in information theory and has been of great importance in ergodic theory where a version of mean entropy serves as an isomorphy invariant, the Kolmogorov–Sinai invariant, for dynamical

systems. Details of these and other applications can be found in the books by Billingsley [[Bil 1]], Jacobs [[Jac 1]], Ornstein [[Orn 1]], Shannon and Weaver [[Sha 1]], and Yaglom and Yaglom [[Yag 1]].

The quantum-mechanical, or noncommutative, definition of entropy $-\mathrm{Tr}(\rho \log \rho)$ was introduced by von Neumann [[Neu 2]] in the early 1930s but there appeared to be no systematic investigation of its basic properties, e.g., subadditivity, concavity, quasi-convexity, until the mid-1960s. Nevertheless, most of these elementary properties appear scattered through the literature. The least known appears to be the quasi-convexity but a proof of this was given in 1947 by Jost [Jos 1]. A survey of these early developments has been given by Huber [Hub 1] who attributes the basic inequality of Lemma 6.2.21 to Delbrück and Moliére in 1936.

Strong subadditivity, Proposition 6.2.24, appears to be the only significant property of $\Lambda \mapsto S_\Lambda(\omega)$ which was not established prior to the 1960s. In 1967 Robinson and Ruelle [Rob 10] pointed out that this property could be derived for classical spin systems from the Kolmogorov–Sinai theory of the entropy of dynamical systems. They also conjectured that it was valid in general. Despite attempts by many authors this conjecture remained unverified for 6 years until Lieb and Ruskai [Lie 3] gave a proof based upon a result of Lieb [Lie 4]. This result states that the map

$$A \mapsto -\mathrm{Tr}(\exp\{L + A\})$$

from the positive $n \times n$ matrices to the reals is convex for each selfadjoint L. Prior to this partial results had been obtained by Baumann and Jost [Bau 1] and Araki and Lieb [Ara 26].

Another proof of strong subadditivity which uses somewhat more sophisticated notions is based on the monotonicity of the relative entropy under Schwarz mappings. This latter property was established by Uhlmann [Uhl 1]. A full exposition of this second proof is given in the book of Ohya and Petz [[Ohy 1]] which also contains an exhaustive discussion of most features of the quantum entropy and related concepts.

The systematic analysis of the entropy and mean entropy as functionals over the states of C^*-algebras began with the papers of Robinson and Ruelle [Rob 10] and Lanford and Robinson [Lan 5]. The first of these dealt with the abelian algebras of classical statistical mechanics and the second extended the formalism to quantum statistical mechanics. The main emphasis of both papers was on invariant states. Their aim was to prepare the ground for a discussion of the free energy, invariant equilibrium states, and the maximum entropy principle of Section 6.2.4. The thermodynamic free energy F was constructed by Gallavotti and Miracle-Sole [Gal 2] for classical spin systems and these authors also described the connection between invariant limits of local Gibbs states and tangent planes to the graph of F. In particular, they proved a version of Theorem 6.2.40 and versions of Observations 1 and 2 at the end of Section 6.2.4. Ruelle [Rue 11] then used the entropy results and the results of Gallavotti and Miracle-Sole to prove property (1) of Theorem 6.2.40. Subsequently,

Robinson [Rob 9] extended the whole discussion to quantum spin systems and proved Theorem 6.2.40 in the form stated.

The identity of the mean entropy and the mean conditional entropy for Gibbs states, mentioned after Proposition 6.2.38, was established by van Enter [Ent 1]. The fact that they do not coincide on the invariant states follows from [Tem 1] (see, also [[Tem 1]], Chapter 8, Sections 5, 6 and 7).

The next step in this development occurred when Robinson [Rob 7] constructed the dynamics of a large class of quantum spin systems as a group of *-automorphisms τ^Φ and proved that if $S - \beta H_\Phi$ is maximized by a unique state, then this state satisfies the (τ^Φ, β)–KMS condition. The extension of this result to all Φ for which τ^Φ exists was subsequently derived by Lanford and Robinson [Lan 6] using results of convex analysis. In particular these authors proved Lemma 6.2.43, the implication (3) $\Rightarrow$ (1) in Theorem 6.2.42, Observations 1 and 2 at the end of Section 6.2.4, and a version of Observation 3 in which the weak* topology replaces the uniform topology. The weak*-version of Observation 3 was derived by proving that tangent functionals to a convex continuous functional F are weak* dense in the F-bounded functionals. Several years later in 1975 Israel [Isr 1] pointed out that the work of Bishop and Phelps [Bis 2] on convex sets implied that this result was true in the uniform topology. Israel also proved Observation 4 and various other interesting results concerning uniqueness and nonuniqueness of invariant equilibrium states. Theorem 6.2.42 was finally completed by Araki [Ara 25] in 1974 with a proof that (2) $\Rightarrow$ (3) and hence, by Corollary 6.2.19, that (1) $\Rightarrow$ (3), i.e., the converse of the Lanford–Robinson result.

An alternative discussion of lattice gases, and in particular the convexity arguments used in the last part of Section 6.2.4, is contained in the book by Israel [[Isr 1]].

Despite the order of the text, analysis of general, i.e., noninvariant, equilibrium states and principles of maximum entropy did not make much headway until the 1970s. The key steps in this analysis were made by Araki and Sewell, both independently and in collaboration. Araki [Ara 27], [Ara 28], [Ara 30] introduced the relative entropy, Definition 6.2.29, and derived most of its basic properties. In particular, Propositions 6.2.32 and 6.2.33 and Corollary 6.2.34 are given in these papers. (Our definition of the conditional entropy differs slightly from that of Araki. One has $S(\varphi|\psi) = -S_{\text{Araki}}(\psi|\varphi)$.)

An independent proof of the monotonicity property of Proposition 6.2.33 was subsequently given by Pusz and Woronowicz [Pus 2] by arguments based on their theory of the functional calculus of sesquilinear forms [Pus 3].

Kosaki [Kos 1] derived an interesting variational expression for the relative entropy, based on some of the ideas of [Pus 2], which can be used to establish the monotonicity together with other basic properties. This line of reasoning is described in [[Ohy 1]], Chapter 5. The review of Wehrl [Weh 1] relates various properties of entropy and relative entropy.

There remain many aspects of non-commutative entropy which we have not described, e.g., the attempts to extend the Kolmogorov-Sinai invariant from

measure theoretic dynamical systems to von Neumann algebras. There are at least three different definitions of dynamical entropy in the non-commutative setting, that of Connes, Narnhofer, Størmer and Thirring [Con 5], that of Alicki and Fannes [Ali 1] and that of Voiculescu [Voi 1] [Voi 2] [Voi 3]. The book by Ohya and Petz [[Ohy 1]] contains more information on these topics and a good bibliography.

Sewell [Sew 2], [Sew 3], introduced the principle of local thermodynamic stability for classical systems, i.e., the principle of maximum conditional entropy described in Proposition 6.2.35 and Theorem 6.2.36, and proved that it was equivalent to the Gibbs condition. Subsequently, Araki and Sewell [Ara 22] extended the notion of local thermodynamic stability to quantum lattice systems, proved that KMS states satisfy this principle, and also proved that the converse is true for invariant states. Finally Sewell [Sew 1] derived the converse without invariance. The key to his proof is the autocorrelation lower bound discussed in Chapter 5.

Attempts to analyze homogeneous systems without invariance, e.g., impurity models, spin glasses, aperiodic systems, from the present perspective can be found in [Rue 9] [Roo 1] [Ent 2] [Gee 1] and references cited therein.

Section 6.2.5

Both results of this section have a relatively long history.

Integral equations of the same basic type that we use for uniqueness at high temperature were first derived by Mayer and by Kirkwood and Salzburg for correlation functions of classical statistical mechanics. They are often referred to as Kirkwood–Salzburg equations. These equations, variants due to Mayer and Montroll, and various related developments of the 1945–1955 period are discussed in the book by Hill [[Hil 1]].

Originally the integral equations were used to study finite-volume equilibrium states. The first application of these techniques to infinite systems occurred in a little known paper of Bogoliubov and Khatset [Bog 3] published in 1949. Basically these authors established the uniqueness of the thermodynamic limit for classical continuous systems at high temperature and low density in the Gibbs canonical ensemble. Much later, in 1963, and quite independently, Ruelle [Rue 6] derived similar results in the grand canonical ensemble. Moreover, Ruelle [Rue 7] developed a technique which leads to spatial cluster properties of the high-temperature states. This is an aspect that we have practically omitted from our general discussion. We mentioned that if $L = \mathbb{Z}^\nu$, uniqueness of the KMS state ω^Φ implies extremality and hence strong clustering of the form

$$\lim_{|x| \to \infty} \{\omega^\Phi(A\tau_x(B)) - \omega^\Phi(A)\omega^\Phi(\tau_x(B))\} = 0$$

for all $A, B \in \mathfrak{A}$. But Ruelle's methods allow the deduction of more precise results, e.g., if $A, B \in \mathfrak{A}_{\{0\}}$ and Φ is a finite-range interaction then

$$|\omega^{\Phi}(A\tau_x(B)) - \omega^{\Phi}(A)\omega^{\Phi}(\tau_x(B))| < e^{-C_{\Phi}|x|}$$

for some C_{Φ}. (The details for quantum spin systems were given by Greenberg [Gre 2].) Ruelle's work was generalized and extended by various authors, Ginibre, Gallavotti and Miracle-Sole, Greenberg, etc. Most of these generalizations are discussed in Ruelle's book [[Rue 1]], the exception being Greenberg's work on quantum spin systems [Gre 1], [Gre 2] which occurred after publication of this book. The popularity of these methods led Bogoliubov and Khatset to extend and republish their work and it now exists in a more accessible English language version [Bog. 4].

In spin language the high-temperature-low-density regime corresponds to high temperature and weak external field. The extension of the uniqueness results to high temperatures and all external fields was given for classical spin systems by Dobrushin [Dob 3] and by Gallavotti, Miracle-Sole, and Robinson [Gal 3]. The latter authors subsequently extended this result to a class of quantum spin systems [Gal 4] using a method of Ginibre [Gin 1] but their work was quickly superseded by that of Greenberg [Gre 1].

The crucial fact that the Kirkwood–Salzburg type equations used by Greenberg could be derived from the KMS condition was first pointed out by Lanford [Lan 7]. Thus, Greenberg's results on uniqueness of the thermodynamic limit immediately translated into statements of uniqueness of KMS states at high temperature.

All these investigations of spin systems were restricted to the simplest case, spin-$\frac{1}{2}$, and the present extension to general spin, Theorem 6.2.46, uses a slightly different technique.

The first proof of uniqueness of equilibrium states for one-dimensional systems was contained in the thesis of Ising [Isi 1]. The simplest method to obtain this result is by a method of Kramers and Wannier [Kra 1] and Montroll [Mon 1]. The basis of this method is the observation that the partition function of a chain of n spins with nearest-neighbor interaction J and external field h,

$$Z_n(J,h) = \sum_{\sigma_1=\pm 1} \cdots \sum_{\sigma_n=\pm 1} \exp\left\{-\sum_{i=1}^{n-1} J\sigma_i\sigma_{i+1} - h\sum_{i=1}^{n}\sigma_i\right\}$$

can be written in the form

$$Z_n(J,h) = \sum_{i=\pm 1}\sum_{j=\pm 1} e^{-ih/2}(M^{n-1})_{ij}e^{-jh/2},$$

where M is the hermitian 2×2 matrix defined by

$$M = \begin{pmatrix} M_{++} & M_{+-} \\ M_{-+} & M_{--} \end{pmatrix} = \begin{pmatrix} e^{-J-h} & e^{J} \\ e^{J} & e^{-J+h} \end{pmatrix} .$$

Thus, Z_n is easily computed in terms of the eigenvalues and eigenfunctions of M, e.g.,

$$\lim_{n \to \infty} n^{-1} \log Z_n(J, h) = \lambda_{\max}(J, h) \ ,$$

where $\lambda_{\max}(J, h)$ is the largest eigenvalue of M. Similarly, one may compute the unique Gibbs state of the model by adroit use of M. The matrix M is called the transfer matrix.

Ruelle has extended this method to classical spin systems with long-range and multispin interactions [Rue 8]. This generalization uses a number of new techniques, e.g., the Perron–Frobenius theorem, and partially relies upon earlier ideas of van Hove [Hov 2]. Subsequently Araki [Ara 15] gave a non-commutative extension applicable to quantum spin systems with finite-range interactions and hence derived a special case of Theorem 6.2.47. The first proof of the general result was also by Araki [Ara29] and relied upon properties of the relative entropy. The proof we have indicated is due to Kishimoto [Kis 5].

It should be emphasized that uniqueness of the equilibrium state for one-dimensional systems is only valid for 'short-range' interactions. Dyson [Dys4] proved that the Ising model with a very long-range ferromagnetic interaction does exhibit a phase transition at low temperatures. Fröhlich and Spencer [Frö 9] subsequently improved Dyson's conclusion by showing that a ferromagnetic interaction $j(x) = 1/|x|^2$ suffices for a spontaneous magnetization at low temperatures.

Finally the transfer matrix method has been of great importance for the analysis of exactly soluble models, and in particular a version called the corner transfer matrix [[Bax 1]]. The method has also been used to prove the 'equivalence' of certain two-dimensional classical systems and appropriate one-dimensional quantum systems and thereby obtain useful information about the classical system. For example, Araki and Evans [Ara 35] analyze the Ising model by this method in the spirit of the current text.

Section 6.2.6

Much of the theoretical understanding of phase transitions has been based upon properties of the ferromagnetic Ising model in two dimensions.

In 1936 Peierls [Pei 1] proved the existence of a nonzero spontaneous magnetization m for the two-dimensional model, with nearest-neighbor coupling $j < 0$, at all sufficiently low temperatures. The proof of Theorem 6.2.48 is based upon Peierls' argument.

Five years later Kramers and Wannier [Kra 1] proved that if the two-dimensional model has a unique critical (inverse) temperature β_c, i.e., if there is a unique β_c such that $m = 0$ for $\beta < \beta_c$ and $m \neq 0$ for $\beta > \beta_c$, then β_c is determined by the equation

$$\sinh 2j\beta_c = 1 \ . \qquad (*)$$

This result was obtained by exploitation of a symmetry between high and low temperatures which allows one to relate high- and low-temperature expansions

of the partition function for the model. Relations of this type are now commonly called duality relations.

Kramers and Wannier also developed the transfer matrix method, described in the Notes and Remarks to the previous section, for the one- and two-dimensional Ising models and used it to calculate the partition function of the one-dimensional model. In 1943 Onsager [Ons 1] extended this method and calculated among other things, the partition function of a two-dimensional cylindrical array with vanishing external field. Onsager's results corroborated the earlier findings of Peierls and Kramers and Wannier. For example, the mean energy per atom of the infinite two-dimensional system is a continuous function of the temperature $T = \beta^{-1}$ and is differentiable except at the Kramers–Wannier critical value T_c. At this value the derivative diverges as $-\log|T - T_c|$.

Subsequently, in 1948, Onsager announced the value

$$m = [1 - \operatorname{cosech}^4 2\beta j]^{1/8}$$

for the spontaneous magnetization m below T_c but he never published a proof of this claim (see [Ons 2]). A proof was given by Yang [Yan 1] 4 years later.

In 1952 Lee and Yang [Lee Y1] devised an alternative method of partially analyzing the ferromagnetic Ising model, in an arbitrary number of dimensions. Their method consists of isolating the zeros of the partition function Z_Λ for the finite-dimensional system. (These zeros potentially lead to singularities of the free energy $F_\Lambda = |\Lambda|^{-1} \log Z_\Lambda$ in the thermodynamic limit and hence herald transition phenomena.) In particular, they discovered the remarkable fact that the zeros of Z_Λ, viewed as a function of the parameter $\exp\{\beta h\}$ where h is the external field, lie on the unit circle. They could conclude that the thermodynamic free energy is differentiable in h except at $h = 0$.

It appears that the success of the Onsager–Yang calculations for the two-dimensional Ising model diverted attention from the general analytic techniques of Peierls and Kramers and Wannier and these methods were not reanalyzed until the post-1964 period. In 1964 the Peierls argument was revived and reformulated by both Dobrushin [Dob 4] and Griffiths [Gri 1]. Griffiths claimed the original Peierls argument was incomplete but this was disputed by Peierls [Pei 2]. An early discussion of Peierls' argument was given by Wannier [[Wan 1]]. After the work of Dobrushin and Griffiths many extensions and generalizations of the Peierls method subsequently appeared. (For reviews up to 1972 see [Gri 2], [Gri3].) In particular Dobrushin [Dob 4] showed how the argument could be applied to anti-ferromagnetic systems, Theorem 6.2.49. Moreover, in 1968, Robinson [Rob 12] realized how the arguments for the classical Ising model could be extended by perturbation theory to the quantum-mechanical anisotropic model. The proof of the weak version of Theorem 6.2.48 is based on Robinson's original argument. Subsequently, Ginibre [Gin 2] reformulated various quantum models as perturbations of classical models by the path method sketched at the end of the proof of Theorem 6.2.48 and thereby improved and extended Robinson's conclusions. Kennedy [Ken 1]

finally optimized Ginibre's arguments for the anisotropic Heisenberg model and established the full statement of Theorem 6.2.48.

Hohenberg [Hoh 1] was the first to realize that Bogoliubov's inequality [Bog 2] could be used to rule out critical phenomena. In particular, he proved the absence of Bose–Einstein condensation for one- and two-dimensional continuous systems. Theorem 6.2.51, the lattice analogue of this result, was subsequently given by Mermin and Wagner [Mer 1] but the absence of a spontaneous magnetization for the isotropic Heisenberg model in two dimensions was already folklore. A heuristic, and apochryphal, argument which supports this result and also indicates the importance of the isotropy, in at least two directions, is discussed by Griffiths in [Gri3].

The origin of the Bogoliubov inequality given in Lemma 6.2.50 has been described in the Notes and Remarks to Section 5.3.

The absence of continuous symmetry breaking described in Theorem 6.2.50 was established by Fröhlich and Pfister in 1981 [Frö 6] [Frö 7] although their method was based on uniform estimates on the relative entropy of suitable local perturbations of the KMS states, in the spirit of the proof of Theorem 6.2.47. But to obtain these estimates they essentially had to estimate $\|\delta_\Phi(U_L)\|$ as in the proof we have given. Our proof is based on the 1984 result of Fannes, Vanheuverzwijn and Verbeure [Fan 4]. It should be emphasized that the absence of spontaneous breaking of symmetries in one-, and two-, dimensional models with short range interactions does not exclude the existence of phase transitions in such systems. Examples of such transitions in the classical case have been given by Dyson [Dys 3] and by Shlosman [Shl 1]. Note also that the estimate on the range on $\|\Phi(\{x, y\})\|$ in Theorem 6.2.50 is the best possible in the sense that there exist two-dimensional systems with a continuous symmetry group G and two-body interactions Φ with $\|\Phi(\{x, y\})\| \sim C|x - y|^{-4+\varepsilon}$, where $\varepsilon > 0$ is arbitrarily small, for which spontaneous symmetry breaking can occur [Kun 1] [Frö 8] [Bon 1] [Ito, K.1].

Theorem 5.3.33A can also be used to establish the absence of discrete symmetry breaking for some one-dimensional models with interaction of so long range that Theorem 6.2.47 does not apply [Fan 4].

The method of infrared bounds was introduced by Fröhlich, Simon, and Spencer [Frö 1] who successfully applied it to a number of classical models, including the multidimensional Ising model. The crucial bounds are obtained by a method of Gaussian domination previously devised by Glimm, Jaffe, and Spencer [Gli 8] to handle phase transitions in constructive field theory. If h is a real functional over $\mathbb{Z}^\nu$, $(\partial_y h)(x) = h(x + y) - h(x)$, and

$$\sigma_3(h) = \sum_x \sigma_3^x h(x) \ ,$$

then the Gaussian domination bounds for the Ising model are

$$\omega_\Lambda\left(\exp\left(\sigma_3\left(\sum_{y;\,\mathrm{n.n.}} \partial_y h\right)\right)\right) \leq \exp\left\{(2\beta j)^{-1} \sum_x |h(x)|^2\right\}$$

where ω_Λ is the local Gibbs state and the y sum is over nearest neighbors. The derivation of these bounds uses the Kramers–Wannier transfer matrix method. It follows from them that

$$\omega_\Lambda(\sigma(h)\sigma(-\Delta h)) \leq (\beta j)^{-1} \sum_x |h(x)|^2 ,$$

where

$$-\Delta h(x) = 2\nu h(x) - \sum_{y;\,\mathrm{n.n.}} (h(x+y) + h(x-y))$$

and this can be used to bound $\omega_\Lambda(\sigma_3^x \sigma_3^y)$. In particular, one finds that the Ising model displays a nonzero spontaneous magnetization whenever

$$2(2\beta j) \geq (2\pi)^{-\nu} \int_{|k_i| \leq \pi} d^\nu k \left(\sum_{i=1}^{\nu} (1 - \cos k_i) \right)^{-1} .$$

This gives a bound on the critical temperature which is within 10% of the correct value for the two-dimensional model.

Applications of the infrared bound technique to quantum spin systems have been given by Dyson, Lieb, and Simon [Dys 2], and Fröhlich and Lieb [Frö 2]. These developments have been reviewed by Lieb [Lieb 5]. In particular, these authors derive the results on the X–Y model mentioned near the end of the section and similar results for the anti-ferromagnetic Heisenberg model.

An interesting connection between the isotropic Heisenberg model and resistance in electrical networks was pointed out by Powers in 1976 [Pow 6] [Pow 7] [Pow 8]. He established a connection between the existence of long range order and the resistance properties of the graph of an associated electrical network.

The multiplicity properties of equilibrium states of the $\mathbb{Z}^2$-invariant two-dimensional ferromagnetic Ising model follow from the work of Ruelle, Messager and Miracle-Sole, Aizenman and Higuchi [Aiz 2] [Hig 1]. Ruelle [Rue 9] proved uniqueness for nonzero external field, or for small β, and Messager and Miracle-Sole proved that there are only two $\mathbb{Z}^2$-invariant extremal (τ, β)-KMS states in the regime for which the spontaneous magnetization is nonzero. In fact, Ruelle proved there is a unique state satisfying the Dobrushin–Lanford–Ruelle equations described in the Notes and Remarks to Section 6.2.2. But these equations are equivalent to the Gibbs condition for classical interactions and hence one deduces uniqueness for the KMS states. Messager and Miracle-Sole [Mes 1] proved that the tangent functionals to the free energy are uniquely determined on the classical interactions defined by even polynomials of the σ_3^x, e.g., on interactions Φ of the form

$$\Phi(\{x_1, \ldots, x_{2n}\}) = \sigma_3^{x_1} \cdots \sigma_3^{x_{2n}}, \quad \text{and} \quad \Phi(\{x_1, \ldots, x_{2n+1}\}) = 0 .$$

It follows from the results of Section 6.2.3 that all the $\mathbb{Z}^2$-invariant (τ, β)-KMS states coincide on the classical subalgebra generated by even polynomials of the σ_3^x. The desired result follows from a simple argument which

uses the fact that the $\mathbb{Z}^2$-invariant (τ, β)-KMS states form a simplex. An alternative derivation of this result has been given by Lebowitz [Leb 1]. Aizenman [Aiz 2] and Higuchi [Hig 1] established independently of each other that all (τ, β)-KMS states of the $\mathbb{Z}^2$-invariant, two-dimensional Ising ferromagnet are $\mathbb{Z}^2$-invariant.

Messager and Miracle-Sole's results exploit the duality techniques introduced by Kramers and Wannier. At very low temperatures more detailed information has been obtained on the phase structure of general classical models by combining duality arguments and the Lee–Yang method of zeros. A comprehensive review of these developments is contained in the monograph of Gruber, Hintermann, and Merlini [[Gru 1]].

There is one important general technique in the theory of phase transitions for classical ferromagnets which we have not touched upon in the text. This is the method of correlation inequalities. This method originated with Griffiths observation [Gri 4] that a ferromagnetic spin system with a positive external field should have a positive magnetization in equilibrium and this magnetization should increase if the interparticle coupling, or the external field, is increased. Quantitatively these observations are expressed by the inequalities

$$\omega_\Lambda(\sigma_3^x) \geq 0 \ ,$$

$$\omega_\Lambda(\sigma_3^x \sigma_3^y) - \omega_\Lambda(\sigma_3^x)\omega_\Lambda(\sigma_3^y) \geq 0 \ ,$$

for the local Gibbs state ω_Λ. Griffiths' results were quickly generalized by Kelly and Sherman [Kell 1] who established the foregoing inequalities remain valid even if σ_3^x, σ_3^y are replaced by products

$$\sigma_X = \prod_{x \in X} \sigma_3^x, \qquad \sigma_Y = \prod_{y \in Y} \sigma_3^y \ .$$

Ginibre has given an easy proof of these basic inequalities [Gin 3]. Subsequently many authors derived extensions, or generalizations, e.g., Fortuin, Ginibre and Kasteleyn [For 1], Lebowitz [Leb 2], [Leb 3], etc. These inequalities have had numerous applications, e.g., to prove the existence of the thermodynamic limits of Gibbs states [Gri 4], to establish uniqueness of equilibrium states [Rue 8], to deduce the existence of phase transitions in one-dimensional systems with long-range interaction [Dys 3], to obtain bounds on critical temperatures [Gri 5], to establish rigorous inequalities on parameters determining critical behavior [Buck 1], and to bound high-order correlation functions by low-order correlation functions [Leb 3]. As an explicit example of this last type of application we remark that Lebowitz has proved that the Gibbs state ω_Λ of an Ising ferromagnet satisfies

$$\omega_\Lambda(n_x n_y) - \omega_\Lambda(n_x)\omega_\Lambda(n_y) \leq \sum_{x \in X} \sum_{y \in Y} \omega_\Lambda(n_x n_y) - \omega_\Lambda(n_x)\omega_\Lambda(n_y) \ ,$$

where n_x is the number operator in the lattice gas interpretation, i.e., $n_x = a_x^* a_x = (\sigma_3^x + \mathbb{1})/2$ and

$$n_X = \prod_{x \in X} n_x \ .$$

Unfortunately, the Griffiths type of correlation inequality has only been derived for classical models and little information is known for genuine quantum systems (see Ginibre's review [Gin 4]).

There are a variety of other general methods which have been used to elucidate the behavior of models of quantum statistical mechanics, e.g., mean field theory and quantum fluctuation theory. The thermostatic part of mean field theory is described in [Rag 1] and the dynamical part in [Duf 1]. The theory of normal fluctuations can be found in [God 1] [God 2] and the theory of abnormal or critical fluctuations in [Bri 1].

Section 6.2.7

This section is based upon the paper of Bratteli, Kishimoto, and Robinson [Bra 15]. But the implication (2) $\Rightarrow$ (1) of Theorem 6.2.58 had already been given by Ruelle [Rue 10]. The condition (3) in the theorem is due to Aizenmann, Davies and Lieb [Aiz 3] [Aiz 4], see also the appendix in [Kom 1]. The conditions that T is positive and $T(A) = A$ for $A \in \mathfrak{A}_{\Lambda^c}$ automatically imply that $T(\mathfrak{A}_\Lambda) \subseteq \mathfrak{A}_\Lambda$, $T(AB) = T(A)B$ for $A \in \mathfrak{A}_\Lambda$, $B \in \mathfrak{A}_{\Lambda^c}$ and T is completely positive.

The detailed structure of the ground states of the X–Y model described in Example 6.2.56 was derived by Araki and Matsui in 1985 [Ara 33] [Ara 34] [Mat 1]. The return to equilibrium for finite temperature states was established in 1984 by Araki [Ara 31].

The ground states of the XXZ model with Hamiltonian

$$H = \sum_{x \in \mathbf{Z}} (\mathbb{1} - \sigma_3^x \sigma_3^{x+1} - \delta(\sigma_1^x \sigma_1^{x+1} + \sigma_2^x \sigma_2^{x+1}))$$

where $0 < \delta < 1$ have been studied by Matsui [Mat 2] and by Gottstein and Werner [Got 1]. In addition to the two translation invariant ground states corresponding to the spins up and down, respectively, there are two families of non-translationally invariant ground states called kinks which interpolate between the spin up and spin down states. The extremal kinks in each of the families are all unitarily equivalent.

The detailed justification for the classical analysis of the ground states of the Ising model given in Example 6.2.56, and the connection between the condition given in Theorem 6.2.52 and the classical condition is as follows. Assume $\mathfrak{A}_{\{x\}} \simeq M_d$ for each $x \in L$ and hence $\mathfrak{A} \simeq \otimes_{x \in L} M_d$. Let $C_d \simeq \mathbb{C}^d$ be the subalgebra of diagonal matrices in M_d and $\mathfrak{C} \simeq \otimes_{x \in L} C_d \simeq C(\mathsf{X}_{x \in L} \mathbb{Z}_d)$ the corresponding maximal abelian subalgebra in $\mathfrak{A}$, the classical spin algebra. The interaction Φ is defined to be *classical* if $\Phi(X) \in \otimes_{x \in X} C_d$ for each $X \in L$ and $\Omega = \mathsf{X}_{x \in L} \mathbb{Z}_d$ is called the *classical configuration space*. If U_d is the unitary group in C_d there is an obvious action of the compact product group $\mathsf{X}_{x \in L} U_d$ on $\mathfrak{A}$

whose fixed point subalgebra is exactly $\mathfrak{C}$ and this is clearly a symmetry group for the classical interactions. This symmetry is never broken for finite temperature equilibrium states, i.e., the KMS states of the quantum model are diagonal states, and the probability measures on Ω one obtains from the restriction to $\mathfrak{C}$ are equilibrium states in the classical sense, i.e., the DLR equations are fulfilled. This follows from the Gibbs condition of Theorem 6.2.18. On the other hand for ground states this symmetry may be broken. This phenomenon can be illustrated already in the matrix case. If, for example, the Hamiltonian has a doubly degenerate lowest eigenvalue the set of ground states is affinely isomorphic to the 3-ball by Example 4.2.7, but there are only two extremal classical ground states. Nevertheless it can be shown, and it is evident in the matrix case, that a state ω on $\mathfrak{A}$ is a ground state in the sense of Theorem 6.2.52 if, and only if, $\omega|_{\mathfrak{C}}$ is a ground state in the classical sense. This means that ω, viewed as a measure on Ω, is supported on the set of ground state configurations, i.e., the set of configurations that has minimal energy with respect to changing the configuration at a finite number of lattice sites. Another characterization is in terms of the projection $g_\Lambda \subseteq \mathfrak{C}_\Lambda \subseteq \mathfrak{C}$ onto those local configurations in $\mathbb{Z}_d^\Lambda$ which have extensions to global ground state configurations; a state $\omega \in E_{\mathfrak{A}}$ is a ground state if and only if $\omega(g_\Lambda) = 1$ for all finite subsets $\Lambda \subseteq L$. Thus the set of ground states is the closed face in $E_{\mathfrak{A}}$ generated by the classical ground states, where a ground state is called classical if it is invariant under the action of the symmetry group $\times_{x \in L} U_d$ on $\mathfrak{A}$, and thus it is uniquely determined by its restriction to the classical subalgebra. Nevertheless, one may have pure quantum ground states which are not unitarily equivalent to any ground state coming from a classical configuration. A simple example of this is given by the trivial interaction, but there may be more interesting ones like the Ising anti-ferromagnet on a triangular lattice [Got 2].

Analysis of the invariant ground states of the one-dimensional Heisenberg model was initiated by Bethe [Bet 1] in 1931. The most extensive rigorous results have been derived by Thomas and Babbitt and Thomas [Tho 1], [Bab 1], [Bab 2]. They describe the spectral properties of H_ω in great detail. It should be emphasized that our brief discussion in terms of the separation of the X–Y and Ising contributions is meant to be purely illustrative. Other descriptions of the model as a lattice Fermi gas (see Example 6.2.14) with two-body interaction or a lattice Bose gas with an additional hard-core interaction (see, for example, [Gin 1]) have also been used extensively.

The X–Y model, or the Ising model, in Example 6.2.56 show that there may be a great multiplicity of ground states, even translationally invariant ground states, in situations for which there is a unique (τ, β)-KMS state for each finite β. Thus one cannot expect to find many general situations where there is a unique ground state. Matsui [Mat 3] proved for a class of translationally invariant interactions with an external field $-\lambda \sum_{x \in \mathbf{Z}^\nu} \sigma_3^x$ that there exists a λ_0 such that there is a unique translationally invariant ground state provided $\lambda > \lambda_0$. The class of interactions include the Heisenberg model with formal Hamiltonian

$$H = -\lambda \sum_{x \in \mathbb{Z}^\nu} \sigma_3^x + \sum_{\substack{x, y \in \mathbb{Z}^\nu \\ |x-y|=1}} (a_1 \sigma_1^x \sigma_1^y + a_2 \sigma_2^x \sigma_2^y + a_3 \sigma_3^x \sigma_3^y)$$

where $a_1 < 0$ and $a_2 a_3 < 0$. The proof uses a representation of translationally invariant ground states as finite temperature states of a classical spin system developed by Kirkwood and Thomas [Kir 1].

Finally we comment on a method of constructing translationally invariant pure states on one-dimensional quantum lattice systems which has been used to analyze the ground states of certain interactions. Let $\mathfrak{A} = \otimes_{-\infty}^{\infty} M_{N+1}$ be the C^*-algebra of a quantum lattice system over $\mathbb{Z}$, fix a $k \in \mathbb{N}$ and let

$$V : \mathbb{C}^k \mapsto \mathbb{C}^k \otimes \mathbb{C}^{N+1}$$

be an isometry. Define a completely positive map $\mathbf{E} : M_k \otimes M_{N+1} \mapsto M_k$ by $\mathbf{E}(A) = V^* A V$. Let ρ be a state on M_k and assume that (ρ, V) satisfies the compatibility condition

$$\rho(\mathbf{E}(B \otimes I)) = \rho(B)$$

for all $B \in M_k$. Define $\mathbf{E}_A : M_k \mapsto M_k$ by $\mathbf{E}_A(B) = \mathbf{E}(B \otimes A)$ for $A \in M_{N+1}$. Then one can define a translationally invariant state ω on $\mathfrak{A}$ by the requirement

$$\omega(A_1 \otimes A_2 \otimes \ldots \otimes A_m) = \rho(\mathbf{E}_{A_m} \circ \mathbf{E}_{A_{m-1}} \circ \ldots \circ \mathbf{E}_{A_1}(I_k)) \ .$$

States constructed in this manner are called *finitely correlated states* by Fannes, Nachtergaele and Werner [Fan 5] [Fan 6]. In the second reference it is established that if ω is a finitely correlated state then the following conditions are equivalent:

(1) ω is pure,
(2) no proper subalgebra of M_k containing I_k is invariant under all $\mathbf{E}_A, A \in M_{N+1}$,
(3) $\mathbf{E}_I$ has trivial peripheral spectrum, i.e., the only eigenvector of

$$\mathbf{E}_I : B \mapsto V^*(B \otimes I)V$$

with eigenvalue of modulus one is I_k.

Using this construction Fannes, Nachtergaele and Werner [Fan 7] have established that the set of all translationally invariant pure states is weakly* dense in the set of all translationally invariant states. Thus the conclusion in Example 4.3.26 that the extremal translationally invariant states is weakly* dense in the set of all translationally invariant states on a quantum spin system can be considerably strengthened in the one-dimensional case.

Results on phase diagrams for genuine quantum statistical mechanical models are relatively sparse compared to the results for classical models [[Sim 2]] [[Sin 1]]. Some results have been obtained as quantum perturbations of classical models on the diagonal algebra. These results rely on the Pirogov–Sinai theory [[Sin 1]] of classical ground states to obtain the complete phase diagram of the quantum perturbation at small temperatures [Bor 1] [Dat 1].

The method is based on the assumption that the classical system has a finite number of pure classical ground states which are then perforce periodic. The models assume that the quantum Hamiltonian has the form $H = H^{(0)} + \delta V$ where $H^{(0)}$ is (formally) in the diagonal algebra and V is the quantum perturbation. The conclusions are drawn by a variation of Ginibre's method [Gin 2] [Ken 1] described in Section 6.2.5. One uses the Trotter formula

$$e^{-\beta H} = \lim_{n \to \infty} \left(e^{-\beta H^{(0)}/n} (\mathbb{1} - \beta V/n) \right)^n$$

to expand the perturbed density matrix $e^{-\beta H}$ around the unperturbed one $e^{-\beta H^{(0)}}$. This expression introduces transitions between classical contours at various times and leads to a representation in terms of 'quantum contours' on $[0, \beta] \times \mathbb{Z}^\nu$. In the case considered in [Gin 2] [Ken 1] the quantum contours could be controlled by standard arguments whilst in the more general situation encountered in [Dat 1] a quantum version the Pirogov–Sinai theory is required. In [Bor 1] one does not, however, consider these quantum contours but uses a map of the ν-dimensional quantum system into a $(\nu + 1)$-dimensional block lattice, where the classical Pirogov–Sinai theory is applicable. This map is somewhat analogous to the maps used in [Ara 35] and [Kle 1].

Section 6.3

The earliest rigorous results on the statistical mechanics of interacting quantum systems were obtained by Ruelle [Rue 12] and Fisher [Fis 1]. Both these papers dealt with properties of the thermodynamic functions, i.e., the pressure, free energy, etc., and the first results concerning the equilibrium states of such systems were given by Fisher [Fis 2] and Ginibre [Gin 5]. In particular, Fisher emphasized the importance of convexity, and differentiability, of the thermodynamic functions in terms of the interaction potentials for the discussion of phase-separation properties. These ideas were subsequently developed in the context of spin systems into the theory of tangent functionals and invariant Gibbs states described in Section 6.2.4. On the other hand, Ginibre introduced the techniques of functional integration. He showed that the quantum-mechanical reduced density matrices could be represented as integrals of functionals which resembled the correlation functionals of classical systems and exploited methods of classical statistical mechanics to obtain a variety of high-temperature, low-activity results. These techniques, which are described in Sections 6.3.2 and 6.3.3, have subsequently played a fundamental role both in quantum statistical mechanics and in constructive field theory. In fact, our statement in the introduction, to the effect that the ideal Bose gas is the only model of continuous quantum systems in which phase transitions have been rigorously established, is a slight exaggeration. In constructive field theory phase transitions have been rigorously derived for the Euclidean $P(\Phi)_2$ theories. To define these theories consider the CCR algebra $\mathfrak{A}_+(\mathfrak{h})$, where the one-particle space $\mathfrak{h}$ consists of the distributions $g \in \mathscr{S}'(\mathbb{R}^2)$ such that

$$||g||_N^2 = \int d^2p\, |\hat{g}(p)|^2 (p^2 + m^2)^{-1} < +\infty \ .$$

Here $\hat{g}$ is the Fourier transform of g and m is a positive constant, i.e., $\mathfrak{h}$ is the completion of $L^2(\mathbb{R}^2)$ in the norm

$$||g||_N = (g, (-\nabla^2 + m^2)^{-1} g)^{1/2} \ .$$

Let $\mathfrak{h}_r$ denote the subspace of $\mathfrak{h}$ consisting of real distributions, i.e., of g such that $\bar{g} = g$, where $\bar{g}(\varphi) = \overline{g(\bar{\varphi})}$ for $\varphi \in \mathscr{S}(\mathbb{R}^2)$ and let ω denote the Fock vacuum state, i.e.,

$$\omega(W(g)) = \exp\left\{-||g||_N^2/4\right\} \ ,$$

where W is the Weyl operator. Note that $W(f)$ and $W(g)$ commute if $f, g \in \mathfrak{h}_r$ and one easily verifies from the decomposition $\mathfrak{h} = \mathfrak{h}_r + i\mathfrak{h}_r$ and Lemma 4.3.15 that $\{W(f); f \in \mathfrak{h}_r\}$ generates a maximal abelian von Neumann algebra $\mathfrak{M}$ on Fock space. Let $\Phi(f)$ be the associated field operators (defined in Proposition 5.2.3.) The restriction of Φ to $\mathfrak{h}_r$ is called the free Euclidean Markov field of mass m in dimension 2. Let $\mathfrak{M} = C(Q)$ be the Gelfand representation of $\mathfrak{M}$, and let μ_0 be the regular Borel measure on Q defined by the Fock vacuum state. μ_0 is called the free measure.

To introduce interacting Euclidean field theories, one perturbs the measure μ_0. Define an operator-valued distribution A^* from a^* by

$$\int d^2p\, A^*(p) f(p) = a^*(\mu \check{f}) \ ,$$

where $\mu = (-\nabla^2 + m^2)^{1/2}$ and $\check{f}$ is the inverse Fourier transform of f. In terms of $A^*(p)$ and its adjoint $A(p)$ the Euclidean field is given by the expression

$$\Phi(x) = (2\pi)^{-1} \int d^2p\, e^{-ipx} [A^*(p) + A(-p)] \mu(p)^{-1} \ ,$$

where $\mu(p) = (p^2 + m^2)^{1/2}$. Note that if $\check{f}$ and $\check{g}$ are real, A and A^* satisfy the commutation relations

$$[A(f), A^*(g)] = \mathbb{1} \int d^2x\, \check{f}(x) \check{g}(x) \ .$$

One defines Wick powers of the field by

$$\begin{aligned} :\Phi^n(x): = &(2\pi)^{-n} \int \prod_{i=1}^{n} (\mu(p_i)^{-1} d^2p_i) e^{-ix(p_1 + \cdots + p_n)} \\ &\times \sum_{j=0}^{n} {}^nC_j A^*(p_1) \cdots A^*(p_j) A(-p_{j+1}) \cdots A(-p_n) \end{aligned}$$

as a quadratic form on finite-particle vectors with smooth components. This corresponds to placing all creation operators to the left and all annihilation operators to the right in the expression for the "operator power" $\Phi(x)^n$. If P is a polynomial of the form

$$P(x) = \sum_{r=0}^{2m} a_r x^r$$

with $a_{2m} > 0$ and g is a sufficiently nice function, one defines

$$\begin{aligned} U(g) &= \int d^2x\, g(x) : P(\Phi(x)) : \\ &= \sum_{r=0}^{2m} a_r \int d^2x\, g(x) : \Phi^r(x) : \quad . \end{aligned}$$

Formally one defines the interacting Gibbs measure by

$$\mu(f) = \frac{\mu_0(e^{-\beta U(1)} f)}{\mu_0(e^{-\beta U(1)})}$$

but $U(1)$ does not make sense as a function on Q, and one has to introduce finite-volume Gibbs measures

$$\mu_{\sigma,\Lambda}(f) = \frac{\mu_{0,\sigma,\Lambda}(e^{-\beta U(\chi_\Lambda)} f)}{\mu_{0,\sigma,\Lambda}(e^{-\beta U(\chi_\Lambda)})}$$

where $\mu_{0,\sigma,\Lambda}$ is the measure defined as μ_0 with $-\nabla^2$ replaced by $T^{(1)}_{\sigma,\Lambda}$, the Laplacian in Λ with the classical boundary conditions given by σ (see Example 5.2.26) and χ_Λ is the characteristic function of Λ. One may also use $\mu_{0,f,\Lambda} = \mu_0$, i.e., the so-called free-boundary conditions, or a measure $\mu_{0,p,\Lambda}$ corresponding to periodic boundary conditions in this definition. It was established by Guerra, Rosen, and Simon [Guer 1], [Guer 2] that the infinite-volume pressure

$$\lim_{\Lambda \to \mathbb{R}^2} \frac{1}{|\Lambda|} \log \mu_{0,\sigma,\Lambda}(e^{-U(\chi_\Lambda)})$$

exists and is independent of the boundary conditions.

Phase transitions in these models were first exhibited by Glimm, Jaffe, and Spencer [Gli 6], [Gli 7]. Specifically, they considered the polynomial

$$P_{k,h}(x) = \frac{(x^2 - k^2)^2}{k^2} + hx \quad .$$

Then, with Dirichlet boundary conditions, the limits of the momenta of the fields

$$\omega_{k,h}(\Phi(f_1) \cdots \Phi(f_n)) = \lim_{\Lambda \to \mathbb{R}^2} \frac{\mu_{0,\infty,\Lambda}(e^{-U(\chi_\Lambda)} \Phi(f_1) \cdots \Phi(f_n))}{\mu_{0,\infty,\Lambda}(e^{-U(\chi_\Lambda)})}$$

exist for $f_1, \ldots, f_n \in \mathscr{D}_r(\mathbb{R}^2)$. However, if k is sufficiently large one can show that

$$\lim_{h \to 0+} \omega_{k,h}(\Phi(f)) \neq \lim_{h \to 0-} \omega_{k,h}(\Phi(f))$$

for positive f, i.e., for $h = 0$ one has pure phases which are not invariant under the symmetry $\Phi \to -\Phi$. This is established by an argument similar to the

Peierls argument of Section 6.2.6. The local nature of the interaction makes these models very similar to lattice models, and one can use all the machinery from the latter models, i.e., correlation inequalities, etc., to prove results about the former. A review of the resulting developments can be found in [Frö 3]. The greatest physical interest of these models comes not from statistical mechanics, but from the fact that they are closely related to quantum field models in one space dimension (see [Guer 1]).

Section 6.3.1

It should be emphasized that the time evolutions

$$\tau_t^\Lambda(A) = e^{itH_{\sigma,\Lambda}} A e^{-itH_{\sigma,\Lambda}}$$

generated by the local Hamiltonians

$$H_{\sigma,\Lambda} = T_{\sigma,\Lambda} + U_\Lambda$$

never can be expected to leave the C^*-algebras $\mathfrak{A}_\pm(\Lambda)$ invariant if $U \neq 0$. A rigorous result in this direction was proved by Fannes and Verbeure [Fan 3]. They consider the CCR algebra $\mathfrak{A}_+(\mathfrak{h})$ over $\mathfrak{h} = \mathbb{C}$, i.e., the C^*-algebra of ordinary quantum mechanics in one dimension. The Schrödinger representation, Example 5.2.16, realizes this algebra on $L^2(\mathbb{R})$ as

$$(W(s)\psi)(x) = e^{isx}\psi(x) \ ,$$
$$(W(is)\psi)(x) = \psi(x-s)$$

for $s \in \mathbb{R}$. Next define

$$P = -\frac{1}{i}\frac{dW(is)}{ds}\bigg|_{s=0} = \frac{1}{i}\frac{d}{dx} \ ,$$
$$Q = \frac{1}{i}\frac{dW(s)}{ds}\bigg|_{s=0} = x$$

and a Hamiltonian

$$H_\lambda = P^2 + \lambda V(Q) \ ,$$

where V is a real, bounded function and $\lambda \in \mathbb{R}$. Define a one-parameter group α_t^λ of $\mathscr{L}(L^2(\mathbb{R}))$ by

$$\alpha_t^\lambda(A) = e^{iH_\lambda t} A e^{-iH_\lambda t} \ .$$

One verifies

$$\alpha_t^0(W(is)) = W(is) \ ,$$

$$\alpha_t^0(W(s)) = e^{i2s^2t} W(s(1-2it)) \ ,$$

i.e., $t \mapsto \alpha_t^0$ defines a one-parameter group of *-automorphisms of $\mathfrak{A}_+(\mathbb{C})$, which is not strongly continuous because of Theorem 5.2.8 (1). Fannes and Verbeure

prove, however, that if $\lambda \neq 0$ and V is either nonconstant and almost periodic (i.e., $V(Q) \in \mathfrak{A}_+(\mathbb{C})\backslash\mathbb{C}\mathbb{1}$) or $V \in L^\infty \cap L^1$ and $V \neq 0$, then α_t^λ does not map $\mathfrak{A}_+(\mathbb{C})$ into itself for $t \neq 0$.

The fact that the local automorphism groups do not leave the local C^*-algebras globally invariant does not lead to any problems since the local Gibbs states ω_Λ are normal in the Fock representation, and therefore have unique normal extensions to $\mathfrak{A}_\pm(\Lambda)'' = \mathscr{L}(\mathfrak{F}_\pm(\Lambda))$. Expressions like

$$\omega_\Lambda(\tau_{t_1}^\Lambda(A_1)\cdots\tau_{t_n}^\Lambda(A_n))$$

for $A_1, \ldots, A_n \in \mathfrak{A}_\pm(\Lambda)$ should therefore be interpreted as

$$\frac{\mathrm{Tr}_{\mathfrak{F}\pm(\Lambda)}(e^{-\beta H_\Lambda}e^{it_1H_\Lambda}A_1e^{i(t_2-t_1)H_\Lambda}A_2\cdots A_ne^{-it_nH_\Lambda})}{\mathrm{Tr}_{\mathfrak{F}\pm(\Lambda)}(e^{-\beta H_\Lambda})}$$

etc.

The literature on perturbations of the infinite-volume Laplacian $-\nabla^2$ by multiplicative operators U is extensive (see, for example, [[Kat 1]], [[Ree 2]], [[Sim 1]]). There does not, however, appear to be any readily available description of the corresponding problem for finite-volume Laplacians with classical boundary conditions although several results can be easily transcribed from the infinite-volume case. For example, the equality of $T_{\sigma,\Lambda}^{(n)} + U_\Lambda^{(n)}$ and $T_{\sigma,\Lambda}^{(n)} + U^{(n)}$ for $U^{(n)} \in L^2(\Lambda)^n$ and $U^{(n)} \geq 0$ follows from an inequality of Kato by the same argument used for $-\nabla^2$ (see Section X.4 in [[Ree 2]] for a description of this technique). Similarly Proposition 6.3.1 is a version of Kato's theorem of 1951 [Kat 2]. The estimates of the kernel of the semigroup used in the proof are discussed in detail in Section 6.3.2.

Stable interactions are discussed in detail in [[Rue 1]], and the statements in Examples 6.3.2 and 6.3.3 are proved there. Example 6.3.2 is originally due to Dobrushin [Dob 5] and 6.3.3 was proved by Ruelle in [Rue 13]. In fact, he proved that if the condition

$$\sum_{i=1}^n\sum_{j=1}^n \Phi(x_i - x_j) \geq 0$$

is not satisfied, then one can find configurations of n particles in a bounded region Λ with a potential energy less than or equal to $-Cn^2$ for infinitely many n, where $C > 0$, which establishes catastrophic behavior of the classical system. Furthermore, it is possible to approximate these configurations by quantum configurations $\varphi_n \in L^2(\Lambda)_\pm^n$ such that

$$(\varphi_n, U_\Lambda\varphi_n) \leq -Cn^2$$

and

$$(\varphi_n, T_{\infty,\Lambda}\,\varphi_n) \leq \begin{cases} C'n & \text{for bosons} \\ C''n^{1+2/\nu} & \text{for fermions} \end{cases}$$

for infinitely many n. This shows that if the classical stability condition

$$U_\Lambda \geq -BN_\Lambda$$

is violated for an upper semi-continuous two-body interaction then the quantum stability condition

$$H_{\infty,\Lambda} \geq -BN_\Lambda$$

is also always violated for bosons, and, if $\nu \geq 3$, also for fermions. This could lead one to believe that the two notions of stability are equivalent, but in the important physical case of the Coulomb interaction of different species of particles they are not. This was pointed out by Dyson and Lenard in 1967–1968 [Dys 4]. Consider, for simplicity, n particles in $\mathbb{R}^3$ with the mass $\frac{1}{2}$ and charges $e_j = \pm 1, j = 1, \ldots, n$. The Hamiltonian of the system is given by

$$H_n = \sum_{j=1}^{n} -\nabla_i^2 + \sum_{1 \leq i < j \leq n} \frac{e_i e_j}{|x_i - x_j|} \quad .$$

The particles may be fermions and/or bosons, of different species or not. In general it is possible to prove the lower bound

$$H_n \geq -Bn^{5/3} \quad ,$$

where B is an absolute constant [Dys 4] and if all the particles are bosons or satisfy Boltzmann statistics, and the total charge is zero, it is also possible to find a unit vector ψ_n such that

$$(\psi_n, H_n \psi_n) \leq An^{7/5} \quad ,$$

where A is an absolute constant [Dys 5]. Thus, in this case the system is not stable in any sense. One can show, however, that if all the n particles are fermions belonging to $q \geq 1$ different species, i.e., if one can partition the arguments $x_1, \ldots, x_n$ in the wave functions into q subsets such that the wave functions are totally antisymmetric under permutations within each subset, then the system is stable

$$H_n \geq -Bq^{2/3}n \quad ,$$

where B is an absolute constant [Dys 4]. This is one of the most striking effects of the Pauli exclusion principle. It is even possible to prove stability of a Coulomb system of fermions of q different species, but all with negative charge, interacting with particles of positive charge, and arbitrary statistics. If the total number of particles is n it is again possible to establish

$$H_n \geq -Bq^{2/3}n$$

where B is an absolute constant [Dys 4], (for the best constants and relativistic cases see [[Lie 1]], [Lie 7], [Lie 8], [Lie 9]) for a simplified proof. It is not only the Pauli exclusion principle which is important for this result, but also the fact that charges interacting via the Coulomb potential tend to screen each other so that all interactions beyond the nearest-neighbor distance can be ignored. The starting point is a classical lemma proved by Onsager in 1939 [Ons 3]. If

$$R_j = \min_{i \neq j} |x_i - x_j|$$

is the distance of a charge e_j at x_j from its nearest neighbor among n charges e_i at x_i, then Onsager's lemma states that

$$\sum_{i<j} \frac{e_i e_j}{|x_i - x_j|} \geq -\sum_{j=1}^{n} \frac{e_j^2}{R_j} \ .$$

All the results on stability of infinitely extended Coulomb systems transfer in a straightforward manner to bounded systems with Dirichlet boundary conditions.

The minimax principle in Proposition 6.3.4 is a standard result which is proved in different versions in [[Kat 1]] and [[Rue 1]]. It was originally proved by Weyl in the beginning of the twentieth century.

Section 6.3.2

The Wiener measure was introduced by Wiener [Wie 1] in 1923. He was partially motivated by the work of Einstein and Smoluchowski on Brownian motion. This phenomenon is the earliest observed effect of microscopic particle structure and was first elucidated by Brown in the early nineteenth century following a trip of exploration to Australia. (It is probably the first physical theory with an Australasian influence.) The monograph by Nelson [[Nel 1]] contains a very readable account of the history and development of the various theories of the phenomenon.

The construction of the Wiener integral that we have given is due to Nelson [Nel 2] (see also [[Ree 2]]). There is a large textbook literature on the Wiener integral from a probabilistic viewpoint. In particular the book of Itô and McKean [[Itô1]] contains a great deal of information about regularity properties of the Wiener measure, including a proof of Theorem 6.3.6.

The idea of the Feynman–Kac formula, Theorem 6.3.7, dates back to Feynman's unpublished Princeton thesis in 1942 (see [Fey 1]). He considered the Schrödinger equation rather than the diffusion equation. If $H_0 = -\nabla^2$ is the free Laplacian on $L^2(\mathbb{R}^\nu)$, one has

$$(e^{-itH_0}\psi)(x) = (4\pi it)^{-\nu/2} \int_{\mathbb{R}^\nu} d^\nu y \, \exp\left\{\frac{i|x-y|^2}{4t}\right\}\psi(y)$$

if ψ is sufficiently smooth, e.g., for $\psi \in \mathscr{S}(\mathbb{R}^\nu)$. If V is a multiplication operator which is H_0-bounded with relative bound less than one, one can use Trotter's theorem to prove that

$$\begin{aligned}&(e^{-it(H_0+V)}\psi)(x_0)\\ &= \lim_{n\to\infty} \left(\frac{4\pi it}{n}\right)^{-\nu n/2} \int_{\mathbb{R}^\nu} \cdots \int_{\mathbb{R}^\nu} d^\nu x_1 \cdots d^\nu x_n \exp\{iS_n(x_0, x_1, \ldots, x_n, t)\}\psi(x_n) \ ,\end{aligned}$$

where

$$S_n(x_0, x_1, \ldots, x_n, t) = \sum_{i=1}^{n} \frac{t}{n} \left[\frac{1}{4} \left(\frac{|x_i - x_{i-1}|}{t/n} \right)^2 - V(x_i) \right] .$$

Feynman's idea was to rewrite the last limit as an integral over paths starting at x_0,

$$(e^{-it(H_0+V)}\psi)(x_0) = \int d\omega \, \exp\{iS_t(\omega)\}\psi(\omega(t)) ,$$

where

$$S_t(\omega) = \int_0^t \frac{1}{4} \left(\frac{d\omega}{d\tau} \right)^2 d\tau - \int_0^t V(\omega(\tau)) d\tau$$

is the action of the path ω. In this way Feynman viewed the Schrödinger dynamics as a "sum over histories" of the particle's motion. Unfortunately, it can be proved rigorously that there does not exist a measure $d\omega$ on the path space Ω_t such that this formula makes sense, see, for example [Cam 1]. Nevertheless, one can construct Feynman "integrals" as linear functionals over suitable function spaces, and this has been used to prove that classical mechanics is the $\hbar \to 0$ limit of quantum mechanics in a suitable sense, i.e., in this limit the Feynman "measure" is "supported" on the path of least action, which is just the classical path. The reader is referred to the monograph of Albeverio and Høegh-Krohn [[Alb 1]] for a review of these developments.

The idea of continuing the Feynman formula to imaginary time so that Wiener measure can be used to establish a rigorous version of the Feynman formula appeared in Kac's 1951 paper [Kac 1].

Theorem 6.3.7 is a generalization of a version of the Feynman–Kac formula given by Reed and Simon ([[Ree 2]], Theorem X 68).

The properties of the finite-volume Green's functions established in Theorem 6.3.8 and the preceding remarks were established by Itô, Sato and Ueno, and Arima [Itô 1], [Sat 1], [Ari 1]. We have largely followed the 1973 paper of Angelescu and Nenciu [Ang 1] in the treatment of the finite-volume Wiener measures. In particular, these authors proved Theorem 6.3.9. The formulas for the Dirichlet boundary condition Wiener measures in Corollary 6.3.10 were used earlier by Ginibre [Gin 5] in his early work on the reduced density matrices in quantum statistical mechanics and by Novikov [Nov 1] in his discussion of the independence of the pressure from the boundary conditions. Example 6.3.11 is due to Novikov.

A comprehensive review of Wiener integral techniques in quantum statistical mechanics prior to 1970 has been given by Ginibre [Gin 6] and the property of Wiener measures used in the proof of Corollary 6.3.10 can be found in this article.

Section 6.3.3

The representation of the reduced density matrices in terms of Wiener integrals was first given by Ginibre [Gin 5] in 1965. In particular, Ginibre derived the combinatorial formulas of Theorem 6.3.14, or really Example 6.3.15 since he dealt exclusively with Dirichlet boundary conditions. Similar combinatorics had previously been considered in the context of perturbation theory (see, for example, the article by Bloch [Blo 1]). This representation is discussed at length in Ginibre's review article [Gin 6] and a good short review of these matters can be found in [Gin 7].

The estimates for the finite-volume reduced density matrices with positive interactions, Theorem 6.3.17 and Corollary 6.3.18, were proved by Bratteli and Robinson in [Bra 17]. The low-density expansions used in proving Theorem 6.3.19 and Theorem 6.3.21 were developed by Ginibre using earlier low-density expansions derived by Ruelle (see [[Rue 1]]) for classical systems. The bounds on the reduced density matrices given in Corollary 6.3.20 were not explicitly stated by Ginibre but they are an easy consequence of his bounds for the associated correlation functionals. These bounds are of the form

$$|\rho_\Lambda(\omega^m)| \leq \left(\frac{R}{\zeta}\right)\left(\frac{\zeta|z|}{R}\right)^q\left(1-\frac{|z|}{R}\right)^{-1}$$

and for bosons or Boltzmann statistics $\rho_\Lambda(\omega^m) \geq 0$. These latter bounds have been generalized and systematized in the classical setting by Ruelle [Rue 16], following earlier ideas of Dobrushin. Ruelle proves that if the interactions are superstable, then the classical correlation functions satisfy bounds

$$0 \leq \rho_\Lambda(x_1, \ldots, x_m) \leq \zeta^n \ .$$

The method for establishing the infinite-volume limit of the pressure with repulsive (Dirichlet) boundary conditions discussed near the end of the section was developed by Fisher [Fis 1] and [Rue 12]. The method for dealing with elastic (Neumann) boundary conditions is due to Robinson [Rob 13]. It is elaborated in the monograph [[Rob 1]] and in particular the pressure is shown to be independent of the boundary conditions whenever the interaction potentials are positive and decreasing. Prior to Robinson's work the only boundary conditions that had been considered in the rigorous analysis of quantum statistical mechanics were Dirichlet boundary conditions. Robinson emphasized that the complementary use of Neumann boundary conditions, which were physically equally compelling, led to upper-lower bound techniques of great analytic utility. These techniques are now commonly referred to as Neumann–Dirichlet bracketing and have been applied in various other fields such as constructive quantum field theory [Guer 2] and quantum-mechanical scattering theory [Marti 1]. For a review of these applications, see [Sim 2].

The functional integration method of proving independence of boundary conditions originated with Novikov [Nov 1] who considered hard-core bosons at low densities. This technique was reviewed by Ginibre [Gin 6] and further

developed by Angelescu and Nenciu [Ang 1]. It has also been extended to other contexts (see [Sim 2]).

The infinite-volume limit of the pressure has also been established for some systems for which classical stability fails, i.e., for different species of bosons and fermions with Coulomb interaction. We mentioned in the end of the Notes and Remarks to Section 6.3.1 that these systems might have a type of quantum-mechanical stability because of the Pauli exclusion principle and the screening effect of the potentials. The infinite-volume limit of the pressure for a system of positively charged bosons interacting via Coulomb forces with negatively charged fermions was proved by Lieb and Lebowitz in 1972 [Lie 6]. If the total system is electrically neutral, the limit is independent of the shapes of the finite volumes Λ, while the limit is shape dependent for systems with a net charge. The existence of the thermodynamic limit for two-dimensional neutral Coulomb systems was demonstrated by Fröhlich in 1976 [Frö 4]. Later Fröhlich and Park were able to use correlation inequality techniques to prove the existence of the thermodynamic limit for the pressure and the correlation functions at arbitrary temperatures and chemical potentials for Boltzmann particles interacting via two-body potentials of positive type [Frö 5] and they announced similar results for bosons. We will give a brief account of their results in the case of distinguishable particles with some simplifying assumptions. Consider a system of Boltzmann particles on $\mathbb{R}^\nu$ consisting of two different species of particles. These species are indexed by a "charge" q, where q may assume the values ± 1. The potential energy between a particle with charge q at the point $x \in \mathbb{R}^\nu$ and one with charge q' at $x' \in \mathbb{R}^\nu$ is given by

$$U(q,x;q',x') = qq'\Phi(x-x') \ ,$$

where Φ is a real symmetric function on $\mathbb{R}^\nu$. The crucial assumption on Φ is that it is positive definite in the sense that

$$\sum_{i,j=1}^{n} \bar{c}_i\, c_j \Phi(x_i - x_j) \geq 0$$

for all finite sequences $c_1, \ldots, c_n \in \mathbb{C}$, $x_1, \ldots, x_n \in \mathbb{R}^\nu$. For more technical reasons one also has to assume that

$$\Phi(0) < +\infty \ .$$

The potential for n particles at the points x^n and with charges q^n is then

$$U^{(n)}(q^n, x^n) = \sum_{1 \leq i < j \leq n} q_i\, q_j\, \Phi(x_i - x_j) \ .$$

The Hilbert space for n particles with charges $q_1, \ldots, q_n$ confined to a bounded region $\Lambda \subseteq \mathbb{R}^\nu$ is

$$\mathfrak{H}_\Lambda^n = \bigotimes_{i=1}^{n} L^2(\Lambda; d^\nu x_i) = L^2(\Lambda^n; d^{n\nu} x^n)$$

and the Hamiltonian is given by

$$H_\Lambda^{(n)}(q^n) = H_{\infty,\Lambda}^{(n)}(q^n) = T_{\infty,\Lambda}^{(n)} + U^{(n)}(q^n, \cdot)$$

where $T_{\infty,\Lambda}^{(1)}$ is $-\nabla^2$ with Dirichlet boundary conditions. The partition function is now

$$\begin{aligned} Z_\Lambda = Z_\Lambda(\beta, z) &= \sum_{n=0}^{\infty} \frac{z^n}{n!} \sum_{q^n} \mathrm{Tr}_{\mathfrak{H}_\Lambda^n}(e^{-\beta H_\Lambda^{(n)}(q^n)}) \\ &= \sum_{n=0}^{\infty} \frac{z^n}{n!} \sum_{q^n} \int_{\Lambda^n} dx^n e^{-\beta H_\Lambda^{(n)}(q^n)}(x^n, x^n) \ , \end{aligned} \tag{1}$$

where the q^n sum runs over all 2^n possible charge configurations and $e^{-\beta H_\Lambda^{(n)}(q^n)}(x^n, y^n)$ is the kernel of $e^{-\beta H_\Lambda^{(n)}(q^n)}$. The finite-volume pressure and the finite-volume particle-density correlation functions are then defined by

$$P_\Lambda(\beta, z) = \frac{1}{\beta|\Lambda|} \log(Z_\Lambda(\beta, z)) \tag{2}$$

and

$$\begin{aligned} &\rho_\Lambda(\beta, z; q^n, x^n) \\ &\quad = Z_\Lambda(\beta, z)^{-1} z^n \left\{ \sum_{m=0}^{\infty} \frac{z^m}{m!} \sum_{q^m} \int_{\Lambda^m} dx'^m e^{-\beta H_\Lambda^{n+m}(q^n q'^m)}(x^n x'^m, x^n x'^m) \right. . \end{aligned} \tag{3}$$

Theorem [Frö 5]. *Adopt the preceding assumptions.*

It follows for arbitrary $\beta > 0$ and $z > 0$ and an arbitrary sequence of bounded regions Λ converging to $\mathbb{R}^\nu$ that

1. $$P(\beta, z) = \lim_{\Lambda \to \mathbb{R}^\nu} P_\Lambda(\beta, z)$$

exists and is independent of the particular sequence chosen, and $P(\beta, z)$ has the standard properties of the thermodynamic pressure;

2. $$\rho(\beta, z; q^n, x^n) = \lim_{\Lambda \to \infty} \rho_\Lambda(\beta, z; q^n, x^n)$$

exists for $n = 0, 1, 2, \ldots$. It is monotonely increasing in z and bounded by

$$\left(z(\pi/\beta)^{\nu/2}\right)^n \exp\{n\beta\Phi(0)/2\} \ .$$

The theorem is proved via the Feynman–Kac formula, which now takes the form

$$e^{-\beta H_\Lambda^{(n)}(q^n)}(x^n, y^n) = \int_{(\Omega_{\Lambda,\beta})^n} d\mu_{x^n, y^n}^{\infty, \Lambda, \beta}(\omega^n) \exp\left\{ -\int_0^\beta dt\, U^{(n)}(q^n, \omega(t)^n) \right\} \ , \tag{4}$$

where

$$d\mu_{x^n, y^n}^{\infty, \Lambda, \beta}(\omega^n) = \prod_{i=1}^{n} d\mu_{x_i, y_i}^{\infty, \Lambda, \beta}(\omega_i) \ .$$

One expresses $\exp\{-\int_0^\beta dt\, U^{(n)}(q^n, \omega(t)^n)\}$ by means of Gaussian integrals as follows. Define a kernel W by

$$W(q, x, t; q', x', t') = qq'\Phi(x - x')\delta(t - t')$$

where $q, q' \in \{-1, 1\}; x, x' \in \mathbb{R}^\nu; t, t' \in [0, \beta]$ and δ is the unit point measure at zero. We identify W with the corresponding quadratic form.

Define

$$\mathfrak{H} = L^2(\{-1, 1\} \times \mathbb{R}^\nu \times [0, \beta]; dq \times d^\nu x \times dt) \ ,$$

where dq is the counting measure on $\{-1, 1\}$, and choose some selfadjoint operator H on $\mathfrak{H}$ such that

(1) $H \geq \mathbb{1}$,
(2) H^{-n} is Hilbert-Schmidt for some $n < +\infty$,
(3) $H^{-n}WH^{-n}$ is a bounded form for some $n < +\infty$.

Let $\mathscr{S}$ consist of the real functions in $\bigcap_{n\geq 1} D(H^n)$, and equip $\mathscr{S}$ with the seminorms

$$f \mapsto ||H^n f||, \quad n = 1, 2, \ldots .$$

The set $\mathscr{S}$ is then a locally convex topological space, and condition (2) ensures that $\mathscr{S}$ is a nuclear space. Condition (3) implies that W is continuous as a form on $\mathscr{S} \times \mathscr{S}$, and hence W extends to a distribution on $\mathscr{S} \otimes \mathscr{S}$ by the nuclear theorem [[Gel 1]]. But W is positive because Φ is positive definite.

By Minlos' theorem [[Gel 1]] there exists a measure $d\mu_W$ on the dual space $\mathscr{S}'$ of $\mathscr{S}$ such that

$$\int_{\mathscr{S}'} d\mu_W(\varphi) e^{i\varphi(f)} = e^{-(1/2)\langle fWf\rangle}$$

where $\langle fWf\rangle$ is the value of the quadratic form W on f. The measure μ_W is often called the *Gaussian measure* with mean 0 and covariance W. Define the *Wick ordered* product of the function $\varphi \in \mathscr{S}' \mapsto e^{i\varphi(f)}$ by

$$:e^{i\varphi(f)}: = e^{(1/2)\langle fWf\rangle} e^{i\varphi(f)}$$

(this is consistent with the definition of Wick ordering in the beginning of the Notes and Remarks to Section 6.3). One can then compute that

$$\int d\mu_W(\varphi) \left[\prod_{j=1}^n :e^{i\varphi(f_j)}: \right] = \exp\left\{ - \sum_{1 \leq i < j \leq n} \langle f_i W f_j \rangle \right\}$$

for $f_1, \ldots, f_n \in \mathscr{S}$. By approximating

$$f_j(q, x, t) = \delta_{q, q_j} \delta(x - \omega_j(t))$$

with functions from $\mathscr{S}$, and using the notation

$$\varphi(f) = \int \varphi(q, x, t) f(q, x, t) dq d^\nu x dt$$

we obtain

$$\int d\mu_W(\varphi)\left[\prod_{j=1}^{n} : \exp\left\{ i\int_0^\beta dt\varphi(q_j,\, \omega_j(t), t)\right\} :\right]$$
$$= \exp\left\{-\int_0^\beta dt\; U^{(n)}(q^n,\, \omega(t)^n)\right\} . \tag{5}$$

This is the desired expansion of $\exp\{-\int_0^\beta dt\; U^{(n)}(q^n, \omega(t)^n)\}$ in terms of Gaussian integrals.

Now, define

$$C_\Lambda^\beta(\varphi) = \sum_{q\in\{-1,1\}} \int_\Lambda d^\nu x \int_{\Omega_{\Lambda,\beta}} d\mu_{x,x}^{\infty,\Lambda,\beta}(\omega) : \exp\left\{ i\int_0^\beta dt\, \varphi(q, \omega(t),\, t)\right\} :$$
$$= \sum_{q\in\{-1,1\}} \int_\Lambda d^\nu x \int_{\Omega_{\Lambda,\beta}} d\mu_{x,x}^{\infty,\Lambda,\beta}(\omega) : \cos\left(\int_0^\beta dt\varphi(q, \omega(t), t)\right) :$$

and substitute the formulas (5) and (4) into (1) to derive

$$Z_\Lambda(\beta,\, z) = \sum_{n=0}^{\infty} \frac{z^n}{n!}\int d\mu_W(\varphi) C_\Lambda^\beta(\varphi)^n = \int d\mu_W(\varphi)\exp\{zC_\Lambda^\beta(\varphi)\} .$$

Combining this with (2) and (3) we obtain

$$P_\Lambda(\beta,\, z) = \frac{1}{\beta|\Lambda|}\log\left(\int d\mu_w(\varphi)\exp\{zC_\Lambda^\beta(\varphi)\}\right)$$

and

$$\rho_\Lambda(\beta,\, z;\, q^n,\, x^n) = Z_\Lambda(\beta,\, z)^{-1} z^n$$
$$\times \int d\mu_W(\varphi)\left[\prod_{j=1}^{n}\int d\mu_{x_j,x_j}^{\infty,\Lambda,\beta}(\omega_j) : \exp\left\{ i\int_0^\beta dt\varphi(q_j,\, \omega_j(t),\, t)\right\} : \exp\{z\, C_\Lambda^\beta(\varphi)\}\right] .$$

One now derives correlation inequalities for quantities like

$$\int d\mu_W(\varphi)\varphi(f_1)\cdots\varphi(f_n)$$

in much the same way as for classical lattice models, and uses these to show the existence of the thermodynamic limit by monotonicity arguments. One can also extend the argument to establish the thermodynamic limit for other correlation functions and imaginary time Green's functions.

Section 6.3.4

The results on the thermodynamic limits of the finite-volume Gibbs states for Bose gases with positive n-body potentials obtained in Theorem 6.3.22 and Corollary 6.3.24 appeared in [Bra 17], where these results were also proved for

general boundary conditions. The result alluded to in the Remark following Theorem 6.3.22 is due to Park in 1985 [Par 1]. Results similar to Theorem 6.3.25 were proved by Duneau and Souillard [Dune 1] in 1973. Theorem 6.3.26 was proved in bits and pieces by several authors. The pointwise convergence of the Green's functions for $\zeta^m \in \mathfrak{D}$ was established by Gruber in 1968 [Gru 1]. (See also [Gin 8].) The full result for fermions was proved by Ruelle [Rue 14], [Rue 15] in 1971–1972 by establishing uniform bounds on the derivatives of the finite-volume Green's functions and essentially applying Lemma 6.3.23, i.e., a technique similar to the one used to prove Proposition 6.3.29. The boson results were established with similar methods by Duneau and Souillard in the paper quoted above.

The study of the infinite-volume limit of Green's functions from a general viewpoint originated in a 1970 paper by Dubin and Sewell [Dub 1], soon to be followed by Ruskai [Rusk 1] and Sirugue and Winnink (see [Win 3]). Some later refinements were made by Bratteli and Robinson [Bra 16] and Jørgensen [Jør 2]. In [Dub 1], [Rusk 1], [Jør 2] the multitime Green's functions are viewed as states on a certain *-algebra essentially introduced by Wightman in 1956 [Wig 3]. This is the free *-algebra $\mathfrak{B}(\mathfrak{A})$ generated by pairs of elements (A, t) with $A \in \mathfrak{A}$ and $t \in \mathbb{R}$ modulo the relations

$$(A_1, t)(A_2, t) = (A_1 A_2, t) \ ,$$
$$\lambda(A_1, t) + (A_2, t) = (\lambda A_1 + A_2, t) \ ,$$

and

$$(\mathbb{1}, t) = (\mathbb{1}, 0)$$

and $A_1, A_2 \in \mathfrak{A}$, $\lambda \in \mathbb{C}$, $t \in \mathbb{R}$. More specifically, let $\mathfrak{W}$ denote the *-algebra linearly spanned, over the complex numbers, by strings of elements

$$P = (A_1, t_1)(A_2, t_2) \cdots (A_k, t_k)$$

with $A_i \in \mathfrak{A}$, $t_i \in \mathbb{R}$. Define the *-operation by

$$P^* = (A_k^*, t_k)(A_{k-1}^*, t_{k-1}) \cdots (A_1^*, t_1)$$

and let $\mathfrak{J}$ be the two-sided ideal generated by the elements

$$(A_1, t)(A_2, t) - (A_1 A_2, t) \ ,$$
$$\lambda(A_1, t) + (A_2, t) - (\lambda A_1 + A_2, t) \ ,$$

and

$$(\mathbb{1}, t) - (\mathbb{1}, 0) \ .$$

Then $\mathfrak{B}(\mathfrak{A})$ is the quotient *-algebra $\mathfrak{W}/\mathfrak{J}$. One next defines a one-parameter group γ of *-automorphisms of $\mathfrak{B}(\mathfrak{A})$ by

$$\gamma_t((A_1, t_1) \cdots (A_k, t_k)) = (A_1, t_1 + t) \cdots (A_k, t_k + t) \ .$$

One can then prove the following analogue of the GNS construction [Dub 1], [Rusk 1], [Jør 2].

Proposition. *Let ω be a positive linear functional ($\omega(P^*P) \geq 0$ for all $P \in \mathfrak{B}(\mathfrak{A})$) on $\mathfrak{B}(\mathfrak{A})$ satisfying the conditions*

(i) $\omega(\gamma_t(P)) = \omega(P)$, *for all* $t \in \mathbb{R}$ *and* $P \in \mathfrak{B}(\mathfrak{A})$.
(ii) *The mapping* $t \mapsto \omega(P^*\gamma_t(P))$ *is continuous on* $\mathbb{R}$ *for all* $P \in \mathfrak{B}(\mathfrak{A})$.

It follows that there exists a **-representation* π *of* $\mathfrak{B}(\mathfrak{A})$ *on a Hilbert space* $\mathfrak{H}$, *a cyclic vector* $\Omega \in \mathfrak{H}$ *and a strongly continuous unitary representation* U *of* $\mathbb{R}$ *on* $\mathfrak{H}$ *such that*

(1) $\omega(P) = (\Omega, \pi(P)\Omega)$,
(2) $U(t)\Omega = \Omega$,
(3) $U(t)\pi(P)U(-t) = \pi(\gamma_t(P))$,

and if we identify $\mathfrak{A}$ *as a subalgebra of* $\mathfrak{B}(\mathfrak{A})$ *by* $A \in \mathfrak{A} \mapsto (A, 0) \in \mathfrak{B}(\mathfrak{A})$ *and* π_0 *is the restriction of* π *to* $\mathfrak{A}$ *it follows that*

(4) $$\omega((A_1, t_1)(A_2, t_2) \cdots (A_k, t_k)) = (\Omega, \pi_0(A_1)U(t_2 - t_1)\pi_0(A_2) \cdots U(t_k - t_{k-1})\pi_0(A_k)\Omega).$$

Furthermore, conditions (1)–(3) *determine* π *and* U *up to unitary equivalence.*

This proposition gives no information on which functions G define states on $\mathfrak{B}(\mathfrak{A})$ through the formula

$$G(A_1, \ldots, A_k; t_1, \ldots, t_k) = \omega((A_1, t_1)(A_2, t_2) \cdots (A_k, t_k))$$

and Theorem 6.3.27 gives the first complete characterization of the two-point functions for this to be true, although [Win 3] and [Bra 16] contain partial characterizations. The technique of dilating the map $t \mapsto X_t$ to a unitary group $t \mapsto U_t$ used in the proof of this theorem goes back to Naimark in 1943 [Nai 3]. An exposition of this and other dilation theorems can be found in [[Eva 1]] and, less complete, in [[Rie 1]]. The separating character of the vector in Theorem 6.3.28 was demonstrated in [Win 3] and the example in the subsequent warning is due to Kishimoto. The reader should be aware that Theorem 2 in [Bra 16] is erroneous, due to disregarding this warning. The semi-abstract setting discussed prior to Proposition 6.3.29 was introduced in [Bra 16], and this proposition and the associated corollary and remark are taken from this paper, although very similar results occur in [Win 3].

The main theorem in Section 6.3.4.2 on Bose gases with repulsive interactions appeared in [Bra 17], and all the estimates in the subsequent lemmas are taken from [Bra 16].

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List of Symbols

Standard Notation

$\mathfrak{A}, \mathfrak{B}, \mathfrak{C}$	C^*-algebras
$\mathfrak{M}, \mathfrak{N}, \mathfrak{Z}$	von Neumann algebras
$\mathfrak{I}$	ideals in C^* and von Neumann algebras
A, B, C	elements in C^* and von Neumann algebras
ω, φ	states
$\tau, \gamma, \alpha, \sigma$	automorphisms or groups of automorphisms
$\mathfrak{H}, \mathfrak{K}$	Hilbert spaces
π	a *-morphism
Ω, ξ, η, ψ	vectors in Hilbert space
P, E, F	orthogonal projections
G	a group
Λ	a bounded region in a Euclidean space or on a lattice
μ, ν	measures

Special Symbols

Roman numerals I and II refer to Volume I and II, respectively, and arabic numerals refer to the page number of the first occurrence in the second editions of the symbol.

$\lvert A \rvert$	Absolute value of A	I 34
$\lVert A \rVert$	C^*-norm of A	I 20

$A_+,\ A_-$	Positive and negative part of A	I 35
A^*	Adjoint of A	I 19
A^{-1}	Inverse of A	I 25
$\hat{A}$	Gelfand transform of A	I 63
$\hat{A}$	Affine functional defined by A	I 339
$[A,\ B]$	Commutator $= AB - BA$	
$\{A,\ B\}$	Anticommutator $= AB + BA$	
$(A,\ B)_\sim$	Canonical correlation	II 94
$A(K)$	The real affine continuous functions on the compact convex set K	I 321
$A(G)$	The almost periodic functions over G	II 36
$A(p),\ A^*(p)$	Fields in momentum space	II 448
$a(f)$	Annihilation operator on Fock space	II 8
$a^*(f)$	Creation operator on Fock space	II 8
$a^{\#}(f)$	Annihilation or creation operator on Fock space	II 9
$a_+(f),\ a_-(f)$	Bose/Fermion annihilation operator on Fock space	II 9
$a_+^*(f),\ a_-^*(f)$	Bose/Fermion creation operator on Fock space	II 9
$a_\pm^{\#}(f)$	Bose/Fermion annihilation or creation operator on Fock space	II 9
$a_\pm(x)$	Annihilation field operator valued distribution	II 10
$a_\pm^*(x)$	Creation field operator valued distribution	II 10
$a_\omega(f)$	Annihilation operator in representation defined by ω	II 25
$a_\omega^*(f)$	Creation operator in representation defined by ω	II 25
a_x, a_x^*	Spin lowering and raising operators	II 258, 425
$\tilde{\mathfrak{A}}$	Unit extension of $\mathfrak{A}$	I 23
$\mathfrak{A}_+$	The positive part of $\mathfrak{A}$	I 32
$\bigotimes_{i=1}^{n} \mathfrak{A}_i$	Finite tensor product of C^*-algebras	I 144
$\bigotimes_{\alpha} \mathfrak{A}_\alpha$	Infinite tensor product of C^*-algebras	I 145
$\mathfrak{A} \otimes_\tau G$	C^*-cross product	I 138
$(\mathfrak{A}, G, \tau)$	C^*-dynamical system	I 136
$(\mathfrak{A}, \tau)$	C^*-dynamical system with $G = \mathbb{R}$	II 76
$\mathfrak{A}_-(\mathfrak{h}), \mathfrak{A}(\mathfrak{h})$	CAR algebra over $\mathfrak{h}$	II 15
$\mathfrak{A}_+(H), \mathfrak{A}(H)$	CCR algebra over H	II 20
$\mathfrak{A}_\tau$	Entire analytic elements for τ	II 76
$\mathfrak{A}^\tau$	Fixed point algebra under action τ	
$\mathfrak{A}_\Lambda$	Local algebra over Λ	II 240
$\hat{\alpha}_\gamma$	Dual action of α_t	I 140
$\alpha_\Lambda(\omega)$	Characteristic function on path space	II 377
$B_{\mathfrak{A}}$	The positive linear functionals on $\mathfrak{A}$ with norm less than or equal to one	I 53

$B(f)$	Fermion field operator	II 17
$B(\chi)$	Fourier coefficients of B	II 206
B_ξ	Banach space of interactions	II 242
B_λ	Banach space of translationally invariant interactions	II 297
$b(\mu)$	Barycenter of μ	I 323
$\mathfrak{B}(\mathfrak{A})$	Free algebra over $\mathfrak{A}$	II 460
β	Inverse temperature	II 5
β_c	Critical inverse temperature	II 331
$\beta_\pm$	Inverse scattering morphisms	II 164
$C_0(X)$	The continuous complex functions on the locally compact Hausdorff space X vanishing at infinity	I 21
$C(X)$	The continuous complex functions on the compact Hausdorff space X	I 21
$C_b(X)$	The bounded continuous complex functions on X	I 24
$C^*(\mathfrak{A}, \tau)$	C^*-crossed product	I 138
C_0	Weakly continuous	I 164
C_0^*	Weakly* continuous	I 164
$Co(\tau_G(A))$	The convex hull of $\{\tau_g(A); g \in G\}$	I 381
C^m	The m times continuously differentiable functions or states	II 37
$\mathbb{C}$	The complex numbers	
$C_{fin}(\Omega_\beta)$	Continuous functions depending on a finite number of coordinates	II 367
$C_\varphi^1(G)$	Functions generated by expectations	II 202
$C_\varphi^2(G)$	Functions generated by expectations	II 206
C_Λ^ω	States asymptotically equal to ω	II 282
c	Lattice configuration	II 329
$\mathfrak{C}_\omega$	Centralizer of ω	II 113
$\mathfrak{C}_\Lambda$	Local algebra of classical lattice system	II 240
$\mathfrak{C}_\Lambda$	Element of isotonic family	II 409
$D(S)$	Domain of linear operator S	
$D(G)$	Domain of graph G	I 186
$(D\psi: D\varphi)_t$	Connes' Radon-Nikodym cocycle	I 147
$D(X)$	Diameter of X	II 242
$d\Gamma(H)$	Second quantization map	II 8
$d(y, \Lambda)$	Distance from y to Λ	II 374
$d\mu^{\sigma,\Lambda,\beta}_{x^m u^n,\, y^m v^n}, (\omega^m, \tilde{\omega}^n)$	Measure on composite paths	II 384
$d\tilde{\omega}$	Path space measure	II 386
$\mathfrak{D}_\beta$	Strip in $\mathbb{C}$	II 81
$\mathfrak{D}_\alpha^{(n)}$	Tube in $\mathbb{C}^n$	II 150
Δ	Modular operator	I 89
$\Delta_{\xi 1,\, \xi 2}$	Relative modular operator	I 109
$\Delta_\mu(A)$	Root mean square deviation	I 349

Δ_Φ	Set of translationally invariant maximal entropy states	II 294
$-\nabla^2$	The Laplacian $= -\sum_{i=1}^{\nu} \frac{\partial^2}{\partial x_i^2}$	II 49
δ_ω	Unit point measure on ω	I 322
δ_Λ	Generator of local evolution	II 244
δ_Φ	Derivation defined by Φ	II 259
$\partial_f(K)$	Boundary set of f	I 326
∂F_x	Derivative of F at x	II 297
$\partial\Lambda$	Boundary of Λ	II 55
$E_{\mathfrak{A}}$	State space of $\mathfrak{A}$	I 53
$E_{\mathfrak{A}}^G$	The G-invariant states on $\mathfrak{A}$	I 374
E_ω	Projection onto $U_\omega(G)$-invariant vectors	I 381
E_ω^τ	The invariant state extensions	II 201
E_χ	Projection onto eigensubspace of regular representation	II 208
$E_\Phi(x)$	Energy of interaction at point x	II 242
E_Λ	Projection onto local subalgebra	II 246
E_Φ	Mean energy at 0 for a translationally invariant interaction Φ	II 291
$:e^{i\varphi(f)}:$	Wick ordered exponential	II 458
$e_{ij}^{(k)}$	Matrix units in CAR algebra	II 16
$e(i_x, j_x)$	Matrix units in lattice systems	II 306
$\mathscr{E}(K)$	The extremal points of the convex set K	I 318
$\mathscr{E}$	Banach space of path space functions	II 390
$\varepsilon(\beta, z)$	Local energy per unit volume	II 53
ε^π	Combinatorial factor	II 385
F	$F = J\Delta^{-1/2}$	I 89
$F_{\mathfrak{A}}$	The set of factor states on $\mathfrak{A}$	I 372
F_ω	$F_\omega = [\pi_\omega(\mathfrak{A}')E_\omega]$	I 383
$F_{A,B}(t)$	$F_{A,B}(t) = \omega(A\tau_t(B))$	II 81, 178
$F(\omega), F_\Lambda(\omega)$	Free energy functional on matrix algebra, $F_\Lambda(\omega) = \beta^{-1}S_\Lambda(\omega) - \omega(H_\Phi(\Lambda))$	II 90, 269
$F_\Lambda(\beta\Phi)$	Free energy on matrix algebra $F_\Lambda(\beta\Phi) = -\beta^{-1}\log \mathrm{Tr}_\Lambda\left(e^{-\beta H_\Phi(\Lambda)}\right)$	II 269
$F_{\beta\Phi}(\omega)$	Mean free energy functional, $F_{\beta\Phi}(\omega) = S(\omega) - \beta H_\Phi(\omega)$	II 292
$F(\Phi)$	Thermodynamic mean free energy	II 292

$\bar{f}(\omega)$	Upper envelope of f	I 326
$\{f, g\}$	Poisson bracket	II 232
$f_\Phi(\Psi)$	Tangential functional to mean free energy	II 302
$\mathfrak{F}(\mathfrak{h})$	Fock space over $\mathfrak{h}$	II 7
$\mathfrak{F}_\pm(\mathfrak{h})$	Bose/Fermi Fock space over $\mathfrak{h}$	II 7
$(\mathfrak{F}, \mathfrak{A}, G, \tau, \gamma, \sigma)$	Field system	II 197
$\mathfrak{F}_\pm(\Lambda)$	Bose/Fermi Fock space over $L^2(\Lambda)$	II 355
$\Phi(f)$	Bose field operator on Fock space	II 12
$\Phi_\omega(f)$	Bose field operator in representation given by ω	II 24
$\Phi(X)$	Spin system interaction	II 241
$\|\|\Phi\|\|_\xi$	Norm on spin interaction	II 242
$\|\|\Phi\|\|_\lambda$	Norm on spin interaction	II 247, 252
$\Phi(x_i - x_j)$	Translationally invariant two-body potential	II 358
$\Phi^{(k)}(x_1, \ldots, x_k)$	k-body potential	II 358
$\Phi(x)$	Free Euclidean field operator valued distribution	II 448
$:\Phi(x)^n:$	Wick ordered power of field	II 448, 458
$\varphi^{(A,B)}$	$\varphi^{(A,B)}(g) = \varphi(A\gamma_g(B))$	II 206
$G(S)$	Graph of the linear operator S	I 186
$\hat{G}$	Dual group of the abelian locally compact group G	I 249
$G_{A,B}(t)$	$G_{A,B}(t) = \omega(\tau_t(A)B) - \omega(A)\omega(B)$	II 83, 178
G_φ	Stabilizer group of φ	II 202
$G_\Lambda(A_0, \ldots, A_n, t_1, \ldots, t_n)$	Finite volume Green functions	II 403
$G_\Lambda(A^m; \xi^m)$	Finite volume Green functions	II 403
$G_\Lambda(A, B; t)$	Finite volume Green functions	II 404
$G(A, B; t)$	Infinite volume Green function	II 404
$\|\|g\|\|_N$	Covariance of free Euclidean measure	II 448
$\Gamma(\mathfrak{M})$	Invariant Γ of $\mathfrak{M}$	I 149
$\Gamma(\alpha)$	Γ-spectrum of α	I 310
$\Gamma(U)$	Second quantization map	II 8
Γ_t	Unitary cocycle	II 127
Γ_t^P	Unitary cocycle defined by the perturbation P	II 145
(γ, t)	$\gamma \in \hat{G}$ acting on $t \in G$	I 250
γ_B	$\gamma_B(A) = B^*AB - \{B^*B, A\}/2$	II 91
$\gamma_\pm$	Scattering morphisms	II 160
γ	Contour in lattice system	II 321
$\|\gamma\|$	ν-1-dimensional area of contour	II 322
H_Λ	Self adjoint extension of the Laplacian on $L^2(\Lambda)$	II 49
H^0	Laplacian with Neumann boundary conditions	II 55
H^σ	Laplacian with σ-boundary conditions	II 55
H^∞	Laplacian with Dirichlet boundary conditions	II 55

H^{per}	Laplacian with periodic boundary conditions	II 55
$H_{A,B}(t)$	$H_{A,B} = F_{A,B} - G_{A,B}$	II 185
$H_\Phi(\Lambda)$	Finite volume Hamiltonian	II 241
$\tilde{H}(\Lambda)$	Locally correct Hamiltonian	II 245
$H_\Phi(\omega)$	Mean energy functional on the translationally invariant state ω	II 291
(H)	Condition (H)	II 410
H	Macroscopic external field strength	II 318
$H(\Phi)$	Ground state energy functional	II 347
$H_{\sigma,\Lambda}$	Total finite volume Hamiltonian	II 356
$H^{(n)}_{\sigma,\Lambda}$	n-particle part of $H_{\sigma,\Lambda}$	II 357
$\hbar$	Planck's constant	I 4
$h(x)$	Microscopic external field strength at x	II 319
$h^{(n)}_{\sigma,\Lambda}$	Form associated to $H^{(n)}_{\sigma,\Lambda}$	II 361
$(\mathfrak{H}, \pi)$	Representation on $\mathfrak{H}$	I 43
$(\mathfrak{H}, \pi, \Omega)$	Cyclic representation on $\mathfrak{H}$ with cyclic vector Ω	I 45
$(\mathfrak{H}_\omega, \pi_\omega, \Omega_\omega)$	Cyclic representation defined by the state ω	I 57
$\mathfrak{H}_\omega$	Hilbert space in cyclic representation defined by ω	I 57
$\bigotimes_{i=1}^{n} \mathfrak{H}_i$	Finite tensor product of Hilbert spaces	I 143
$\bigotimes_\alpha^{\Omega_\alpha} \mathfrak{H}_\alpha$	Infinite tensor product of Hilbert spaces	I 144
$\mathfrak{H}_\Lambda$	Bounded domain Hilbert space	II 240
$\overline{\mathfrak{H}}$	Conjugate Hilbert space of $\mathfrak{H}$	I 70
$\mathfrak{h}^n$	n-fold tensor product of $\mathfrak{h}$ with itself	II 7
$\mathfrak{h}^n_+, \mathfrak{h}^n_-$	Symmetrized/antisymmetrized part of $\mathfrak{h}^n$	II 7
I	Identity on a Banach space	
$\mathbb{1}$	Identity of an operator algebra	I 21
$\mathfrak{I}^U_Y$		I 250
$\imath$	Identity automorphism of an operator algebra	
J	Modular conjugation	I 89
J_{ξ_1,ξ_2}	Relative modular conjugation	I 109
$j(A)$	$j(A) = JAJ$	I 102
$j(x, y)$	Ising interaction	II 257, 319
K_μ	Modified Hamiltonian, $K_\mu = H - \mu N$	II 46
K_β	The set of KMS states at value β	II 113
K_∞	The set of ground states	II 131
$\mathfrak{K}(\mathfrak{A}, G)$	Continuous functions $G \mapsto \mathfrak{A}$ with compact support	I 137

$\kappa_\mu(f)$		I 341
$L^p(\mu), L^p(X,\mu)$	L^p-spaces of complex functions	I 83
$L^p(X,G)$	The L^p-functions from the locally compact group G into the Banach space X	I 138
$L^1(\mathfrak{A}_0)$	Notion of asymptotic abelianness	II 160
$L^P(\omega)$	Work in cyclic process	II 213
L	Lattice	II 239
$L^1_{\text{loc}}(\mathbb{R}^\nu \backslash S)$	Local L^1-space	II 360
$\mathscr{L}(X)$	The bounded linear operators on the Banach space X	I 20
$\mathscr{L}\mathscr{C}(\mathfrak{H})$	The compact operators on $\mathfrak{H}$	I 21
$\mathscr{L}_*(\mathfrak{H})$	The predual of $\mathscr{L}(\mathfrak{H})$	I 69
$\lvert \Lambda \rvert$	Area of Λ, or number of points in Λ	
Λ^c	Complement of Λ	
λ	Thermal wavelength, $\lambda = (4\pi\beta)^{1/2}$	II 53
$M_+(K)$	The positive Radon measures on the convex compact set K	I 321
$M_1(K)$	The probability measures on K	I 321
$M_\omega(K)$	The probability measures with barycenter ω	I 323
$M(A)$	Mean of A	I 383
$M(\beta, h_x)$	Mean magnetization of atom at point x	II 314
M	Overall magnetization	II 318
$\overline{M}(h)$	Maximum mean magnetization	II 335
$\mathfrak{M}', \mathfrak{M}''$	Commutant, and bicommutant respectively, of set $\mathfrak{M}$	I 71
$[\mathfrak{M}\mathfrak{K}]$	The closed linear span of $\mathfrak{M}\mathfrak{K}$, or the projection into this	I 72
$\mathfrak{M}_*$	The predual of $\mathfrak{M}$	I 75
$(\mathfrak{M}, G, \tau)$	W^*-dynamical system	I 136
$(\mathfrak{M}, \tau)$	W^*-dynamical system with $G = \mathbb{R}$	II 77
$\mathfrak{M} \otimes_\tau G$	W^*-crossed product	I 139
$\mathfrak{M}^\tau$	The fixed point algebra under the action τ	II 113
$\mathfrak{M}_\tau$	The entire analytic elements for the action τ	I 78
$\bigotimes_{i=1}^{N} \mathfrak{M}_i$	Finite W^*-tensor product	I 144
$\bigotimes_\alpha^{\Omega_\alpha} \mathfrak{M}_\alpha$	Infinite W^*-tensor product	I 144
$\mathfrak{M}_E$	$\mathfrak{M}_E = E\mathfrak{M}E$	I 389
$\mu \vee \nu$	Least upper bound	I 323
$\mu \wedge \nu$	Greatest lower bound	I 323
$\mu \succ \nu$	Choquet ordering	I 325
$\mu \succcurlyeq \nu$	Bishop-de Leeuw ordering	I 458
μ	Chemical potential	II 5

μ_A	Spectral measure of automorphism group in invariant state	II 88
μ_K	KMS-measure on $E_{\mathfrak{A}}$	II 117
μ_C	Central measure	II 117
μ_E	Measure of ergodic decomposition	II 120
μ_X	Maximal measure on $E_{\mathfrak{A}}$	II 131
$\mu^{\beta}_{x,y}$	Conditional Wiener measure	II 368
μ_x	Wiener measure	II 369
$\mu^{\sigma,\Lambda,\beta}_{x,y}$	Conditional finite volume Wiener measure with boundary conditions σ	II 375
μ	$\mu = (-\nabla^2 + m^2)^{1/2}$	II 449
$\mu_{\sigma,\Lambda}$	Finite volume Euclidean Gibbs measure	II 449
μ_w	Gaussian measure with square mean W	II 458
$N_{\mathfrak{A}}$	The normal states on the C^*-algebra $\mathfrak{A}$ on a Hilbert space	I 131
N^G_ω	The G-invariant, ω-normal states on $\mathfrak{A}$	I 385
N	Number operator on Fock space	II 7
N_f	$N_f = a^*(f)a(f)$	II 26
$N_{\omega,f}$	$N_{\omega,f} = a^*_\omega(f)a_\omega(f)$	II 27
N_ω	Number operator on $\mathfrak{H}_\omega$	II 31
$\hat{N}(\omega)$	Number functional, $\hat{N}(\omega) = \hat{\omega}(N_\omega)$	II 37
$\hat{N}_\Lambda(\omega)$	Local number functional	II 52
N_Λ	Local number operator	II 363
$NN(\Lambda)$	Set of nearest neighbours in Λ	II 321
$n_{\omega,f}$	$n_{\omega,f}(\psi) = \|\|a_\omega(f)\psi\|\|^2$	II 27
n_ω	Form associated to N_ω	II 30
n_Λ	$n_\Lambda = \sum_{x\in\Lambda} a^*_x a_x$	II 425
ν_A	Spectral measure of automorphism group in invariant state	II 88
$O(t)$	Order t	I 202
$o(t)$	Smaller order than t	I 202
$\mathcal{O}_\omega(E_{\mathfrak{A}})$, $\mathcal{O}_\omega$	The orthogonal probability measures on $E_{\mathfrak{A}}$ with barycenter ω	I 340
$\mathcal{O}_n$	Cuntz' algebra	II 110
Ω_ω	Cyclic vector associated to the state ω	I 57
Ω^P	Perturbed vector	II 149
Ω_β	Path space	II 367
Ω^α_β	Space of Hölder continuous paths	II 369
Ω	Path space	II 368
$\Omega_{\Lambda,\beta}$	Space of bounded paths	II 375
ω_Ω	Vector state associated to the vector Ω	I 48
$\omega_1 \perp \omega_2$	Orthogonal states	I 340
$\omega_1 \overset{\downarrow}{\circ} \omega_2$	Disjoint states	I 370
ω_F	Fock vacuum state	II 44
ω_T	Truncated state	II 39, 43

ω_Λ, ω_Λ^Φ	Local Gibbs state	II 50, 61, 263, 377
$\hat{\omega}$	Normal extension of ω to $\pi_\omega(\mathfrak{A})''$	II 80
$\tilde{\omega}$	Extension of ω to $\tilde{\mathfrak{A}}$	II 116
ω^P	Perturbed (KMS-) state	II 149
ω_A	Quasi-free state	II 219
$\omega_{\sigma,\Lambda}^{\beta,\mu}$	Local Gibbs state for interacting quantum gas	II 381
$\omega_\sigma^{\beta,\mu}$	Infinite volume limit of $\omega_{\sigma,\Lambda}^{\beta,\mu}$	II 381
ω^m	Family of m trajectories	II 384
$\hat{P}_\omega$	Projection onto U_ω-almost periodic vectors	I 408
$P_\pm$	Projection onto even/odd subspaces of Fock space	II 7
$P(\beta, z)$	Thermodynamic pressure	II 53
$P_\pm^x$	$P_\pm^x = (\mathbb{1} \pm \sigma_3^x)/2$	II 320
$P(\Phi)_2$	Polynomial local interaction	II 449
$p_\Phi(x)$	$p_\Phi(x) = \sum_{X \ni x} \|\|\Phi(X)\|\|$	II 244
$p(x, y; t)$	$p(x, y, t) = (e^{t\nabla^2})(x, y)$	II 367
$p_{\sigma,\Lambda}(x, y; t)$	$P_{\sigma,\Lambda}(x, y; t) = (e^{-tT_{\sigma,\Lambda}^{(1)}})(x, y)$	II 373
$p_{\mathrm{per},\Lambda}(x, y; t)$	Green function with periodic boundary conditions	II 380
$\mathscr{P}, \mathscr{P}_\Omega$	Natural positive cone	I 102
$\mathscr{P}_I$	Partition of I into ordered subsets	II 39
$\Pi(f)$	Bose field operator on Fock space, $\Pi(f) = \Phi(if)$	II 12
π_ω	The *-morphism in the cyclic representation defined by ω	I 53
$\pi_1 \simeq \pi_2$	Unitarily equivalent representations	I 48
$\pi_1 \approx \pi_2$	Quasi-equivalent representations	I 80
$\pi_1 \mathrel{\underset{\circ}{\perp}} \pi_2$	Disjoint representations	I 370
$R(S)$	Range of linear operator S	
$R(G)$	Range of the graph G	I 186
$\mathbb{R}$	The real numbers	
$\mathbb{R}_+$	The non-negative real numbers	
$\rho(A)$	Spectral radius of A	I 26
$\rho(\beta, z)$	Particle density	II 52
$\rho_\Lambda(\beta, z)$	Finite volume particle density	II 56
$\rho_c(\beta)$	Critical density of Bose gas	II 64
$\rho_0(\beta)$	Density of Bose-Einstein condensate	II 69
$\tilde{\rho}_{\sigma,\Lambda}^U(y^m; x^m)$, $\tilde{\rho}_\Lambda(y^m; x^m)$	Finite volume reduced density matrix	II 382
$\overline{\rho}_\Lambda$	Density matrix of finite volume Gibbs state	II 383
$\rho_\Lambda(\omega^m)$	Density functional on trajectories	II 384
$\rho_\Lambda(\beta, z; q^n, x^n)$	Finite volume particle-density correlation functions	II 457

S	$S = J\Delta^{1/2}$	I 89
S_{ξ_1, ξ_2}	$S_{\xi_1, \xi_2} = J_{\xi_1, \xi_2}\Delta^{1/2}_{\xi_1, \xi_2}$	I 109
$S(\mathfrak{M})$	Invariant S of $\mathfrak{M}$	I 149
$S(K)$	The real continuous convex functions on the compact convex set K	I 321
$S_\lambda(U)$	Convex combinations of $U(g)$'s	I 382
$S_\lambda(\tau(A))$	Convex combinations of $\tau_g(A)$'s	I 382
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