CHAPTER 3

Equilibrium States

3.1. States for finite systems

We start by describing states for finite systems, i.e. systems with finitely many sites. Later we will consider states for infinite systems with no reference to a Hilbert space. But for now we have a finite-dimensional Hilbert space $\mathcal{H}$ with an inner product $\langle \cdot, \cdot \rangle$ and norm $\|v\| = \langle v, v \rangle^{1/2}$. We let $\mathcal{B}(\mathcal{H})$ be its space of bounded operators, i.e. the space of linear maps $A : \mathcal{H} \to \mathcal{H}$ which have finite operator norm

$$\|A\| = \sup_{v \in \mathcal{H}} \|Av\| / \|v\|. \tag{3.1}$$

An operator $A \in \mathcal{B}(\mathcal{H})$ is called positive-semi-definite if it can be written $A = B^* B$ for some $B \in \mathcal{B}(\mathcal{H})$. One can show (using the spectral theorem) that this is equivalent to $\langle v, Av \rangle \geq 0$ for all $v \in \mathcal{H}$.

A **state** on $\mathcal{H}$ is a positive, normalised linear functional on $\mathcal{B}(\mathcal{H})$; that is, it is a map $\langle \cdot \rangle : \mathcal{B}(\mathcal{H}) \to \mathbb{C}$ that is

(i) linear: $\langle sA + tB \rangle = s\langle A \rangle + t\langle B \rangle$ for all $s, t \in \mathbb{C}$ and $A, B \in \mathcal{B}(\mathcal{H})$;
(ii) positive: $\langle A^* A \rangle \geq 0$ for all $A \in \mathcal{B}(\mathcal{H})$;
(iii) normalised: $\langle \mathbb{1} \rangle = 1$.

One can check that the operator norm $\|\langle \cdot \rangle\| = \sup_{A \in \mathcal{B}(\mathcal{H})} |\langle A \rangle| / \|A\|$ of any state $\langle \cdot \rangle$ is 1. It turns out that states on Hilbert spaces can be represented by density operators, a very useful property. A **density operator** ρ is a trace-class (meaning that $\operatorname{Tr} |\rho| < \infty$) positive-definite hermitian operator such that $\operatorname{Tr} \rho = 1$. Given a density operator, there corresponds the state

$$\langle A \rangle = \operatorname{Tr} \rho \, A. \tag{3.2}$$

The converse is also true, that is, each state is represented by a density operator.

Proposition 3.1 (**Riesz representation of states**). *Let $\langle \cdot \rangle$ be a state on a finite-dimensional Hilbert space $\mathcal{H}$. Then there exists a unique density operator ρ such that $\langle A \rangle = \operatorname{Tr} \rho A$ for all $A \in \mathcal{B}(\mathcal{H})$.*

Proof of Proposition 3.1. Let us introduce the Hilbert-Schmidt inner product that turns $\mathcal{B}(\mathcal{H})$ into a Hilbert space:

$$\langle A, B \rangle_{\mathrm{HS}} = \operatorname{Tr} A^* B. \tag{3.3}$$

for all $A, B \in \mathcal{B}(\mathcal{H})$. The standard Riesz representation theorem implies that $\mathcal{B}(\mathcal{H})$ is self-dual, that is, every linear functional $\langle \cdot \rangle : \mathcal{B}(\mathcal{H}) \to \mathbb{C}$ is represented by a unique operator ρ such that

$$\langle A\rangle = \langle \rho, A\rangle_{\mathrm{HS}} = \operatorname{Tr} \rho^* A. \tag{3.4}$$

for all $A \in \mathcal{B}(\mathcal{H})$. We check that if $\langle\cdot\rangle$ is a state, then ρ is a density operator. We have for all $\varphi \in \mathcal{H}$ with $\|\varphi\| = 1$ that

$$\langle \varphi, \rho^* \varphi\rangle = \operatorname{Tr} P_\varphi \rho^* = \langle P_\varphi\rangle = \langle P_\varphi^2\rangle \geq 0. \tag{3.5}$$

(Here, P_φ denotes the projector onto φ.) Then ρ^* is positive-definite; it is therefore hermitian (Exercise 3.1) so $\rho \geq 0$ as well. Finally, $\operatorname{Tr} \rho = \operatorname{Tr} \rho \mathbb{1} = \langle \mathbb{1}\rangle = 1$. □

Note that the "Gibbs state" $\langle A\rangle_{\Lambda,\beta,h} = \frac{1}{Z_{\Lambda,\beta,h}} \operatorname{Tr} A\, \mathrm{e}^{-\beta H_{\Lambda,h}}$ of (1.39) is indeed a state in the sense of the definition above (the Hilbert space $\mathcal{H}_\Lambda$ is finite-dimensional). The only condition which may not be obvious is the positivity, see Exercise 3.5.

The set of states is *convex*: If $\langle\cdot\rangle_1, \langle\cdot\rangle_2$ are two states, the convex combination $t\langle\cdot\rangle_1 + (1-t)\langle\cdot\rangle_2$ is also a state for all $t \in [0,1]$. A state is **mixed** if it can be written as a convex combination of distinct states. A state is **pure** if it is not mixed; in other words, pure states are the extremal points of the convex set of states.

Given $\varphi \in \mathcal{H}$ with $\|\varphi\| = 1$, the corresponding projector $P_\varphi = |\psi\rangle\langle\psi|$ is a special case of a density operator, hence it gives a state. It is perhaps expected that this state is pure, and that all pure states are represented by projectors.

PROPOSITION 3.2. *A state is pure if and only if its density operator is equal to P_φ for some $\varphi \in \mathcal{H}$.*

(That $\|\varphi\| = 1$ follows from the properties of states.)

PROOF. The density operator ρ of the state is hermitian and it can be written as

$$\rho = \sum_{i=1}^n \lambda_i P_{\varphi_i}, \tag{3.6}$$

where the φ_is form an orthonormal basis of eigenvectors. This can be viewed as a convex combination of density operators. This shows that if ρ is not equal to a projector, then the corresponding state is mixed.

It remains to show that if $\rho = P_\varphi$ is a projector, then the state is pure. Assume that $\langle\cdot\rangle = t\langle\cdot\rangle_1 + (1-t)\langle\cdot\rangle_2$ with $t \in (0,1)$. By Proposition 3.1, there exist density matrices ρ_1, ρ_2 such that $\langle\cdot\rangle_i = \operatorname{Tr} \rho_i \cdot$ for $i = 1, 2$. Then

$$P_\varphi = t\rho_1 + (1-t)\rho_2. \tag{3.7}$$

We have

$$\begin{aligned} 1 = \operatorname{Tr} \rho = \operatorname{Tr} P_\varphi = \operatorname{Tr} P_\varphi^2 &= \operatorname{Tr} P_\varphi\bigl(t\rho_1 + (1-t)\rho_2\bigr) \\ &= t\langle \varphi, \rho_1\varphi\rangle + (1-t)\langle\varphi, \rho_2\varphi\rangle \leq t + (1-t) = 1. \end{aligned} \tag{3.8}$$

In the last inequality we used that for any density matrix ρ and any vector φ, we have that $\langle\varphi, \rho\varphi\rangle \leq \|\varphi\|^2$ as can easily be checked. Equality holds here only if ρ is the projector onto the subspace spanned by φ. Since equality must hold for both ρ_1 and ρ_2 in (3.8), we conclude that $\rho_1 = \rho_2 = P_\varphi = \rho$ as claimed. □

3.2. Gibbs states in Hilbert spaces

We now discuss equilibrium (or Gibbs) states in the context of a Hilbert space $\mathcal{H}$. The main example is $\mathcal{H} = \mathcal{H}_\Lambda$. Let $H = H^* \in \mathcal{B}(\mathcal{H})$ be a Hermitian operator, which we call a **Hamiltonian**. Since it is Hermitian, H has only real eigenvalues. For $\beta \geq 0$, we define the **Gibbs state** with Hamiltonian H (at inverse temperature β) as the state $\langle\cdot\rangle_{H,\beta}$ with density matrix

$$\rho = \frac{1}{Z_\beta}\,\mathrm{e}^{-\beta H}\,, \qquad Z_\beta = \mathrm{Tr}\;\mathrm{e}^{-\beta H}\,. \tag{3.9}$$

Explicitly,

$$\langle A\rangle_{H,\beta} = \frac{1}{Z_\beta}\mathrm{Tr}\,A\,\mathrm{e}^{-\beta H}\,. \tag{3.10}$$

The normalizing factor Z_β is called the **partition function**. The Gibbs state arises through the following four characterizations. Each of the four characterizations carries over to infinite systems, with suitable adjustements, as will be discussed in later sections.

PROPOSITION 3.3. *The Gibbs state $\langle\cdot\rangle_{H,\beta}$ is the unique state $\langle\cdot\rangle = \mathrm{Tr}\,\cdot\,\rho$ satisfying any of the following four conditions:*

(a) Tangent condition: *Let $F_\beta(H) := -\frac{1}{\beta}\log\mathrm{Tr}\;\mathrm{e}^{-\beta H}$. Then*

$$F_\beta(H+A) \leq F_\beta(H) + \langle A\rangle$$

for all $A = A^* \in \mathcal{B}(\mathcal{H})$.

(b) Gibbs variational principle: *The density matrix ρ minimizes the function*

$$\mathcal{F}_\beta(\rho) := \mathrm{Tr}\,H\rho + \tfrac{1}{\beta}\mathrm{Tr}\,\rho\log\rho.$$

(c) KMS condition: *Define the time evolution*

$$\alpha_t(A) = \mathrm{e}^{\mathrm{i}tH}\,A\,\mathrm{e}^{-\mathrm{i}tH}\,, \qquad t \in \mathbb{C}. \tag{3.11}$$

Then

$$\langle AB\rangle = \big\langle B\,\alpha_{\mathrm{i}\beta}(A)\big\rangle$$

for all $A, B \in \mathcal{B}(\mathcal{H})$.

(d) RAS condition: *For all $A \in \mathcal{B}(\mathcal{H})$ such that $\langle AA^*\rangle > 0$,*

$$\langle A^*[H,A]\rangle \geq \frac{1}{\beta}\langle A^*A\rangle\log\frac{\langle A^*A\rangle}{\langle AA^*\rangle} \tag{3.12}$$

The first two conditions are common also in classical statistical mechanics, while the last two are mainly encountered for quantum systems. Regarding the tangent condition, one can prove that

PROPOSITION 3.4. *The free energy F_β is a concave function: $F_\beta(\theta H + (1-\theta)K) \geq \theta F_\beta(H) + (1-\theta)F_\beta(K)$ for $\theta \in [0,1]$.*

This follows from the Golden–Thompson and Hölder inequalities. The tangent condition may be interpreted geometrically as saying that $\langle\cdot\rangle$ defines a supporting hyperplane at H. Note also that $F_\beta(H + sA)$ is differentiable in s for any A and that $\frac{\mathrm{d}}{\mathrm{d}s}F_\beta(H + sA)\big|_{s=0} = \langle A\rangle$, so the hyperplane at H is indeed the Gibbs state.

In the variational principle, the expression to be minimized may be written as $U - TS$ where $U = \mathrm{Tr}\, H\rho$ is the energy and $S = -\mathrm{Tr}\, \rho \log \rho$ the entropy in the state ρ (and $T = \frac{1}{\beta}$ is the temperature). This form is common in thermodynamics. The condition also extends naturally to the **ground state** (zero temperature) case $\beta = \infty$, where the problem becomes to minimize $\mathrm{Tr}\, H\rho$. It is not hard to see that this is achieved by any density matrix ρ which is restricted to the eigenspace for H with lowest eigenvalue. We can write this as $\rho \le P_{E_0}$ where P_{E_0} is the projector onto the latter eigenspace.

In the KMS condition (named after Kubo, Martin and Schwinger) the evolution operators α_t, $t \in \mathbb{R}$, are related to the Heisenberg framework of quantum mechanics. Note that we need to allow complex values of the 'time' parameter t.

Finally, the RAS condition (named after Roepstorff, Araki and Sewell) also extends straightforwardly to the ground state $\beta = \infty$, where the condition becomes $\langle A^*[H, A]\rangle \ge 0$. The intuition becomes clearer if we take $\langle\cdot\rangle$ to be a pure state with density matrix $\rho = |\phi\rangle\langle\phi|$ with $|\phi\rangle$ a unit eigenvector for H satisfying $H|\phi\rangle = e|\phi\rangle$. The condition becomes

$$e \le \frac{\langle A\phi|H|A\phi\rangle}{\langle A\phi|A\phi\rangle}.$$

In the right-hand-side, $|A\phi\rangle$ is a perturbation of $|\phi\rangle$, and the condition says that the average energy in the pure state associated with $|A\phi\rangle$ is higher than in the state associated with $|\phi\rangle$.

We prove part (c) of Proposition 3.3 here, leaving the other parts for the exercises.

Proof of Proposition 3.3(c). If $\rho = \mathrm{e}^{-\beta H}/Z_\beta$, then using the cyclicity of the trace

$$\begin{aligned}\langle AB\rangle &= \frac{1}{Z_\beta}\mathrm{Tr}\ \mathrm{e}^{-\beta H} AB = \frac{1}{Z_\beta}\mathrm{Tr}\, B\,\mathrm{e}^{-\beta H} A = \frac{1}{Z_\beta}\mathrm{Tr}\ \mathrm{e}^{-\beta H} B(\mathrm{e}^{-\beta H} A\,\mathrm{e}^{\beta H}) \\ &= \langle B\alpha_{\mathrm{i}\beta}(A)\rangle.\end{aligned} \tag{3.13}$$

So the Gibbs state is indeed a solution.

Next, let ρ be the density matrix of a state that satisfies the KMS condition. We have for all $A, B \in \mathcal{B}(\mathcal{H})$,

$$\mathrm{Tr}\,(\rho A)B = \mathrm{Tr}\,\rho B(\mathrm{e}^{-\beta H} A\,\mathrm{e}^{\beta H}) = \mathrm{Tr}\,(\mathrm{e}^{-\beta H} A\,\mathrm{e}^{\beta H}\rho)B. \tag{3.14}$$

Since this holds for all $B \in \mathcal{B}(\mathcal{H})$ (including $B = |i\rangle\langle j|$ for an orthonormal basis), we have that

$$\rho A = \mathrm{e}^{-\beta H} A\,\mathrm{e}^{\beta H}\rho \tag{3.15}$$

for all $A \in \mathcal{B}(\mathcal{H})$. Choosing $A = \mathrm{e}^{\beta H}$ we get $\mathrm{e}^{\beta H}\rho = \rho\,\mathrm{e}^{\beta H}$, so ρ commutes with $\mathrm{e}^{\beta H}$. Now observe that (3.15) implies that $\rho\,\mathrm{e}^{\beta H}$ commutes with all $A \in \mathcal{B}(\mathcal{H})$. Then $\rho\,\mathrm{e}^{\beta H}$ is proportional to the identity and ρ must be equal to the Gibbs operator. $\square$

3.3. Infinite volume Gibbs states

The goal of statistical mechanics is to describe the “bulk properties” of the system, far away from its boundaries. The large system is approximated by an *infinite* regular graph, the “lattice”. For simplicity we consider $\mathbb{Z}^d$, although all of the setting and many of the properties hold more generally. For an infinite system one cannot define equilibrium states using a density matrix, instead we proceed using appropriate analogs of the properties in Proposition 3.3 to define them. To prepare for this, we need some definitions.

At each site $x \in \mathbb{Z}^d$ is associated a Hilbert space $\mathcal{H}_x$. We write $n = \dim \mathcal{H}_x$, which we assume to be finite and independent of x. For $X \Subset \mathbb{Z}^d$ we let $\mathcal{H}_X = \otimes_{x\in X}\mathcal{H}_x$ and we let $\mathcal{A}_X = \mathcal{B}(\mathcal{H}_X)$ denote the algebra of bounded linear operators on $\mathcal{H}_X$. We consider two norms on $\mathcal{A}_X$. First, the usual operator norm $\|A\| = \sup_{\varphi\in\mathcal{H}_X} \|A\varphi\|/\|\varphi\|$. Second, the Hilbert-Schmidt norm $\|A\|_2 = \sqrt{\operatorname{tr} A^*A}$, where tr denotes the **normalised trace**

$$\operatorname{tr} A = \frac{1}{\dim \mathcal{H}_X} \operatorname{Tr} A = \frac{1}{n^{|X|}} \operatorname{Tr} A. \tag{3.16}$$

If $X \subset Y \Subset \mathbb{Z}^d$, there is a natural injection $\iota : \mathcal{A}_X \to \mathcal{A}_Y$ defined by

$$\iota A = A \otimes \mathbb{1}_{Y\setminus X}. \tag{3.17}$$

Notice that $\|\iota A\| = \|A\|$ (Exercise 3.2) and $\|\iota A\|_2 = \|A\|_2$ (because of the normalised trace). Then we can view $\mathcal{A}_X$ as a subalgebra of $\mathcal{A}_Y$. We define the algebra of **local observables** as the inductive union

$$\mathcal{A}_{\text{loc}} = \bigvee_{X\Subset\mathbb{Z}^d} \mathcal{A}_X. \tag{3.18}$$

If $A \in \mathcal{A}_{\text{loc}}$, then there exists $X \Subset \mathbb{Z}^d$ such that $A \in \mathcal{A}_X$. Finally, we let $\mathcal{A}$ denote the completion of $\mathcal{A}_{\text{loc}}$ with respect to the operator norm; this is the algebra of **quasi-local observables**. We also let $\mathcal{A}_{\text{h}}$ denote the algebra of hermitian quasi-local operators.

From the definition of $\mathcal{A}$ above we see that a local operator can be represented by several distinct elements, since $A \in \mathcal{A}_X$ has a counterpart $\iota(A) \in \mathcal{A}_Y$ for all $Y \supset X$. If we define a map α on operators $A \in \mathcal{A}_X$, simultaneously for all $X \Subset \mathbb{Z}^d$, we need to check that it is **consistent**, namely that $\alpha(A) = \alpha(\iota(A))$.

We denote by τ_x the lattice translation by $x \in \mathbb{Z}^d$. The action of τ_x is intuitive but let us define it formally. First we view τ_x as a linear map between $\mathcal{H}_X$ and $\mathcal{H}_{X+x}$ for any $X \Subset \mathbb{Z}^d$ such that

$$\tau_x \otimes_{y\in X} \varphi_y = \otimes_{y\in X}\varphi_{y+x} \tag{3.19}$$

for any set of vectors (φ_y) in $\mathcal{H}_0$. This extends by linearity to all vectors of $\mathcal{H}_X$. Notice that $\tau_x^{-1} = \tau_{-x}$. Then we define $\tilde{\tau}_x$ as the linear map $\mathcal{A}_X \to \mathcal{A}_{X+x}$ whose action on the local observable $A \in \mathcal{A}_X$ is

$$(\tilde{\tau}_x A)\varphi = \tau_x A(\tau_x^{-1}\varphi), \qquad \forall \varphi \in \mathcal{H}_{X+x}. \tag{3.20}$$

We dismiss the tilde from now on and we write τ_x for translations of vectors and of operators. Notice that for any $A \in \mathcal{A}_{X-x}$ and $B \in \mathcal{A}_X$ we have

$$(\tau_x A)B = \tau_x(A(\tau_x^{-1}B)), \tag{3.21}$$

indeed for $\varphi \in \mathcal{H}_X$

$$[\tau_x(A(\tau_x^{-1}B))]\varphi = \tau_x A(\tau_x^{-1}B)\tau_x^{-1}\varphi = \tau_x A\tau_x^{-1}B(\tau_x\tau_x^{-1}\varphi) = [(\tau_x A)B]\varphi. \tag{3.22}$$

An **interaction** is a collection of local self-adjoint observables indexed by finite subsets, $\Phi = (\Phi_X)_{X \Subset \mathbb{Z}^d}$. We only consider translation-invariant interactions, i.e. we assume that $\Phi_{X+x} = \tau_x \Phi_X$ for all $X \Subset \mathbb{Z}^d$ and all $x \in \mathbb{Z}^d$. Interactions form a (real) linear space and we consider the following norms:

$$\begin{aligned} |||\Phi||| &= \sum_{X \ni 0} \frac{\|\Phi_X\|}{|X|}, \\ \|\Phi\|_r &= \sum_{X \ni 0} \mathrm{e}^{r(|X|-1)} \, \|\Phi_X\| \qquad \text{for } r \geq 0. \end{aligned} \tag{3.23}$$

We denote by $\mathcal{I}$ and $\mathcal{I}_r$ the corresponding Banach spaces of interactions.

The **hamiltonian** in a finite domain $\Lambda \Subset \mathbb{Z}^d$ is

$$H_\Lambda^\Phi = \sum_{X \subseteq \Lambda} \Phi_X. \tag{3.24}$$

In the finite domain $\Lambda \Subset \mathbb{Z}^d$ the **Gibbs state** for the interaction Φ, at inverse temperature β, is defined as before: it is the linear functional $\langle\cdot\rangle_{\Lambda,\beta}^\Phi : \mathcal{A}_\Lambda \to \mathbb{C}$ given by

$$\langle A\rangle_{\Lambda,\beta}^\Phi = \frac{1}{Z_{\Lambda,\beta}(\Phi)} \operatorname{Tr} A \, \mathrm{e}^{-\beta H_\Lambda^\Phi}, \tag{3.25}$$

where $Z_{\Lambda,\beta}(\Phi) = \operatorname{Tr} \mathrm{e}^{-\beta H_\Lambda^\Phi}$.

We want to extend this notion to the infinite lattice $\mathbb{Z}^d$. There is no hamiltonian on the infinite lattice. In fact, we also avoid the Hilbert space for $\mathbb{Z}^d$ since it would be an infinite tensor product and would not be separable; this would cause many pathologies. The way out is to extend the linear functionals from $\mathcal{A}_\Lambda$ to $\mathcal{A}$, the space of quasi-local observables.

Definition 3.5. *A* **state** $\langle\cdot\rangle$ *is a normalised, positive linear functional on* $\mathcal{A}$. *That is,* $\langle\cdot\rangle$ *satisfies*

(i) $\langle sA + tB\rangle = s\langle A\rangle + t\langle B\rangle$ *for all* $A, B \in \mathcal{A}$ *and* $s, t \in \mathbb{C}$.
(ii) $\langle \mathbb{1}\rangle = 1$.
(iii) $\langle A^*A\rangle \geq 0$ *for all* $A \in \mathcal{A}$.

We write $\mathfrak{E}$ *for the set of states. A state is called* **translation-invariant** *if* $\langle A\rangle = \langle \tau_x A\rangle$ *for all* $x \in \mathbb{Z}^d$.

All states have norm 1 (Exercise 3.2).

In the following subsections, we summarise the definitions for equilibrium states in $\mathbb{Z}^d$, and how they are related.

3.3.1. Gibbs states as cluster points. The first notion of infinite-volume Gibbs states is to simply define them as limits of finite-volume Gibbs states. By the Banach–Alaoglu theorem the set of states is compact in the weak-* topology (that is, the topology of pointwise convergence of linear functionals). In plain words, this means that from any sequence of states $(\langle\cdot\rangle_n)$, we can extract a subsequence (n_k) such that $\langle A\rangle_{n_k}$ converges for any $A \in \mathcal{A}$.

DEFINITION 3.6 (Gibbs state as cluster point). *Let $\Phi \in \mathcal{I}$, and let Ψ_n be a sequence of interactions in $\mathcal{I}$ such that $\|\!|\Psi_n|\!\| \to 0$ as $n \to \infty$. Let $\Lambda_n = \{-n, \dots, n\}^d$ and for $A \in \mathcal{A}_{\rm loc}$, let*

$$\langle A\rangle^{\Phi}_{\Lambda_n,\beta} = \frac{1}{Z_{\Lambda_n,\beta}(\Phi+\Psi_n)} \operatorname{Tr} A\, \mathrm{e}^{-\beta H^{\Phi+\Psi_n}_{\Lambda_n}}.$$

The cluster points of the sequence $(\langle\cdot\rangle^{\Phi}_{\Lambda_n,\beta})_{n\geq 1}$ are infinite-volume Gibbs states for the interaction Φ.

While useful in many concrete situations, the set of cluster-points lacks relevant mathematical properties. For this reason, we consider four other definitions which are analogs of the properties in Proposition 3.3.

3.3.2. Gibbs states as tangent functionals. The finite-volume **free energy** in the domain $\Lambda \Subset \mathbb{Z}^d$ is defined as the following function of interactions:

$$f_\Lambda(\Phi,\beta) = -\frac{1}{\beta|\Lambda|} \log \operatorname{tr} \mathrm{e}^{-\beta H^{\Phi}_{\Lambda}}. \tag{3.26}$$

Notice the use the normalised trace tr , see (3.16). This is convenient for the connection to the variational principle.)

PROPOSITION 3.7.

(a) The free energy f_Λ is a concave function of the interactions.
(b) $(f_\Lambda)_{\Lambda\Subset\mathbb{Z}^d}$ are equicontinuous: for any $\Phi, \Phi' \in \mathcal{I}$ we have

$$\big|f_\Lambda(\Phi,\beta) - f_\Lambda(\Phi',\beta)\big| \leq \|\!|\Phi - \Phi'|\!\|.$$

PROOF. (a) follows from Proposition 3.4.

(b) We use that for any hermitian matrices A, B we have

$$\operatorname{Tr} \mathrm{e}^{A-\|B\|} \leq \operatorname{Tr} \mathrm{e}^{A+B} \leq \operatorname{Tr} \mathrm{e}^{A+\|B\|}. \tag{3.27}$$

With $A = -\beta H^{\Phi}_{\Lambda}$ and $B = \beta H^{\Phi}_{\Lambda} - \beta H^{\Phi'}_{\Lambda}$ we easily get that

$$\big|f_\Lambda(\Phi,\beta) - f_\Lambda(\Phi',\beta)\big| \leq \tfrac{1}{|\Lambda|}\|H^{\Phi}_{\Lambda} - H^{\Phi'}_{\Lambda}\|. \tag{3.28}$$

Finally,

$$\begin{aligned}\|H^{\Phi}_{\Lambda} - H^{\Phi'}_{\Lambda}\| &\leq \sum_{X\subset\Lambda} \|\Phi_X - \Phi'_X\| \underbrace{\sum_{y\in\Lambda} \tfrac{1}{|X|} 1_{y\in X}}_{=1} \\ &= \sum_{y\in\Lambda}\sum_{X\ni y} \tfrac{1}{|X|}\|\Phi_X - \Phi'_X\|\, 1_{X\subset\Lambda} \\ &\leq |\Lambda|\, \|\!|\Phi - \Phi'|\!\|.\end{aligned} \tag{3.29}$$

□

Definition 3.8. *A sequence of finite domains* $(\Lambda_n)_{n\geq 1}$ *converges to* $\mathbb{Z}^d$ **in the sense of van Hove** *if*

(i) *it is increasing:* $\Lambda_{n+1} \supset \Lambda_n$ *for all* n*;*
(ii) *it invades* $\mathbb{Z}^d$*:* $\cup_{n\geq 1}\Lambda_n = \mathbb{Z}^d$*;*
(iii) *the ratio boundary/bulk vanishes:* $\frac{|\partial_r \Lambda_n|}{|\Lambda_n|} \to 0$ *as* $n \to \infty$*,* $\forall\, r$*.*

Here, the r*-boundary is* $\partial_r \Lambda = \{x \in \Lambda^{\rm c} : {\rm dist}(x,\Lambda) \leq r\}$*.*

We now state one of the major results in statistical mechanics, namely the existence of the infinite volume free energy.

Theorem 3.9. *Assume that* $\Phi \in \mathcal{I}$*, i.e.* $|\!|\!|\Phi|\!|\!| < \infty$*. Then the limit*

$$f(\Phi,\beta) := \lim_{n\to\infty} f_{\Lambda_n}(\Phi,\beta)$$

exists and is the same along all van Hove sequences $\Lambda_n \Uparrow \mathbb{Z}^d$*. It is a concave function of the interactions.*

Proof. We prove the theorem for $\Phi \in \mathcal{I}_0 \subsetneq \mathcal{I}$. It is enough, because of Proposition 3.7 (b) and of the Arzolà-Ascoli theorem.

We check that $|\Lambda|\, f_\Lambda(\Phi,\beta)$ meets the conditions of Lemma A.13. If $\Lambda \Subset \mathbb{Z}^d$ is the disjoint union of $\Lambda_i, \dots, \Lambda_k$, we have

$$H_\Lambda^\Phi = \sum_{i=1}^k H_{\Lambda_i}^\Phi + B, \tag{3.30}$$

where B is the sum of all Φ_X where $X \subset \Lambda$ but $X \not\subset \Lambda_i$ for any i. Then

$$\|B\| \leq \sum_{i=1}^k \sum_{\substack{X\cap\Lambda_i\neq\emptyset \\ X\not\subset\Lambda_i}} \|\Phi_X\| \leq \sum_{i=1}^k \|\Phi\|_0\, |\partial_1 \Lambda_i|. \tag{3.31}$$

Using (3.27) we easily get that

$$\Bigl| |\Lambda|\, f_\Lambda(\Phi,\beta) - \sum_{i=1}^k |\Lambda_i|\, f_{\Lambda_i}(\Phi,\beta) \Bigr| \leq \|\Phi\|_0 \sum_{i=1}^k |\partial_1 \Lambda_i|. \tag{3.32}$$

The result then follows from Lemma A.13, taking $a_\Lambda = |\Lambda|\, f_\Lambda(\Phi,\beta)$. ☐

We use the infinite-volume free energy to define infinite-volume states. The definition is restricted to translation-invariant states. Let us introduce

$$A_\Psi = \sum_{X\ni 0} \frac{1}{|X|} \Psi_X. \tag{3.33}$$

Notice that $\|A_\Psi\| \leq |\!|\!|\Psi|\!|\!|$.

DEFINITION 3.10 (Gibbs states as tangent functionals). *A translation-invariant state $\langle\cdot\rangle$ on $\mathcal{A}$ is an equilibrium state for the interaction $\Phi \in \mathcal{I}$, in the sense of tangent functionals to the free energy, if*

$$f(\Phi + \Psi) \leq f(\Phi) + \langle A_\Psi \rangle$$

for all $\Psi \in \mathcal{I}$.

To motivate the use of A_Ψ, note from Proposition 3.3 that $\langle\cdot\rangle = \langle\cdot\rangle^{\Phi}_{\Lambda,\beta}$ satisfies

$$f_\Lambda(\Phi + \Psi, \beta) \leq f_\Lambda(\Phi, \beta) + \langle \tfrac{1}{|\Lambda|} H^{\Psi}_{\Lambda} \rangle. \tag{3.34}$$

For a translation-invariant state $\langle\cdot\rangle$ we have $\langle \frac{1}{|\Lambda|} H^{\Psi}_{\Lambda} \rangle = \langle A_\Psi \rangle$.

We denote by $\mathcal{G}^{\Phi}_{\text{t.i.}}$ the set of translation invariant states on $\mathcal{A}$ that are tangent to the free energy at Φ in the sense that they satisfy Definition 3.10. This definition is more general than that of states as cluster points:

PROPOSITION 3.11. *Any translation-invariant cluster state for Φ (Definition 3.6) is tangent to the free energy at Φ (i.e. satisfies Definition 3.10).*

3.3.3. The variational definition of Gibbs states. We now introduce the entropy of states on the quasi-local observables $\mathcal{A}$. This is a function on finite subsets of $\mathbb{Z}^d$, that are defined using the von Neumann entropy of the corresponding density matrices.

Recall that we defined the von Neumann entropy $S(\rho)$ of a density matrix ρ by $S(\rho) = -\operatorname{Tr} \rho \log \rho$. If $(\lambda_i)_{i\geq 1}$ are the eigenvalues of ρ, then $S(\rho) = -\sum_i \lambda_i \log \lambda_i$. The formula also applies when some eigenvalues are 0, using $0 \log 0 = 0$, and it applies to all positive semi-definite matrices, not only density matrices.

Since we consider sequences $\Lambda \Subset \mathbb{Z}^d$, it is important to note that the trace Tr actually depends on Λ, so we write here $\operatorname{Tr}_\Lambda$. For example, the trace of the identity operator $\mathbb{1}$ depends on which $\mathcal{H}_\Lambda$ we view it as acting on: $\operatorname{Tr}_\Lambda \mathbb{1} = \dim \mathcal{H}_\Lambda$. For this reason, we instead use the normalized trace $\operatorname{tr} = \frac{1}{\dim \mathcal{H}_\Lambda} \operatorname{Tr}_\Lambda$, introduced in (3.16). Then for $A \in \mathcal{A}_{\text{loc}}$, the trace $\operatorname{tr} A$ does not depend on which $\mathcal{H}_\Lambda$ we view it as acting on. With respect to the normalized trace, a density matrix is positive semi-definite and satisfies $\operatorname{tr} \rho = 1$, so (if $\rho \in \mathcal{A}_\Lambda$) $\operatorname{Tr}_\Lambda \rho = \dim \mathcal{H}_\Lambda$.

For notational convenience, here we write $\boldsymbol{\rho}$ rather than $\langle\cdot\rangle$ for states. Let $\boldsymbol{\rho}$ be a state on $\mathcal{A}$. For $\Lambda \Subset \mathbb{Z}^d$, we let ρ_Λ be the density matrix (with respect to normalized trace) of the restriction of $\boldsymbol{\rho}$ to $\mathcal{A}_\Lambda$. We define the entropy in $\Lambda \Subset \mathbb{Z}^d$ to be

$$s_\Lambda(\boldsymbol{\rho}) := -\operatorname{tr} \rho_\Lambda \log \rho_\Lambda. \tag{3.35}$$

Note that $s_\Lambda(\boldsymbol{\rho}) = S_\Lambda\big(\frac{1}{\dim \mathcal{H}_\Lambda} \rho_\Lambda\big) - \log(\dim \mathcal{H}_\Lambda)$, where $S_\Lambda(A) = -\operatorname{Tr}_\Lambda A \log A$ is the usual von Neumann entropy in $\mathcal{A}_\Lambda$ and $\frac{1}{\dim \mathcal{H}_\Lambda} \rho_\Lambda$ is a density matrix with respect to $\operatorname{Tr}_\Lambda$.

For a translation-invariant state $\boldsymbol{\rho}$ we can define the infinite-volume mean (or specific) entropy by

$$s(\boldsymbol{\rho}) = \lim_{\Lambda \Uparrow \mathbb{Z}^d} \frac{1}{|\Lambda|} s_\Lambda(\boldsymbol{\rho}). \tag{3.36}$$

Proposition 3.12. *Let $\boldsymbol{\rho}$ be a translation-invariant state on $\mathcal{A}$.*

(a) The limit (3.36) exists along any van Hove sequence of domains and is the same along all such sequences.

(b) The functional s is affine: $s(t\boldsymbol{\rho} + (1-t)\boldsymbol{\rho}') = ts(\boldsymbol{\rho}) + (1-t)s(\boldsymbol{\rho}')$.

Let $\boldsymbol{\rho}$ be a translation-invariant state on $\mathcal{A}$. We define the **infinite-volume free energy functional** by

$$f^{\beta,\Phi}(\boldsymbol{\rho}) = \boldsymbol{\rho}(A_\Phi) - \tfrac{1}{\beta} s(\boldsymbol{\rho}), \tag{3.37}$$

where $A_\Phi = \sum_{X \ni 0} \frac{1}{|X|} \Phi_X$ is defined in (3.33). We have that $f^{\beta,\Phi}(\boldsymbol{\rho})$ is affine in Φ and in $\boldsymbol{\rho}$.

Recall that $f(\Phi,\beta) = -\lim_{\Lambda \Uparrow \mathbb{Z}^d} \frac{1}{\beta|\Lambda|} \log \operatorname{tr}_\Lambda \mathrm{e}^{-\beta H_\Lambda^\Phi}$ is the free energy density. While $f(\Phi,\beta)$ is a function of the interaction Φ, the functional $f^{\beta,\Phi}(\boldsymbol{\rho})$ depends also on a state $\boldsymbol{\rho}$

Definition 3.13. *Let $\boldsymbol{\rho}$ be a translation-invariant state on $\mathcal{A}$. Then it is called a Gibbs state for the interacton Φ, in the variational sense, if it is a minimizer of $f^{\beta,\Phi}(\cdot)$ over all translation-invariant states.*

The following result explains the connection between the free energy $f(\beta,\Phi)$ and the free energy functional $f^{\beta,\Phi}(\cdot)$, and establishes the equivalence of the definitions of Gibbs states in terms of tangent functionals and the variational problem:

Theorem 3.14 (Gibbs variational principle, infinite volume).

(a) The free energy is equal to the minimum of the free energy functional:

$$f(\beta,\Phi) = \inf_{\boldsymbol{\rho} \in \mathfrak{E}_{\mathrm{t.i.}}} f^{\beta,\Phi}(\boldsymbol{\rho}).$$

The infimum is over all infinite-volume translation-invariant states on $\mathcal{A}$.

(b) The minimisers are Gibbs states: If $\boldsymbol{\rho}$ is a translation-invariant state, then

$$f(\beta,\Phi) = f^{\beta,\Phi}(\boldsymbol{\rho}) \quad \Longleftrightarrow \quad f(\beta,\Phi+\Psi) \le f(\beta,\Phi) + \boldsymbol{\rho}(A_\Psi) \quad \forall \Psi \in \mathcal{I}.$$

3.3.4. The KMS definition of Gibbs states. We now turn to the KMS definition of equilibrium states. An advantage of this definition is that, unlike the tangent and variational definitions, it is not restricted to translation-invariant states. But the interaction belongs to the smaller space $\mathcal{I}_r$ for some $r > 0$.

Given an interaction $\Phi \in \mathcal{I}_r$ we consider the family of evolution operators $\alpha^\Phi_{\Lambda,t}$, with $t \in \mathbb{C}$ and $\Lambda \Subset \mathbb{Z}^d$, that acts on local operators of $\mathcal{A}_\Lambda$ as in (3.11):

$$\alpha^\Phi_{\Lambda,t}(A) = \mathrm{e}^{\mathrm{i}tH^\Phi_\Lambda}\, A\, \mathrm{e}^{-\mathrm{i}tH^\Phi_\Lambda}\,. \tag{3.38}$$

To prove the existence of the infinite-volume limit of $\alpha^\Phi_{\Lambda,t}$, we proceed along the following steps:

(1) For $|t| < \frac{r}{2\|\Phi\|_r}$, we show that $(\alpha^{\Phi}_{\Lambda,t})_{\Lambda \Subset \mathbb{Z}^d}$ is Cauchy for each fixed $A \in \mathcal{A}_{\rm loc}$. We denote the limit $\alpha^{\Phi}_t(A)$.
(2) For $t \in \mathbb{R}$, we have $\|\alpha^{\Phi}_{\Lambda,t}(A)\| = \|A\|$ for all Λ, so $\|\alpha^{\Phi}_t\| = 1$.
(3) We use the group property to extend α^{Φ}_t to the whole real line.

For the infinite-volume limit, the notation $\Lambda_n \uparrow \mathbb{Z}^d$ means that $\Lambda_n \Subset \mathbb{Z}^d$, $\Lambda_n \subset \Lambda_{n+1}$, and $\cup_n \Lambda_n = \mathbb{Z}^d$ (we do not need the ration boundary/bulk to go to 0 here). If the limit along each diverging sequence (Λ_n) exists, then the limit is the same along any sequence (Exercise 3.15).

LEMMA 3.15. *Assume that $\Phi \in \mathcal{I}_r$ for some $r > 0$ and that $t \in \mathbb{C}$ with $|t| < \frac{r}{2\|\Phi\|_r}$. Then $(\alpha^{\Phi}_{\Lambda,t})_{\Lambda \Subset \mathbb{Z}^d}$ is a Cauchy sequence for each fixed $A \in \mathcal{A}_{\rm loc}$.*

We need the multicommutator ("Lie-Schwinger") expansion. Let $\mathrm{ad}_A(B) = [A, B]$ denote the "adjoint endomorphism".

LEMMA 3.16 (Lie-Schwinger multicommutator expansion). *Let A and B be two operators on the same finite-dimensional Hilbert space. Then*

$$\mathrm{e}^{A}\, B\, \mathrm{e}^{-A} = \sum_{n \geq 0} \frac{1}{n!} \mathrm{ad}^n_A(B).$$

PROOF. We show that $\mathrm{e}^{sA}\, B\, \mathrm{e}^{-sA}$ and $\sum_n \frac{s^n}{n!} \mathrm{ad}^n_A(B)$ satisfy the same differential equation. First,

$$\frac{\mathrm{d}}{\mathrm{d}s} \mathrm{e}^{sA}\, B\, \mathrm{e}^{-sA} = \big[A, \mathrm{e}^{sA}\, B\, \mathrm{e}^{-sA}\big]. \tag{3.39}$$

Second,

$$\frac{\mathrm{d}}{\mathrm{d}s} \sum_{n \geq 0} \frac{s^n}{n!} \mathrm{ad}^n_A(B) = \sum_{n \geq 1} \frac{s^{n-1}}{(n-1)!} \mathrm{ad}_A\Big(\mathrm{ad}^{n-1}_A(B)\Big) = \Big[A, \sum_{n \geq 0} \frac{s^n}{n!} \mathrm{ad}^n_A(B)\Big]. \tag{3.40}$$

□

PROOF OF LEMMA 3.15. Let $A \in \mathcal{B}_Y$ for some $Y \Subset \mathbb{Z}^d$. We show that $(\alpha^{\Phi}_{\Lambda,t}(A))_{\Lambda \Subset \mathbb{Z}^d}$ is Cauchy. By Lemma 3.16, we have

$$\begin{aligned} \alpha^{\Phi}_{\Lambda,t}(A) &= \sum_{n \geq 0} \frac{(\mathrm{i}t)^n}{n!} \mathrm{ad}^n_{H^{\Phi}_{\Lambda}}(A) \\ &= \sum_{n \geq 0} \frac{(\mathrm{i}t)^n}{n!} \sum_{X_1, \dots, X_n \subset \Lambda} [\Phi_{X_n}, [\Phi_{X_{n-1}}, \dots [\Phi_{X_1}, A] \dots]]. \end{aligned} \tag{3.41}$$

We show that this series converges absolutely for small $|t|$. In order for the commutators to differ from zero, the sets must satisfy

$$\begin{aligned}&X_1 \cap Y \neq \emptyset,\\&X_2 \cap (X_1 \cup Y) \neq \emptyset,\\&\quad\vdots\\&X_n \cap (X_1 \cup \dots \cup X_{n-1} \cup Y) \neq \emptyset.\end{aligned} \tag{3.42}$$

The sum over such sets can be realised by first summing over sets that contain the origin, then by summing over translations so that (3.42) is satisfied. One needs to divide by the cardinality of the set in order not to over-count. Then

$$\begin{aligned}\alpha^{\Phi}_{\Lambda,t}(A) = \sum_{n\geq 0} \frac{(\mathrm{i}t)^n}{n!} \sum_{X_1,\dots,X_n \ni 0} \Bigl(\prod_{i=1}^{n} \frac{1}{|X_i|}\Bigr)\\ \sum_{\substack{x_1,\dots,x_n \in \mathbb{Z}^d\\ X_i + x_i \subset \Lambda\ \forall i}} [\Phi_{X_n+x_n}, [\Phi_{X_{n-1}+x_{n-1}}, \dots [\Phi_{X_1+x_1}, A] \dots]].\end{aligned} \tag{3.43}$$

For given $X_1, \dots, X_n$ there are no more than

$$\begin{aligned}&|Y| \cdot |X_1| \text{ possible choices for } x_1,\\&\bigl(|Y| + |X_1| - 1\bigr) \cdot |X_2| \text{ possible choices for } x_2,\\&\quad\vdots\\&\bigl(|Y| + |X_1| + \dots + |X_{n-1}| - (n-1)\bigr) \cdot |X_n| \text{ possible choices for } x_n.\end{aligned} \tag{3.44}$$

We get

$$\begin{aligned}&\Bigl\| \sum_{X_1,\dots,X_n} \Bigl(\prod_{i=1}^{n} \frac{1}{|X_i|}\Bigr) \sum_{x_1,\dots,x_n} [\Phi_{X_n+x_n}, \dots [\Phi_{X_1+x_1}, A] \dots] \Bigr\|\\&\qquad \leq \|A\| 2^n \sum_{X_1,\dots,X_n \ni 0} \bigl(|X_1| + \dots + |X_n| - n + |Y|\bigr)^n \prod_{i=1}^{n} \|\Phi_{X_i}\|\\&\qquad \leq \|A\|\, \mathrm{e}^{r|Y|}\, n! \Bigl(\frac{2\|\Phi\|_r}{r}\Bigr)^n.\end{aligned} \tag{3.45}$$

We used $c^n \leq n! r^{-n} \mathrm{e}^{rc}$, which is obvious from the Taylor series of e^{rc}. The factor 2^n is due to the n commutators. It follows that $\alpha^{\Phi}_{\Lambda,t}(A)$ is absolutely convergent whenever $|t| < \frac{r}{2\|\Phi\|_r}$ if $\|\Phi\|_r < \infty$. Notice the bound

$$\|\alpha^{\Phi}_{\Lambda,t}(A)\| \leq \|A\|\, \mathrm{e}^{r|Y|} \Bigl(1 - |t| \frac{2\|\Phi\|_r}{r}\Bigr)^{-1}. \tag{3.46}$$

for all $A \in \mathcal{A}_Y$. It is uniform in Λ but not in Y.

If $\Lambda' \supset \Lambda$, we have

$$\alpha^{\Phi}_{\Lambda',t}(A) - \alpha^{\Phi}_{\Lambda,t}(A) = \sum_{n\geq 0} \frac{(\mathrm{i}t)^n}{n!} \sum_{\substack{X_1,\dots,X_n : Y\\ \cup X_i \not\subset \Lambda}} [\Phi_{X_n}, [\Phi_{X_{n-1}}, \dots [\Phi_{X_1}, A] \dots]]. \tag{3.47}$$

The second sum is over sets in Λ' that satisfy the constraint (3.42) and whose union is not contained in Λ. For small $|t|$, it follows from the absolute convergence of the series that (3.47) is as small as we want by taking Λ large enough, uniformly in $\Lambda' \supset \Lambda$. Hence $(\alpha^{\Phi}_{\Lambda,t}(A))_{\Lambda}$ is Cauchy. □

THEOREM 3.17 (Infinite-volume limit of the evolution operator).
Let $\Phi \in \mathcal{I}_r$ for some $r > 0$. There exists a family of $*$-automorphisms α^{Φ}_t on $\mathcal{A}$ such that

(a) $\lim_{n\to\infty} \alpha^{\Phi}_{\Lambda_n,t}(A) = \alpha^{\Phi}_t(A)$ along any sequence $\Lambda_n \uparrow \mathbb{Z}^d$, for any $t \in \mathbb{R}$, and for any $A \in \mathcal{A}_{\rm loc}$.
(b) $\|\alpha^{\Phi}_t\| = 1$ for any $t \in \mathbb{R}$.
(c) It satisfies the group property

$$\alpha^{\Phi}_{s+t}(A) = \alpha^{\Phi}_s\big(\alpha^{\Phi}_t(A)\big) \qquad \text{for all } A \in \mathcal{A}, s,t \in \mathbb{R}.$$

In case clarification is needed, α^{Φ}_t is an homomorphism in the sense that it is linear and $\alpha^{\Phi}_t(AB) = \alpha^{\Phi}_t(A)\alpha^{\Phi}_t(B)$. It is an automorphism since it is also a bijection, and a $*$-automorphism since $\alpha^{\Phi}_t(A)^* = \alpha^{\Phi}_t(A^*)$ when t is real.

PROOF. It is convenient to extend $\alpha^{\Phi}_{\Lambda,t}$ to the whole of $\mathcal{A}$. Namely, for $A \in \mathcal{A}_{\rm loc}$ of the form $A = B \otimes C$ with $B \in \mathcal{A}_{\Lambda}$ and $C \in \mathcal{A}_{\Lambda^{\rm c}}$[1] we define

$$\alpha^{\Phi}_{\Lambda,t}(A) = \, {\rm e}^{{\rm i}tH^{\Phi}_{\Lambda}}\, B\, {\rm e}^{-{\rm i}tH^{\Phi}_{\Lambda}} \otimes C. \tag{3.48}$$

The norm of the extension is still 1, so $\alpha^{\Phi}_{\Lambda,y}$ can be extended to the whole of $\mathcal{A}$.

For t small (precisely $|t| < \frac{r}{2\|\Phi\|_r}$) we can use Lemma 3.15 and define α^{Φ}_t to be the pointwise limit of $\alpha^{\Phi}_{\Lambda,t}$. Now let $t, t_1, \dots, t_k \in \mathbb{R}$ such that $t = \sum_i t_i$ and $|t_i| < \frac{r}{2\|\Phi\|_r}$ for $i = 1, \dots, k$. We have

$$\alpha^{\Phi}_{\Lambda,t_k} \circ \dots \alpha^{\Phi}_{\Lambda,t_1}(A) - \alpha^{\Phi}_{t_k} \circ \dots \alpha^{\Phi}_{t_1}(A) = \sum_{j=1}^{k} \alpha^{\Phi}_{\Lambda,t_k} \circ \dots \big(\alpha^{\Phi}_{\Lambda,t_j} - \alpha^{\Phi}_{t_j}\big) \circ \dots \alpha^{\Phi}_{t_1}(A). \tag{3.49}$$

Then

$$\big\|\alpha^{\Phi}_{\Lambda,t_k} \circ \dots \alpha^{\Phi}_{\Lambda,t_1}(A) - \alpha^{\Phi}_{t_k} \circ \dots \alpha^{\Phi}_{t_1}(A)\big\| \le \sum_{j=1}^{k} \big\|\alpha^{\Phi}_{\Lambda,t_j} - \alpha^{\Phi}_{t_j}\big\|\, \|A\|. \tag{3.50}$$

Then

$$\lim_{n\to\infty} \alpha^{\Phi}_{\Lambda_n,t}(A) = \alpha^{\Phi}_{t_k} \circ \dots \circ \alpha^{\Phi}_{t_1}(A), \tag{3.51}$$

and this holds for any small $t_1, \dots, t_k$ that add up to t. This establishes the infinite-volume limit and the group property at the same time. The right side does not depend on the choice of the t_is. We then define α^{Φ}_t by the above limit. □

[1] If $X \subset \mathbb{Z}^d$ and $|X| = \infty$, we define $\mathcal{A}_X$ to be the completion of the space of local observables with support in X.

In order to state the KMS condition for infinite volume states, we rely on complex analysis to extend the definition of α_t^Φ from $t \in \mathbb{R}$ to $t \in \mathbb{C}$. More precisely, we rely on an extension of complex analysis that involves maps from $\mathbb{C}$ to an algebra of bounded operators. Convergent series can be defined in the same way, so the notion of analytic functions and their extensions still makes sense.

Consider a function $f \in C_c^\infty(\mathbb{R})$, the space of smooth functions $\mathbb{R} \to \mathbb{C}$ with compact support, and set

$$\widehat{f}(z) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} e^{i\xi z} f(\xi) d\xi, \qquad z \in \mathbb{C}. \tag{3.52}$$

Then $\widehat{f}$ is analytic in the whole complex plane (it is "entire"). Given $A \in \mathcal{A}$ and $f \in C_c^\infty(\mathbb{R})$, let

$$A_f = \int_{\mathbb{R}} \widehat{f}(t) \alpha_t^\Phi(A) dt. \tag{3.53}$$

Then $\tilde{\mathcal{A}} = \{A_f : A \in \mathcal{A}, f \in C_c^\infty(\mathbb{R})\}$ is a dense subspace of $\mathcal{A}$ (sometimes called Paley–Wiener operators). For $A_f \in \tilde{\mathcal{A}}$ and $z \in \mathbb{C}$ we *define*

$$\alpha_z^\Phi(A_f) := \int_{\mathbb{R}} \widehat{f}(t-z) \alpha_t^\Phi(A) dt. \tag{3.54}$$

Thus $\alpha_z^\Phi(A_f) = A_{f_z} \in \tilde{\mathcal{A}}$, where $f_z \in C_c^\infty(\mathbb{R})$ is the function given by $f_z(t) = e^{-izt} f(t)$. Note that $(f_z)_w = f_{z+w}$. To summarize:

PROPOSITION 3.18. *With the definition (3.54), α_z^Φ maps $\tilde{\mathcal{A}}$ to $\tilde{\mathcal{A}}$ and satisfies the group property $\alpha_z^\Phi \circ \alpha_w^\Phi = \alpha_{z+w}^\Phi$ for all $z, w \in \mathbb{C}$.*

DEFINITION 3.19. *We say that the state $\langle \cdot \rangle$ on $\mathcal{A}$ satisfies* **the KMS condition** *for the interaction $\Phi \in \mathcal{I}_r$ at inverse temperature β if for all $A \in \tilde{\mathcal{A}}$ and all $B \in \mathcal{A}$, we have*

$$\langle AB \rangle = \langle B \alpha_{i\beta}^\Phi(A) \rangle. \tag{3.55}$$

Equivalently, we have for all $A, B \in \mathcal{A}$, and all functions f such that $\widehat{f} \in C_c^\infty$, that

$$\int_{\mathbb{R}} f(t) \langle \alpha_t^\Phi(A) B \rangle dt = \int_{\mathbb{R}} f(t - i\beta) \langle B\, \alpha_t^\Phi(A) \rangle dt. \tag{3.56}$$

We write $\mathcal{G}_\beta^\Phi$ for the set of states satisfying the KMS-condition for Φ at inverse temperature β. Notice that the states $\langle \cdot \rangle \in \mathcal{G}_\beta^\Phi$ are not assumed to be translation-invariant (even though the interaction Φ is). For translation-invariant states, the three definitions agree:

PROPOSITION 3.20. *Let $\langle \cdot \rangle$ be a translation-invariant state on $\mathcal{A}$. Then $\langle \cdot \rangle$ satisfies the KMS-condition if and only if it satisfies the tangent- and variational definitions.*

Let S_β denote the strip $S = \{z \in \mathbb{C} : 0 \le \operatorname{Im} z \le \beta\}$ in the complex plane. Another common formulation of the KMS condition is the following:

PROPOSITION 3.21. *A state $\langle\cdot\rangle$ is a KMS state on $\mathcal{A}$ if and only if for each $A, B \in \mathcal{A}$ there is a continuous, bounded function $F = F_{A,B} : S_\beta \to \mathbb{C}$ that is analytic in the interior of the strip S_β and satisfies for all $t \in \mathbb{R}$ that*

$$\langle A\,\alpha_t^\Phi(B)\rangle = F(t), \qquad \langle \alpha_t^\Phi(B)A\rangle = F(t+\mathrm{i}\beta).$$

PROOF. First assume that $\langle\cdot\rangle$ is a KMS state. If $A \in \mathcal{A}$ and $B_f \in \tilde{\mathcal{A}}$, set $F_{A,B_f}(z) = \langle A\,\alpha_z^\Phi(B_f)\rangle$. Then $F_{A,B_f}(z)$ is indeed analytic (indeed, entire) and it satisfies the first identity by definition. As for the second identity, we have using (3.56) and the group property:

$$\begin{aligned} F_{A,B_f}(t+\mathrm{i}\beta) &= \langle A\,\alpha_{t+\mathrm{i}\beta}^\Phi(B_f)\rangle = \int_{\mathbb{R}} f(s-t-\mathrm{i}\beta)\langle A\,\alpha_s^\Phi(B)\rangle \mathrm{d}s \\ &= \int_{\mathbb{R}} f(u-\mathrm{i}\beta)\langle A\,\alpha_u^\Phi(\alpha_t^\Phi(B))\rangle \mathrm{d}u = \int_{\mathbb{R}} f(u)\langle \alpha_u^\Phi(\alpha_t^\Phi(B))A\rangle \mathrm{d}u \\ &= \Big\langle \alpha_t^\Phi\Big(\int_{\mathbb{R}} f(u)\alpha_u^\Phi(B)\mathrm{d}u\Big)A\Big\rangle = \langle \alpha_t^\Phi(B_f)A\rangle. \end{aligned} \tag{3.57}$$

This extends to arbitrary $B \in \mathcal{A}$ by continuity. Indeed, if $B_{f_n} \to B$, then $\alpha_t^\Phi(B_{f_n}) \to \alpha_t^\Phi(B)$ and $\langle A\,\alpha_t^\Phi(B_{f_n})\rangle$, $\langle \alpha_t^\Phi(B_{f_n})A\rangle$ converge. Further, the functions $F_{A,B_{f_n}}(z)$ converge by the Phragmén–Lindelöf theorem.

We now establish the other implication. If $A \in \mathcal{A}$ and $B \in \tilde{\mathcal{A}}$, the function $z \mapsto \langle A\,\alpha_z^\Phi(B)\rangle$ is entire. We have $\langle A\,\alpha_z^\Phi(B)\rangle = F_{A,B}(z)$ for all $z \in \mathbb{R}$. The identity is then also valid for z in the strip, so that

$$\langle A\,\alpha_{\mathrm{i}\beta}^\Phi(B)\rangle = F_{A,B}(\mathrm{i}\beta) = \langle BA\rangle. \qquad \square$$

3.3.5. The RAS definition of Gibbs states. Finally, the RAS-condition extends straightforwardly from finite to infinite volume. We need the interaction Φ to be in $\mathcal{I}_0$. Then, for each $\Lambda \Subset \mathbb{Z}^d$ and each $A \in \mathcal{A}_{\mathrm{loc}}$ we define

$$[H^\Phi, A] := \sum_{X \Subset \mathbb{Z}^d} [\Phi_X, A]. \tag{3.58}$$

To check that the sum converges in norm, first note that

$$\sum_{X \Subset \mathbb{Z}^d} [\Phi_X, A] = \sum_{X \ni 0} \frac{1}{|X|} \sum_{x \in \mathbb{Z}^d} [\Phi_{X+x}, A] = \sum_{X \ni 0} \frac{1}{|X|} \sum_{x : (X+x)\cap\Lambda \neq \varnothing} [\Phi_{X+x}, A] \tag{3.59}$$

Then

$$\|[H^\Phi, A]\| \le 2\|A\| \sum_{X \ni 0} \frac{1}{|X|} \|\Phi_X\| \cdot |X||\Lambda| = 2\|A\||\Lambda| \sum_{X \ni 0} \|\Phi_X\| < \infty. \tag{3.60}$$

Here $|X||\Lambda|$ is an upper bound for the number of x such that $X+x$ intersects Λ.

Definition 3.22. *A state $\langle\cdot\rangle$ on $\mathcal{A}$ satisfies the* **RAS condition** *for the interaction $\Phi \in \mathcal{I}_0$ and inverse temperature β if*

$$\langle A^*[H^\Phi, A]\rangle \geq \frac{1}{\beta}\langle A^*A\rangle \log \frac{\langle A^*A\rangle}{\langle AA^*\rangle}$$

for all $A \in \mathcal{A}_{\mathrm{loc}}$ such that $\langle AA^*\rangle > 0$.

Theorem 3.23. *A state on $\mathcal{A}$ satisfies the RAS condition if and only if it satisfies the KMS condition.*

An advantage of the RAS-condition is that it gives a definition of ground-states by taking $\beta \to \infty$:

Definition 3.24. *A state $\langle\cdot\rangle$ on $\mathcal{A}$ is called a* **ground state** *for the interaction $\Phi \in \mathcal{I}$ if*

$$\langle A^*[H^\Phi, A]\rangle \geq 0$$

for all $A \in \mathcal{A}_{\mathrm{loc}}$.

3.4. Extremal Gibbs states

The goal now is to understand better the structure of the set of (translation invariant) infinite-volume Gibbs states for a given interaction. We see in this section that it is a convex set, that extremal points enjoy special properties, and that any Gibbs state can be written as a convex combination of extremal states. It is remarkable that these properties can be established in a large class of systems without identifying the actual Gibbs states.

It is easy to see that if $\langle\cdot\rangle^{(1)}, \langle\cdot\rangle^{(2)} \in \mathfrak{E}$ are two states, then the convex combination $t\langle\cdot\rangle^{(1)} + (1-t)\langle\cdot\rangle^{(2)}$, $t \in [0,1]$, is also a state: the set $\mathfrak{E}$ of states is convex. It is also not hard to check that the set of equilibrium states $\mathcal{G}_\beta^\Phi$ and the set of translation-invariant states $\mathcal{G}_{\mathrm{t.i.}}^\Phi$, for a given interaction $\Phi \in \mathcal{I}$, is convex. Indeed, the tangent functional property, the variational principle, and the KMS and RAS conditions are all preserved by taking convex combinations. Recall that $\mathfrak{E} \supseteq \mathcal{G}_\beta^\Phi \supseteq \mathcal{G}_{\mathrm{t.i.}}^\Phi$.

Definition 3.25. *An element x of a convex set $\mathcal{X}$ is called* **extremal** *if it cannot be written as a convex combination $tx_1 + (1-t)x_2$, $t \in (0,1)$, of distinct elements $x_1, x_2 \in \mathcal{X}$. In particular, this definition applies to elements of $\mathfrak{E}$, $\mathcal{G}_\beta^\Phi$ and $\mathcal{G}_{\mathrm{t.i.}}^\Phi$.*

Another relevant property of states is to have short-range correlations.

DEFINITION 3.26. *A state $\langle\cdot\rangle$ is said to have* **short-range correlations** *if*

$$\lim_{\Lambda\Uparrow\mathbb{Z}^d} \sup_{\substack{B\in\mathcal{A}_{\Lambda^c}\\ \|B\|=1}} \big|\langle AB\rangle - \langle A\rangle\langle B\rangle\big| = 0.$$

It is said to be **mixing** *if for all $A, B \in \mathcal{A}$ we have*

$$\lim_{\|x\|\to\infty} \big(\langle A\tau_x B\rangle - \langle A\rangle\langle\tau_x B\rangle\big) = 0.$$

Clearly short-range correlations implies mixing. For translation-invariant Gibbs states we will see that they are actually equivalent. In the definition of short-range correlations we may assume that the operators B are Hermitian: if the limit is 0 when restricted to Hermitian B then, by considering $B + \mathrm{i}B'$, it follows that the limit is 0 for all B.

Finally we introduce a notion that is reminiscent of ergodic measures in dynamical systems, which are equal to the time averages. Here the time evolution is replaced by space translations. We consider the averaging operator m_n whose action on $A \in \mathcal{A}$ is

$$m_n(A) = \frac{1}{n^d} \sum_{x\in\{1,\dots,n\}^d} \tau_x A. \tag{3.61}$$

For translation-invariant states we always have $\langle m_n(A)\rangle = \langle A\rangle$. Notice that $m_n(A) \in \mathcal{A}$ for finite n but the limit $n \to \infty$ does not exist in general.

DEFINITION 3.27. *A translation-invariant state $\langle\cdot\rangle$ is* **ergodic** *if*

$$\limsup_{n\to\infty} \Big\langle \big(m_n(A) - \langle A\rangle\big)^2 \Big\rangle = 0$$

for all $A \in \mathcal{A}$.

A pleasing aspect of the theory of translation-invariant states is that these properties of states (extremal, short-range correlations, ergodic) are all equivalent.

THEOREM 3.28. *Let $\langle\cdot\rangle \in \mathcal{G}^{\Phi}_{\text{t.i.}}$. The following properties are equivalent.*

(a) $\langle\cdot\rangle$ is extremal in $\mathcal{G}^{\Phi}$.
(b) $\langle\cdot\rangle$ is extremal in $\mathfrak{E}$.
(c) $\langle\cdot\rangle$ has short-range correlations.
(d) $\langle\cdot\rangle$ is mixing.
(e) $\langle\cdot\rangle$ is ergodic.

Note that we restrict to translation-invariant Gibbs states. Without translation-invariance, the equivalence of (a), (b) and (c) should still hold.

PROOF. We prove that (b) $\Longrightarrow$ (a) $\Longrightarrow$ (c) $\Longrightarrow$ (d) $\Longrightarrow$ (e) $\Longrightarrow$ (b).

(b) $\Longrightarrow$ (a): The contrapositive is clear; indeed, if the state can be decomposed in distinct states in $\mathcal{G}^{\Phi}$, it can also be decomposed among all states.

(a) $\Longrightarrow$ (c): We show the contrapositive, namely that if $\langle\cdot\rangle$ does not have short-range correlations, it is not extremal in the set of KMS states.

Since $\langle\cdot\rangle$ does not have short-range correlations, there exist quasilocal observables A and B_n, with $B_n \in \mathcal{A}_{\Lambda_n^c}$ where $\Lambda_n \Uparrow \mathbb{Z}^d$ and $\|B_n\| = 1$, such that

$$\liminf_{n\to\infty} \big|\langle AB_n\rangle - \langle A\rangle \langle B_n\rangle\big| > 0. \tag{3.62}$$

As pointed out above, we can assume here that the B_n are Hermitian. We can further assume without loss of generality that $A, B_n \in \mathcal{A}_{\rm loc}$, and by adding constants and multiplying by constants we can also assume that $\frac14 \mathbb{1} \leq B_n \leq \frac34 \mathbb{1}$.

By extracting a subsequence, we may assume that $\theta = \lim_{n\to\infty}\langle B_n\rangle$ exists. By further extracting a diagonal subsequence (using separability) we can assume that the following limits exist:

$$\begin{aligned} \langle\cdot\rangle^{(1)} &:= \lim_{n\to\infty} \frac{\langle \cdot B_n\rangle}{\langle B_n\rangle} = \lim_{n\to\infty} \frac{\langle \cdot B_n\rangle}{\theta} \\ \langle\cdot\rangle^{(2)} &:= \lim_{n\to\infty} \frac{\langle \cdot(\mathbb{1} - B_n)\rangle}{1-\langle B_n\rangle} = \lim_{n\to\infty} \frac{\langle\cdot\rangle - \langle \cdot B_n\rangle}{1-\theta} \end{aligned} \tag{3.63}$$

It is not hard to verify that $\langle\cdot\rangle^{(1)}$ and $\langle\cdot\rangle^{(2)}$ are Gibbs states (Exercise 3.13). We also have

$$\langle\cdot\rangle = \theta\langle\cdot\rangle^{(1)} + (1-\theta)\langle\cdot\rangle^{(2)}. \tag{3.64}$$

It remains to check that these states are not all identical. With A the operator in (3.62), we have

$$\langle A\rangle^{(1)} = \lim_{n\to\infty} \frac{\langle AB_n\rangle}{\langle B_n\rangle} \neq \langle A\rangle, \tag{3.65}$$

so $\langle\cdot\rangle^{(1)} \neq \langle\cdot\rangle$.

(c) $\Longrightarrow$ (d): This is obvious.

(d) $\Longrightarrow$ (e): Let $A \in \mathcal{A}$. For every $\varepsilon > 0$ there exists R such that

$$\big|\langle A\tau_x A\rangle - \langle A\rangle^2\big| < \varepsilon \tag{3.66}$$

for all $\|x\| \geq R$. Then

$$\begin{aligned} \langle m_n(A)^2\rangle - \langle A\rangle^2 &= \frac{1}{n^{2d}} \sum_{x,y\in\{1,\dots,n\}^d} \big(\langle \tau_x A \tau_y A\rangle - \langle A\rangle^2\big) \\ &= \frac{1}{n^{2d}} \sum_{\substack{x,y\in\{1,\dots,n\}^d \\ \|x-y\|<R}} \big(\langle \tau_x A \tau_y A\rangle - \langle A\rangle^2\big) + \frac{1}{n^{2d}} \sum_{\substack{x,y\in\{1,\dots,n\}^d \\ \|x-y\|\geq R}} \big(\langle \tau_x A \tau_y A\rangle - \langle A\rangle^2\big). \end{aligned} \tag{3.67}$$

The first term is less than $2\|A\|^2 n^{-d}(2R)^d$ and it vanishes in the limit $n \to \infty$. The second term is less than ε. It follows that

$$\lim_{n\to\infty} \big|\langle m_n(A)^2\rangle - \langle A\rangle^2\big| \leq \varepsilon \tag{3.68}$$

for any $\varepsilon > 0$.

(e) $\Longrightarrow$ (b): We prove the contrapositive, namely that if the state is not extremal, it is not ergodic. If the state $\langle\cdot\rangle$ is not extremal, it is possible to find $\langle\cdot\rangle^{(1)}$ and $\langle\cdot\rangle^{(2)}$

such that $\langle\cdot\rangle = \frac{1}{2}\langle\cdot\rangle^{(1)} + \frac{1}{2}\langle\cdot\rangle^{(2)}$ and with $\langle A\rangle^{(1)} \neq \langle A\rangle^{(2)}$ for some hermitian $A \in \mathcal{A}$. Recalling that $(s+t)^2 < 2s^2 + 2t^2$ if $s \neq t$ we have, for all n,

$$\begin{aligned} \langle A\rangle^2 =& \big(\tfrac{1}{2}\langle A\rangle^{(1)} + \tfrac{1}{2}\langle A\rangle^{(2)}\big)^2 < \tfrac{1}{2}\big(\langle A\rangle^{(1)}\big)^2 + \tfrac{1}{2}\big(\langle A\rangle^{(2)}\big)^2 \\ \leq& \Big(\tfrac{1}{2}\langle m_n(A)^2\rangle^{(1)} + \tfrac{1}{2}\langle m_n(A)^2\rangle^{(2)}\Big) = \langle m_n(A)^2\rangle. \end{aligned} \tag{3.69}$$

The second inequality holds because the variance is nonnegative:

$$0 \leq \langle (m_n(A) - \langle A\rangle)^2\rangle = \langle (m_n(A)^2\rangle - \langle A\rangle^2. \tag{3.70}$$

Taking $n \to \infty$ in (3.69) we get

$$\liminf_{n\to\infty} \langle m_n(A)^2\rangle > \langle A\rangle^2. \tag{3.71}$$

Because of the strict inequality the state $\langle\cdot\rangle$ is not ergodic. □

3.5. Decomposition of states

We now show that any equilibrium state is a convex combination of extremal states. Since $\mathcal{G}^\Phi \subset \mathcal{A}^*$, and $\mathcal{A}^*$ is a Banach space with the usual operator norm, the set of Gibbs states is a metric space. It is also a measurable space with the Borel σ-algebra (the one that is generated by open sets).

THEOREM 3.29. *Let $\Phi \in \mathcal{I}$ and $\langle\cdot\rangle \in \mathcal{G}^\Phi_{\text{tr.inv}}$. There exists a measure μ on $\mathcal{G}^\Phi$, that is concentrated on the extremal states of $\mathcal{G}^\Phi$, such that for all $A \in \mathcal{A}$, we have*

$$\langle A\rangle = \int_{\mathcal{G}^\Phi} \gamma(A)\,\mu(\mathrm{d}\gamma).$$

If the measure is concentrated on $\mathcal{G}^\Phi_{\text{tr.inv.}}$, it is unique.

Theorem 3.29 is based on Choquet's theory, whose main result can be formulated as follows.

PROPOSITION 3.30 (Choquet). *Let K be a metrisable compact convex set and $\kappa \in K$. Then there exists a probability measure μ on K such that*

(a) μ is concentrated on the extremal points of K.
(b) For any affine function $f : K \to \mathbb{R}$ we have $f(\kappa) = \int_K f(\eta)\mu(\mathrm{d}\eta)$.

PROOF OF THEOREM 3.29. We apply Choquet's result to $K = \mathcal{G}^\Phi$. For this, note that $\mathcal{A}$ is separable, that the linear functionals on $\mathcal{A}$ of norm 1 form a compact set in the weak* topology (Banach-Alaoglu Theorem), and any weak* compact Hausdorff space is metrisable (the topology is generated by a countable family of seminorms, so it is second countable, which is enough for the existence of a metric[2]). Finally, closed subsets of compact sets are compact, and it is easy to see that $\mathcal{G}^\Phi$ is a closed subset

[2]Reference: Theorem 2.6.23 of Megginson's An Introduction to Banach Space Theory.

of the set of observables of norm 1: If $\langle\cdot\rangle_n \in \mathcal{G}^\Phi$ is a net that converges to $\langle\cdot\rangle$ (in the weak* topology), then for any $A, B \in \tilde{\mathcal{A}}$:

$$\langle AB\rangle = \lim_n \langle AB\rangle_n = \lim_n \langle B\alpha_{\mathrm{i}}^\Phi(A)\rangle_n = \langle B\alpha_{\mathrm{i}}^\Phi(A)\rangle. \tag{3.72}$$

Then $\langle\cdot\rangle \in \mathcal{G}^\Phi$. (One can prove in the same way that positive normalised linear functionals form a closed set.)

For $A \in \mathcal{A}$ we consider the affine function $f_A(\gamma) = \gamma(A)$, $\gamma \in \mathcal{G}^\Phi$. The existence of the measure in Theorem 3.29 then follows from Proposition 3.30.

There remains to establish uniqueness. Let $\langle\cdot\rangle$ be a state and μ a measure on $\mathcal{G}^\Phi_{\text{tr.inv.}}$ such that $\langle\cdot\rangle = \int \gamma(\cdot)\mu(\mathrm{d}\gamma)$ and where μ is concentrated on extremal states. We check that the μ-expectation of any continuous function depends solely on the state. Then μ is indeed unique.

Recall the Stone–Weierstrass theorem (continuous functions can be approximated by polynomials); it is then enough to check expectations of polynomials. Let $f_{A_1}, \dots, f_{A_k}$ be functions as above, for some $A_1, \dots, A_k \in \mathcal{A}$. Then, since the measure μ is concentrated on extremal states with short-range correlations, we have

$$\begin{aligned} \mu(f_{A_1} \dots f_{A_k}) &= \int_K \gamma(A_1) \dots \gamma(A_k)\mu(\mathrm{d}\gamma) \\ &= \lim_{n\to\infty} \int_K \gamma(m_n(A_1)) \dots \gamma(m_n(A_k))\mu(\mathrm{d}\gamma) \\ &= \lim_{n\to\infty} \int_K \gamma\big(m_n(A_1) \dots m_n(A_k)\big)\mu(\mathrm{d}\gamma) \\ &= \lim_{n\to\infty} \big\langle m_n(A_1) \dots m_n(A_k)\big\rangle. \end{aligned} \tag{3.73}$$

The last term does not depend explicitly on μ, but solely on the state. □

Remark 3.1 (On the variational characterisation). *In Theorem 3.14, Gibbs states $\boldsymbol{\rho}$ are characterised as the minimisers of the free energy functional $f^{\beta,\Phi}(\boldsymbol{\rho})$. Note that the latter is an affine function of states. The minimum of an affine function on a convex set is attained at an extreme point. Thus, in the infimum in Theorem 3.14, we can restrict to* extremal *states $\boldsymbol{\rho}$.*

3.6. Exercises

Here $\mathcal{H}$ always denotes a separable Hilbert space, possibly infinite-dimensional.

Exercise 3.1.

(a) *Show that any $A \in \mathcal{B}(\mathcal{H})$ can be written as $A = B + \mathrm{i}C$ where $B, C \in \mathcal{B}(\mathcal{H})$ are Hermitian.*

(b) *Show that the operator norm (3.1) on $\mathcal{B}(\mathcal{H})$ satisfies $\|AB\| \le \|A\|\|B\|$ for all matrices A, B.*

Exercise 3.2. *Consider a state $\langle\cdot\rangle$ on $\mathcal{B}(\mathcal{H})$ and $A, B \in \mathcal{B}(\mathcal{H})$.*

(a) Show that $\langle A^* \rangle = \overline{\langle A \rangle}$.
(b) Prove the Cauchy–Schwarz inequality, $|\langle A^* B\rangle|^2 \leq \langle A^* A\rangle\langle B^* B\rangle$.
(c) Show that $|\langle A\rangle|^2 \leq \langle A^* A\rangle$. *Deduce that* $\|\langle\cdot\rangle\| = 1$.

EXERCISE 3.3. *Consider a tensor product* $\mathcal{H}_1 \otimes \mathcal{H}_2$ *of two Hilbert spaces. Show that*
(a) $\|v \otimes w\| = \|v\|\|w\|$ *for all* $v \in \mathcal{H}_1$, $w \in \mathcal{H}_2$
(b) $\|A \otimes B\| = \|A\|\|B\|$ *for all* $A \in \mathcal{B}(\mathcal{H}_1)$, $B \in \mathcal{B}(\mathcal{H}_2)$.
Deduce that $\|\iota A\| = \|A\|$ *where* ι *is the injection given in (3.17).*

EXERCISE 3.4 (Bloch sphere). *Let* $\vec{\sigma} = (\sigma^{(1)}, \sigma^{(2)}, \sigma^{(3)})$ *denote the Pauli matrices and* $\vec{a} = (a_1, a_2, a_3)$ *a vector in* $\mathbb{R}^3$. *Consider the matrix*

$$X = \tfrac{1}{2}(\mathbb{1} + \vec{a}\cdot\vec{\sigma}).$$

(a) Find the eigenvalues of X *in terms of* $\vec{a}$ *and use this to determine conditions on* $\vec{a}$ *under which* X *is positive definite.*
(b) Show that any 2×2 *density matrix* X *can be written this way.*
(c) Now suppose $Y = \frac{1}{2}(\mathbb{1} + \vec{b}\cdot\vec{\sigma})$. *Write* $\mathrm{Tr}\,(XY)$ *in terms of* $\vec{a}$ *and* $\vec{b}$, *and using this (or otherwise) prove the inequality*

$$x_1 y_2 + x_2 y_1 \leq \mathrm{Tr}\,(XY) \leq x_1 y_1 + x_2 y_2$$

for arbitrary positive definite 2×2 *matrices* X, Y *where* $x_1 \geq x_2 \geq 0$ *are the eigenvalues of* X *and where* $y_1 \geq y_2 \geq 0$ *are the eigenvalues of* Y.

EXERCISE 3.5. *Show that* $A \mapsto \langle A\rangle_{H,\beta} = \frac{1}{Z_{H,\beta}} \mathrm{Tr}\, A\, \mathrm{e}^{-\beta H}$ *satisfies the definition of states on a Hilbert space* $\mathcal{H}$.

Exercises 3.6, 3.7 and 3.7 establish the remaining parts of Proposition 3.3. We let $\mathcal{H}$ be a Hilbert space and $H = H^* \in \mathcal{B}(\mathcal{H})$.

EXERCISE 3.6 (Tangent condition). *Let* $F_\beta(H) := -\frac{1}{\beta}\log \mathrm{Tr}\; \mathrm{e}^{-\beta H}$. *Show that the Gibbs state* $\langle\cdot\rangle_{H,\beta}$ *is the unique state such that* $F_\beta(H + A) \leq F_\beta(A) + \langle A\rangle$ *for all* $A = A^* \in \mathcal{B}(\mathcal{H})$. *You may assume the concavity of* $F_\beta(\cdot)$.

EXERCISE 3.7 (Variational principle). *Show that* $\mathrm{e}^{-\beta H}/\mathrm{Tr}\; \mathrm{e}^{-\beta H}$ *is the unique density matrix* ρ *which minimizes the function* $\mathcal{F}_\beta(\rho) := \mathrm{Tr}\, H\rho + \frac{1}{\beta}\mathrm{Tr}\,\rho\log\rho$.

EXERCISE 3.8 (RAS condition). *Show that the Gibbs state* $\langle\cdot\rangle_{H,\beta}$ *is the unique state such that*

$$\langle A^*[H, A]\rangle \geq \frac{1}{\beta}\langle A^* A\rangle \log\frac{\langle A^* A\rangle}{\langle AA^*\rangle} \tag{3.74}$$

for all $A \in \mathcal{B}(\mathcal{H})$.

Hints: To show that the Gibbs state satisfies RAS, use the inner product

$$A, B \mapsto (A, B)_s = \langle\alpha_{-\mathrm{i}s}(A^*)B\rangle = \langle A^*\alpha_{\mathrm{i}s}(B)\rangle \tag{3.75}$$

(you may assume that this is an inner product) and show that the function $f(s) = (A, A)_s$ *is log-convex. For the other direction, consider the RAS-inequality for* $A = 1 + tB$ *with* t *small and show that* H *commutes with the density matrix.*

EXERCISE 3.9. *Use Proposition 3.3(b) to show that, for any translation-invariant state* $\boldsymbol{\rho}$,

$$f^{\beta,\Phi}(\boldsymbol{\rho}) \geq f(\Phi,\beta).$$

EXERCISE 3.10. *Show that* $A \mapsto \operatorname{tr} A$ *is the unique Gibbs state at* $\beta = 0$.

EXERCISE 3.11. *Prove that a state* $\langle\cdot\rangle$ *satisfies the KMS condition if and only if* $\langle A^*A\rangle = \langle A\alpha_{\mathrm{i}\beta}(A^*)\rangle$ *for all* $A \in \tilde{\mathcal{A}}$.

EXERCISE 3.12. *Use Liouville's theorem to show that if a state* $\langle\cdot\rangle$ *satisfies the KMS condition, then it is invariant under the time evolution given by* α_z^Φ, *i.e.* $\langle\alpha_z^\Phi(A)\rangle = \langle A\rangle$ *for all* $z \in \mathbb{C}$.

EXERCISE 3.13. *Let* $\langle\cdot\rangle$ *be a KMS state,* $\Lambda_n \Uparrow \mathbb{Z}^d$ *and let* $B_n \in \mathcal{A}_{\Lambda_n^c}$ *be positive semidefinite operators such that the limits* $\theta := \lim_{n\to\infty}\langle B_n\rangle > 0$ *and* $\langle\cdot\rangle' := \lim_{n\to\infty}\langle\cdot B_n\rangle/\langle B_n\rangle$ *exist. Show that* $\langle\cdot\rangle'$ *is a KMS state.*

Hint: use the fact that for any local observable C *we have* $[C, B_n] = 0$ *for* n *large enough and check the RAS condition.*

EXERCISE 3.14. *Let* $\langle\cdot\rangle \in \mathcal{G}^{\beta\Phi}$ *be a Gibbs state and let* U *be a unitary matrix such that for each* $X \Subset \mathbb{Z}^d$ *we have*

$$\bigotimes_{x\in X} U_x^* \Phi_X \bigotimes_{x\in X} U_x = \Phi_X.$$

Define a state $\langle\cdot\rangle'$ *by, for each* $\Lambda \Subset \mathbb{Z}^d$ *and each* $A \in \mathcal{A}_\Lambda$,

$$\langle A\rangle' := \Big\langle \bigotimes_{x\in\Lambda} U_x^* A \bigotimes_{x\in\Lambda} U_x \Big\rangle.$$

Show that $\langle\cdot\rangle' \in \mathcal{G}^{\beta\Phi}$.

EXERCISE 3.15. *Let* $(a_\Lambda)_{\Lambda\Subset\mathbb{Z}^d}$ *be a set-indexed sequence. Assume that, along any sequence* $\Lambda_n \uparrow \mathbb{Z}^d$, *the limit* $\lim_n a_{\Lambda_n}$ *exists. Check that this limit does not depend on the choice of the sequence.*

The same property holds for van Hove sequences, with the same proof.

BIBLIOGRAPHICAL REFERENCES

The topics of this chapter are covered in the books of Ruelle [**28**], Israel [**21**], Simon [**29**]. We are grateful to Mathieu Lewin for sharing his notes on the RAS condition [**23**].