CHAPTER 3

# Pressure and tangent functionals

The statistical mechanics definition of the pressure, see Eq. (3.4) below, is a fundamental notion. It relates the microscopic description (based on the local knowledge encoded in interactions) to a macroscopic quantity (the pressure is a thermodynamic notion). The connection to physics is a bit indirect, as it relates to models of particles in the grand-canonical ensemble. Besides, the heuristics are better explained in the context of the Boltzmann entropy in the microcanonical ensemble. The curious reader is encouraged to read more about it in introductory textbooks of statistical physics. Here we take it as a mathematical definition.

## 3.1. Finite-volume pressure

Given a Hilbert space $\mathcal{H}$ and the space of hermitian operators $\mathcal{B}_{\mathrm{h}}(\mathcal{H})$, we consider the following function:

$$P(a) = \log \operatorname{Tr} \mathrm{e}^{-a}, \qquad a \in \mathcal{B}_{\mathrm{h}}(\mathcal{H}). \tag{3.1}$$

If $\mathcal{H}$ is infinite-dimensional it is possible (and allowed) that $P(a) = \infty$. We should take $a = \beta H$, with $\beta$ the inverse temperature and $H$ the hamiltonian of the system, to get the physical pressure.

Proposition 3.1.

(a) *The function $P$ is a convex function on the space of hermitian operators.*

(b) *We have the bound $|P(a) - P(b)| \leq \|a - b\|$.*

*Let $H$ be a fixed hermitian operator such that $P(H)$ is finite.*

(c) *The Gibbs state $\langle a \rangle = \operatorname{Tr} a \, \mathrm{e}^{-H} / \operatorname{Tr} \mathrm{e}^{-H}$ is tangent to the pressure at $H$ in the sense that for all self-adjoint operators $a$, we have*

$$P(H + a) \geq P(H) - \langle a \rangle.$$

See Figure 3.1 for an illustration of the last item. Notice that the tangent is unique here; later, in the infinite-volume situation, it may not be unique.

Proof. For the claim (a) we use the Golden–Thompson inequality (Proposition 2.4) and then the Hölder inequality (Proposition 2.3). For $s \in [0, 1]$, we

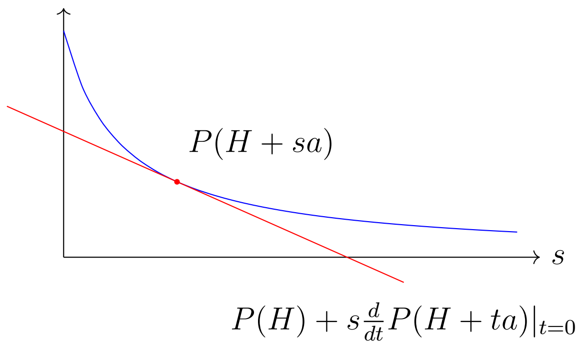


FIGURE 3.1. An illustration of tangents to the pressure: we have that $P(H+sa) \geq P(H) - s\langle a \rangle$ where $-\langle a \rangle = \frac{d}{dt}P(H+ta)|_{t=0}$. Note that $P(H+sa)$ is non-increasing in $s$ for positive-definite $a$, which motivates the choice of sign in front of $\langle a \rangle$.

have

$$\begin{aligned} P(sa+(1-s)b) &= \log \operatorname{Tr} \mathrm{e}^{-sa-(1-s)b} \\ &\leq \log \operatorname{Tr} \mathrm{e}^{-sa}\, \mathrm{e}^{-(1-s)b} \\ &\leq \log\Big[\Big(\operatorname{Tr}\big(\mathrm{e}^{-sa}\big)^{\frac{1}{s}}\Big)^{s}\Big(\operatorname{Tr}\big(\mathrm{e}^{-(1-s)b}\big)^{\frac{1}{1-s}}\Big)^{1-s}\Big] \\ &= sP(a) + (1-s)P(b). \end{aligned} \tag{3.2}$$

For the claim (b), let $(\varphi_j)$ be an orthonormal basis of eigenvectors of $a$ with eigenvalues $(\alpha_j)$. Starting with Peierls inequality (Proposition 2.7) we have

$$\operatorname{Tr} \mathrm{e}^{-b} \geq \sum_j \mathrm{e}^{-\langle \varphi_j, b\varphi_j \rangle} \geq \mathrm{e}^{-\|a-b\|} \sum_j \mathrm{e}^{-\alpha_j} = \mathrm{e}^{-\|a-b\|} \operatorname{Tr} \mathrm{e}^{-a}. \tag{3.3}$$

It follows that $P(b) - P(a) \geq -\|a-b\|$. The same inequality holds after exchanging $a$ and $b$, which gives (b).

For the claim (c), let $H$ and $a$ be fixed self-adjoint operators and consider the function $f : s \mapsto P(H+sa)$. It is convex by (a) and the derivative at $s=0$ is equal to $-\langle a \rangle$. □

### 3.2. Infinite-volume limit of the pressure

Recall the definition (2.35) of the hamiltonian $H_\Lambda^\Phi$; the finite-volume **pressure** in the domain $\Lambda \Subset \mathbb{Z}^d$ is defined as a function of interactions, namely

$$p_\Lambda(\Phi) = \frac{1}{|\Lambda|} \log \operatorname{Tr} \mathrm{e}^{-H_\Lambda^\Phi}. \tag{3.4}$$

(The inverse temperature $\beta$ has been included in the interaction.) The following property is important and, since $H_\Lambda^{\Phi+\Psi} = H_\Lambda^\Phi + H_\Lambda^\Psi$, it follows straightforwardly from Proposition 3.1:

PROPOSITION 3.2. *The pressure $p_\Lambda$ is a convex function of the interactions.*

We now study the infinite volume limit of the pressure. We first consider the boxes $\Lambda_n = \{1, \dots, n\}^d$ of size $n$ and volume $n^d$. We consider more general "van Hove sequences" of increasing domains below.

LEMMA 3.3. *Assume that $\Phi \in \mathcal{I}$, i.e. $|||\Phi||| < \infty$. Then there exists a function $p : \mathcal{I} \to \mathbb{R}$ such that*

$$p(\Phi) = \lim_{n\to\infty} p_{\Lambda_n}(\Phi)$$

*where $\Lambda_n = \{1, \dots, n\}^d$. Further, the function $p$ is convex and it satisfies*

$$|p(\Phi) - p(\Psi)| \le |||\Phi - \Psi|||.$$

PROOF. We have for all $\Lambda \Subset \mathbb{Z}^d$ that

$$\|H_\Lambda^\Phi\| \le \sum_{X\subset\Lambda} \|\Phi_X\| = \sum_{x\in\Lambda} \sum_{\substack{X\subset\Lambda \\ X\ni x}} \frac{\|\Phi_X\|}{|X|} \le |\Lambda| \, |||\Phi|||. \tag{3.5}$$

Together with Proposition 3.1 (b), this implies that

$$\big|p_\Lambda(\Phi) - p_\Lambda(\Psi)\big| \le \frac{1}{|\Lambda|} \|H_\Lambda^\Phi - H_\Lambda^\Psi\| \le |||\Phi - \Psi|||. \tag{3.6}$$

This property allows us to prove convergence for a dense set of interactions, namely the set of $\Phi$ satisfying $\|\Phi\|_0 = \sum_{X\ni 0} \|\Phi_X\| < \infty$, and to invoke a continuity argument to extend it to all of $\mathcal{I}$. This also proves the last claim of the theorem. Notice that convexity of $p_\Lambda$ was stated in Proposition 3.2.

The proof of the existence of the infinite volume limit uses a subadditive argument. The pressure in a big domain is compared with that of smaller domains inside the big one, by neglecting interactions between the small domains. In order to do this, we need the following inequality for hermitian matrices $A, B$ (its proof is Exercise 3.1).

$$\mathrm{Tr}\, \mathrm{e}^{a-\|b\|} \le \mathrm{Tr}\, \mathrm{e}^{a+b} \le \mathrm{Tr}\, \mathrm{e}^{a+\|b\|}. \tag{3.7}$$

Let $m, n, k, r$ be integers such that $n = km + r$ and $0 \le r < m$. The box $\Lambda_n$ is the disjoint union of $k^d$ boxes of size $m$ and of some remaining sites, see Figure 3.2 for an illustration. We get an inequality for the partition function in

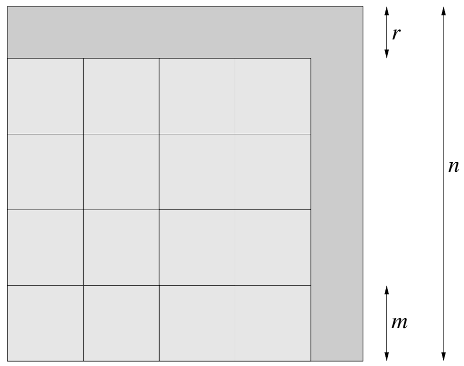


FIGURE 3.2. The large box of size $n$ is decomposed in $k^d$ boxes of size $m$; there are no more than $drn^{d-1}$ remaining sites in the darker area.

$\Lambda_n$ by replacing all $\Phi_X$, where $X$ is not inside a single box of size $m$, by the norm $\|\Phi_X\|_0$. The boxes $\Lambda_m$ become independent, and

$$\begin{aligned} Z_{\Lambda_n}(\Phi) &= \operatorname{Tr}_{\Lambda_n} \exp\Bigl(-\sum_{X\subset\Lambda} \Phi_X\Bigr) \\ &\geq \Bigl[\operatorname{Tr}_{\mathcal{H}_{\Lambda_m}} \exp\Bigl(-\sum_{X\subset\Lambda_m} \Phi_X\Bigr)\Bigr]^{k^d} \mathrm{e}^{-(dk^d m^{d-1}+drn^{d-1})\|\Phi\|_0} \\ &= [Z_{\Lambda_m}(\Phi)]^{k^d} \mathrm{e}^{-(dk^d m^{d-1}+drn^{d-1})\|\Phi\|_0}. \end{aligned} \tag{3.8}$$

The term $dk^d m^{d-1}$ is an upper bound for the number of sites at the boundary between boxes; each set $X$ that involves two boxes or more, must contain at least one of these sites. The term $drn^{d-1}$ is an upper bound for the number of sites in the region of $\Lambda_n$ outside the small boxes. We then obtain a subbaditive relation for the pressure:

$$p_{\Lambda_n}(\Phi) \geq \frac{(km)^d}{n^d} p_{\Lambda_m}(\Phi) - \frac{dk^d m^{d-1} + drn^{d-1}}{n^d} \|\Phi\|_0. \tag{3.9}$$

Then, since $\frac{km}{n} \to 1$ as $n \to \infty$,

$$\liminf_{n\to\infty} p_{\Lambda_n}(\Phi) \geq p_{\Lambda_m}(\Phi) - \frac{d}{m}\|\Phi\|_0. \tag{3.10}$$

Taking the lim sup over $m$ in the right side, we see that it is smaller or equal to the lim inf. It is not hard to verify that $p_\Lambda(\Phi)$ is bounded uniformly in $\Lambda$, so the limit necessarily exists. □

Periodic boundary conditions are convenient since finite-volume expressions are translation invariant. The notions are natural and intuitive but should be clarified nonetheless. Let $\Lambda_n^{\rm per} = (\mathbb{Z}/n\mathbb{Z})^d$ denote the periodic box of size $n$. Formally, elements of $\Lambda_n^{\rm per}$ are equivalence classes of sites where $x \sim y$ whenever

$x_i - y_i = 0 \mod n$ for $i = 1, \dots, d$. Given the interaction $\Phi = (\Phi_X)_{X \Subset \mathbb{Z}^d}$ the hamiltonian is

$$H^{\Phi}_{\Lambda_n^{\text{per}}} = \sum_{\substack{X \ni 0 \\ \text{diam} X \leq n}} \frac{1}{|X|} \sum_{x \in \{1,\dots,n\}^d} \Phi_{X+x}. \tag{3.11}$$

In the above equation the interaction $\Phi_{X+x}$ is supported on the set in $\Lambda_n^{\text{per}}$ that consists of equivalence classes of sites of $X + x$.

The pressure can also be obtained by taking a sequence of periodic boxes of increases sizes.

Corollary 3.4 (Thermodynamic limit with periodic boundary conditions). *Let $(\Lambda_n^{\text{per}})$ be the sequence of cubes in $\mathbb{Z}^d$ of size $n$ with periodic boundary conditions. Then $(p_{\Lambda_n^{\text{per}}}(\Phi))_{n \geq 1}$ converges pointwise to the same function $p(\Phi)$ as in Theorem 3.6.*

This follows from $|p_{\Lambda_n^{\text{per}}}(\Phi) - p_{\Lambda_n}(\Phi)| \leq \frac{d}{n} \|\Phi\|_0$, which is not too hard to prove, and Theorem 3.6.

The next step is to take the limit of infinite domains, in such a way that boundary effects vanish. This prompts the following notion.

Definition 3.5. *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 $\partial_r \Lambda = \{x \in \Lambda^{\text{c}} : \text{dist}(x, \Lambda) \leq r\}$.*

We use the notation $\Lambda_n \Uparrow \mathbb{Z}^d$ to say that the sequence converges to $\mathbb{Z}^d$ in the sense of van Hove. Notice that $(\Lambda_n = \{1, \dots, n\}^d)$ is not a van Hove sequence since it does not invade $\mathbb{Z}^d$. We now state one of the major results in statistical mechanics, namely the existence of the infinite volume pressure.

Theorem 3.6. *Assume that $\Phi \in \mathcal{I}$, i.e. $\|\Phi\| < \infty$. Then*

$$p(\Phi) = \lim_{n \to \infty} p_{\Lambda_n}(\Phi)$$

*along all sequences of domains such that $\Lambda_n \Uparrow \mathbb{Z}^d$. The function $p$ is the same as in Lemma 3.3.*

Proof. Let us pave $\mathbb{Z}^d$ with boxes of size $m$ and let $B_i$, $i = 1, \dots, k$, denote those boxes that are inside $\Lambda_n$. Let

$$C = \Lambda_n \setminus \cup_{i=1}^k B_i. \tag{3.12}$$

We have the bounds

$$Z_B(\Phi)^k \,\mathrm{e}^{-(dkm^{d-1}+|C|)\|\Phi\|_0} \leq Z_{\Lambda_n}(\Phi) \leq Z_B(\phi)^k \,\mathrm{e}^{(dkm^{d-1}+|C|)\|\Phi\|_0} N^{|C|}. \tag{3.13}$$

Then

$$\tfrac{km^d}{|\Lambda_n|} p_B(\Phi) - \tfrac{dkm^{d-1}+|C|}{\Lambda_n|} \|\Phi\|_0 \leq p_{\Lambda_n}(\Phi) \leq \tfrac{km^d}{|\Lambda_n|} p_B(\Phi) + \tfrac{dkm^{d-1}+|C|}{\Lambda_n|} \|\Phi\|_0 + \tfrac{|C| \log N}{|\Lambda_n|}. \tag{3.14}$$

There remains to verify to find the limits $n \to \infty$ of the various terms above. We have $\frac{km^d}{|\Lambda_n|} \leq 1$ and $\frac{km^d + |\partial\Lambda_n| m^d}{|\Lambda_n|} \geq 1$, so that

$$1 - m^d \tfrac{|\partial\Lambda_n|}{|\Lambda_n|} \leq \tfrac{km^d}{|\Lambda_n|} \leq 1. \tag{3.15}$$

Then $\frac{km^d}{|\Lambda_n|} \to 1$ as $n \to \infty$. Next we have $|C| \leq m^d |\partial\Lambda_n|$ so that $\frac{|C|}{|\Lambda_n|} \to 0$. We can then take the limit $n \to \infty$ and we get for any $m$ that

$$p_B(\Phi) - \tfrac{d}{m} \|\Phi\|_0 \leq \limsup_{n\to\infty} p_{\Lambda_n}(\Phi) \leq p_B(\Phi) + \tfrac{d}{m} \|\Phi\|_0. \tag{3.16}$$

(The inequalities hold with lim inf too.) Taking $m \to \infty$, both the left and right sides converge to the function $p(\Phi)$ of Lemma 3.3. □

## 3.3. Tangent functionals and Gibbs states

We use the infinite-volume pressure to define infinite-volume states. Since the definition is somewhat abstract we first discuss the finite domain $\Lambda_n^{\rm per}$. This is actually similar to Proposition 3.1 (c). Given the local hermitian operator $a \in \mathcal{A}_\Lambda$ for some $\Lambda \Subset \mathbb{Z}^d$, we define the interaction $\Psi_a$ using translates of $a$, namely

$$(\Psi_a)_X = \begin{cases} \tau_x a & \text{if } X = \Lambda + x \text{ for some } x \in \mathbb{Z}^d, \\ 0 & \text{otherwise.} \end{cases} \tag{3.17}$$

Now let $\lambda$ be a linear functional on $\mathcal{I}$ that is tangent to the pressure $p_{\Lambda_n^{\rm per}}$ at $\Psi$, in the sense that[1]

$$p_{\Lambda_n^{\rm per}}(\Phi + \Psi) \geq p_{\Lambda_n^{\rm per}}(\Phi) - \lambda(\Psi) \qquad \forall \Psi \in \mathcal{I}. \tag{3.18}$$

Since $p_{\Lambda_n^{\rm per}}$ is a smooth convex function of interactions, the linear functional exists and is unique. Further we have for all $a \in \mathcal{A}_\Lambda$, $\Lambda \subset \Lambda_n^{\rm per}$, that

$$\lambda(\Psi_a) = -\frac{\mathrm{d}}{\mathrm{d}t} p_{\Lambda_n^{\rm per}}(\Phi + t\Psi_a)\Big|_{t=0} = \frac{1}{Z_{\Lambda_n^{\rm per}}(\Phi)} \operatorname{Tr} a \,\mathrm{e}^{-H^\Phi_{\Lambda_n^{\rm per}}}. \tag{3.19}$$

We can define the state $\langle\cdot\rangle$ using the relation $\langle a \rangle = \lambda(\Psi_a)$; then $\langle\cdot\rangle$ is in fact the finite-volume Gibbs state.

We now generalise this setting to infinite volumes. We consider tangent functionals to the (infinite-volume) pressure and prove that they indeed define states.

[1] To be precise: $-\lambda$ is tangent to the pressure.

DEFINITION 3.7 (Tangent functional). *A linear functional $\lambda \in \mathcal{I}^*$ is tangent to the pressure $p$ at $\Phi \in \mathcal{I}$ if*

$$p(\Phi + \Psi) \geq p(\Phi) - \lambda(\Psi)$$

*for all $\Psi \in \mathcal{I}$. The set of tangent functionals at $\Phi$ is denoted $\mathcal{L}^\Phi$.*

If $\lambda \in \mathcal{I}^*$, we define the following linear functional on $\mathcal{A}$; for $a$ self-adjoint, let

$$\langle a \rangle_\lambda = \lambda(\Psi_a). \tag{3.20}$$

This is a real linear functional, and there is a unique extension to a complex linear functional on $\mathcal{A}$ (see Exercise 3.2). We now check that $\langle \cdot \rangle_\lambda$ is a state; we assume that $\lambda$ is tangent to the pressure.

PROPOSITION 3.8. *Let $\lambda \in \mathcal{L}^\Phi$. Then*

(a) *Suppose $\Lambda \subset \Lambda'$, $a \in \mathcal{A}_\Lambda$, $a' \in \mathcal{A}_{\Lambda'}$ such that $a' = a \otimes \mathbb{1}_{\Lambda' \setminus \Lambda}$; then $\langle a \rangle_\lambda = \langle a' \rangle_\lambda$.*
(b) *$\langle \mathbb{1} \rangle_\lambda = 1$.*
(c) *$\langle a \rangle_\lambda \geq 0$ for all $a \geq 0$.*

Item (a) verifies that the definition is consistent, as $a$ and $a'$ are two different ways to write the same observable. It is clear that $\langle \cdot \rangle_\lambda$ is linear and (b) and (c) imply that it is indeed a state.

PROOF. (a) One can check that $\| H_{\Lambda''}^{\Psi_a} - H_{\Lambda''}^{\Psi_{a'}} \| \leq \text{const } |\partial \Lambda''|$ where the constant depends on $\Lambda, \Lambda', a, a'$ but not on $\Lambda''$. It follows that $p(\Phi + t(\Psi_a - \Psi_{a'})) = p(\Phi)$ for all $t \in \mathbb{R}$. If $\lambda$ is tangent to the pressure we must have $\lambda(\Psi_a - \Psi_{a'}) = 0$, so that $\lambda(\Psi_a) = \lambda(\Psi_{a'})$ and $\langle a \rangle = \langle a' \rangle$.

(b) Let us define the constant interaction by

$$\Psi_X = \begin{cases} \mathbb{1} & \text{if } X = \{x\} \text{ for some } x \in \mathbb{Z}^d, \\ 0 & \text{otherwise.} \end{cases} \tag{3.21}$$

Then $p(\Phi + t\Psi) = p(\Phi) - t$ and Definition 3.7 implies that $-t \geq -t \langle \mathbb{1} \rangle$ for all $t \in \mathbb{R}$; hence $\langle \mathbb{1} \rangle = 1$.

(c) If $a \geq 0$ we have $H_\Lambda^{\Psi_a} \geq 0$; using the Golden-Thompson inequality we have

$$\operatorname{Tr} \mathrm{e}^{-H_\Lambda^\Phi - H_\Lambda^{\Psi_a}} \leq \operatorname{Tr} \mathrm{e}^{-H_\Lambda^\Phi} \mathrm{e}^{-H_\Lambda^{\Psi_a}} \leq \operatorname{Tr} \mathrm{e}^{-H_\Lambda^\Phi}, \tag{3.22}$$

so that $p(\Phi + \Psi_a) \leq p(\Phi)$. Together with Definition 3.7 we get $\langle a \rangle \geq 0$. □

We now check that linear functionals are in one-to-one correspondence with states. We consider here a more general setting where the functionals are not necessarily tangent to the pressure. There is a minor annoyance, namely that states need to be consistent, although we have not defined this notion for the functionals of interactions. This is why we study the inverse map, which starts with states and therefore enforces consistency. Let us introduce

$$a_\Psi = \sum_{X \ni 0} \frac{1}{|X|} \Psi_X. \tag{3.23}$$

Notice that $\|a_\Psi\| \leq |||\Psi|||$. Given $\langle\cdot\rangle \in \mathcal{A}^*$, let us define the linear functional on $\mathcal{I}$ by

$$\lambda(\Psi) = \langle a_\Psi \rangle. \tag{3.24}$$

PROPOSITION 3.9.

(a) *If $\lambda$ satisfies (3.24), then $\langle a \rangle = \lambda(\Psi_a)$ for all $a \in \mathcal{A}$.*

(b) *The map $\langle\cdot\rangle \mapsto \lambda$ in (3.24) is an isometry ($\|\langle\cdot\rangle\| = \|\lambda\|$) and a homeomorphism in the weak-* topologies (i.e. if $\langle a \rangle_n \to \langle a \rangle$ for all $a \in \mathcal{A}$, then $\lambda_n(\Psi) \to \lambda(\Psi)$ for all $\Psi \in \mathcal{I}$).*

Remark: the proposition implies that if $\langle\cdot\rangle$ and $\langle\cdot\rangle'$ are two states, and $\lambda$ and $\lambda'$ their images by the map (3.24), then $\|\langle\cdot\rangle - \langle\cdot\rangle'\| = \|\lambda - \lambda'\|$.

PROOF. (a) Straightforward, using translation invariance.
(b) Since $\|a_\Psi\| \leq |||\Psi|||$ we have

$$\|\lambda\| = \sup_{|||\Psi|||=1} |\lambda(\Psi)| = \sup_{|||\Psi|||=1} |\langle a_\Psi \rangle| \leq \sup_{|||\Psi|||=1} \|\langle\cdot\rangle\| \, \|a_\Psi\| \leq \|\langle\cdot\rangle\|. \tag{3.25}$$

Conversely, using the identity (a) and $|||\Psi_a||| = \|a\|$, we have

$$\|\langle\cdot\rangle\| = \sup_{\|a\|=1} |\langle a \rangle| = \sup_{\|a\|=1} |\lambda(\Psi_a)| \leq \|\lambda\|. \tag{3.26}$$

The second property is straightforward: If $\langle a \rangle_n \to \langle a \rangle$ for all $a \in \mathcal{A}$, then $\lambda_n(\Psi) = \langle a_\Psi \rangle_n \to \langle a_\Psi \rangle = \lambda(\Psi)$. □

These considerations allow for our second definition of infinite-volume equilibrium states.

DEFINITION 3.10 (States as tangent functionals). *A state $\langle\cdot\rangle$ on $\mathcal{A}$ is an equilibrium state for the interaction $\Phi$, in the sense of tangent functionals to the pressure, if*

$$p(\Phi + \Psi) \geq p(\Phi) - \langle a_\Psi \rangle$$

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

We denote by $\mathcal{G}^{\Phi}_{\text{tr.inv.}}$ the set of (translation invariant) states on $\mathcal{A}$ that are tangent to the pressure at $\Phi$. This definition is more general than that of states as cluster points.

PROPOSITION 3.11. *Any cluster state of Definition 2.10 satisfies Definition 3.10.*

PROOF. Let $\Phi, \Psi_n \in \mathcal{I}$ such that $|||\Psi_n||| \to 0$, and $\Lambda_n \Uparrow \mathbb{Z}^d$, such that the finite-volume Gibbs states $\langle\cdot\rangle_{\Lambda_n}^{\Phi+\Psi_n}$ converge as $n \to \infty$ (pointwise in $\mathcal{A}_{\rm loc}$). By Proposition 3.1 we have

$$p_{\Lambda_n}(\Phi + \Psi_n + \Upsilon) \geq p_{\Lambda_n}(\Phi + \Psi_n) - \langle a_\Upsilon \rangle_{\Lambda_n}^{\Phi+\Psi_n} \tag{3.27}$$

for all $\Upsilon \in \mathcal{I}$. Using (3.6), it is not too hard to generalise Lemma 3.3 and Theorem 3.6 to show that $p_{\Lambda_n}(\Phi + \Psi_n) \to p(\Phi)$ as $\Lambda_n \Uparrow \mathbb{Z}^d$, whenever $|||\Psi_n||| \to 0$. This allows to take the limit $n \to \infty$ in Eq. (3.27), and we get the property of Definition 3.10. □

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EXERCISE 3.1. *Prove the matrix inequality (3.7).*

EXERCISE 3.2. *Let $\mathcal{B}$ be a space of bounded operators and $\mathcal{B}_{\rm h}$ be the subspace of hermitian operators. Let $\rho$ be a linear functional $\mathcal{B}_{\rm h} \to \mathbb{R}$. Show that there exists a unique extension to a (complex) linear functional on $\mathcal{B}$. Hint: An operator can be uniquely decomposed as $a = b + {\rm i}c$ with $b, c$ hermitian; indeed, take $b = \frac{1}{2}(a^* + a)$ and $c = \frac{\rm i}{2}(c^* - c)$.*

CHAPTER 4

# Gibbs variational principle

## 4.1. Finite-volume entropy

In order to motivate this section, let us consider a finite-dimensional Hilbert space, and define the **von Neumann entropy** as the following function on density operators in the Hilbert space $\mathcal{H}_\Lambda$:

$$S_\Lambda(\rho) = -\mathrm{Tr}\,\rho\log\rho. \tag{4.1}$$

Next, given a bounded hermitian operator $H$, we define the **free energy** of a density operator as the functional

$$F(\rho) = \mathrm{Tr}\,\rho H - S_\Lambda(\rho). \tag{4.2}$$

(People familiar with thermodynamics will have recognised the relation $F = U - TS$, with the temperature $T$ equal to 1.)

PROPOSITION 4.1 (Gibbs variational principle). *The Gibbs operator* $\mathrm{e}^{-H}/\mathrm{Tr}\,\mathrm{e}^{-H}$ *is the unique minimiser of the free energy functional.*

PROOF. We first check that the minimiser is in the interior of the set of density operators. Indeed, let $\rho$ belong to its boundary. Then its kernel has positive dimension and there exists a density operator $\rho'$ that lives in the kernel. We can check that

$$F\big((1-\varepsilon)\rho + \varepsilon\rho'\big) = (1-\varepsilon)F(\rho) + \varepsilon F(\rho') + (1-\varepsilon)\log(1-\varepsilon) + \varepsilon\log\varepsilon. \tag{4.3}$$

It is clear that $\varepsilon = 0$ is not a minimum, as the last term is negative and stronger than linear. We now know that any minimiser $\rho_0$ is in the interior of the set of density operators. For any operator $\eta$ such that $\mathrm{Tr}\,\eta = 0$, we have

$$0 = \frac{\mathrm{d}}{\mathrm{d}s}F(\rho_0 + s\eta)\Big|_{s=0} = \mathrm{Tr}\,\eta(H + \log\rho_0). \tag{4.4}$$

It follows that $H + \log\rho_0$ is proportional to the identity, so that $\rho_0 = \mathrm{const}\,\mathrm{e}^{-H}$ is the only solution. The constant is $1/\mathrm{Tr}\,\mathrm{e}^{-H}$ in order for $\rho_0$ to be a density operator.

Although this is redundant, one can check that

$$\frac{\mathrm{d}^2}{\mathrm{d}s^2}F(\rho_0 + s\eta)\Big|_{s=0} = \mathrm{Tr}\,\eta\rho_0^{-1}\eta \geq 0, \tag{4.5}$$

which confirms that $\rho_0$ is a minimiser. □

The goal now is to extend these notions so we can decide whether a give infinite volume state is an equilibrium state.

### 4.2. Infinite-volume limit of the mean entropy

Let $\langle\cdot\rangle$ be a state on $\mathcal{A}$ and $\Lambda \Subset \mathbb{Z}^d$. The restriction of the state to $\mathcal{A}_\Lambda$ is represented by the density matrix $\rho_\Lambda$. This allows to define

$$S_\Lambda = S_\Lambda(\langle\cdot\rangle) = \operatorname{tr} \rho_\Lambda \log \rho_\Lambda. \tag{4.6}$$

(We dropped the reference to the state in the notation for $S_\Lambda$.) The dependence of the entropy on the domain, given a fixed infinite-volume state, turns out to be important. We have the following properties.

LEMMA 4.2. *Given a fixed state, its entropy satisfies*
(a) $-log \dim \mathcal{H}_\Lambda \leq S_\Lambda \leq 0$.
(b) *If* $\Lambda \subset \Lambda'$, *then* $S_\Lambda \geq S_{\Lambda'}$.
(c) *If* $\Lambda \cap \Lambda' = \emptyset$, *then* $S_{\Lambda\cup\Lambda'} \leq S_\Lambda + S_{\Lambda'}$.

PROOF. Cf Israel [1979], Lemma II.2.5. □

Remark: It is possible to prove that the entropy displays "strong subadditivity"; if $\Lambda \cap \Lambda' \neq \emptyset$, then $S_{\Lambda\cup\Lambda'} + S_{\Lambda\cap\Lambda'} \leq S_\Lambda + S_{\Lambda'}$.
For a translation-invariant state $\langle\cdot\rangle$ we can define the infinite-volume mean entropy by

$$s(\langle\cdot\rangle) = \lim_{\Lambda \Uparrow \mathbb{Z}^d} \frac{1}{|\Lambda|} S_\Lambda(\langle\cdot\rangle). \tag{4.7}$$

PROPOSITION 4.3. *The limit (4.7) exists along any van Hove sequence of domains.*

PROOF. It is similar to the proof for the pressure, see Lemma 3.3 and Theorem 3.6. We can use Lemma 4.2 (c) to decouple different domains and we obtain a suitable subadditivity property. □

### 4.3. Gibbs variational principle and Gibbs states

Thermodynamic potentials are related by Legendre transforms. Here is a generalisation to infinite-dimensional spaces, which turns out to be relevant for us.

THEOREM 4.4.

(a) *Let* $\Phi \in \mathcal{I}$ *and recall the definition (3.23) of* $a_\Phi$*. The pressure is then equal to*

$$p(\Phi) = \sup_{\langle\cdot\rangle} \big\{ s(\langle\cdot\rangle) - \langle a_\Phi \rangle \big\}.$$

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

(b) *Let* $\Phi \in \mathcal{I}$ *and* $\langle\cdot\rangle$ *a translation-invariant state on* $\mathcal{A}$*. Then*

$$p(\Phi) = s(\langle\cdot\rangle) - \langle a_\Phi \rangle \quad \Longleftrightarrow \quad p(\Phi + \Psi) \geq p(\Phi) - \langle a_\Psi \rangle \quad \forall \Psi \in \mathcal{I}.$$

PROOF. See Israel [1979], Theorem II.3.2, Corollary II.3.3, and Theorem II.3.4. □

Theorem 4.4 allows to formulate a 3rd definition of infinite volume states, that is equivalent to states from tangent functionals.

DEFINITION 4.5. *A translation-invariant state* $\langle\cdot\rangle$ *is an equilibrium state for the interaction* $\Phi \in \mathcal{I}$ *if it satisfies the Gibbs variational principle, i.e. if*

$$p(\Phi) = s(\langle\cdot\rangle) - \langle a_\Phi \rangle.$$

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EXERCISE 4.1. *Check the validity of Eqs (4.3)–(4.5).*