

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}_Λ :

$$S_\Lambda(\rho) = -\text{Tr } \rho \log \rho. \quad (4.1)$$

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

$$F(\rho) = \text{Tr } \rho H - S_\Lambda(\rho). \quad (4.2)$$

(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 $e^{-H} / \text{Tr } e^{-H}$ 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 ρ belong to its boundary. Then its kernel has positive dimension and there exists a density operator ρ' that lives in the kernel. We can check that

$$F((1 - \varepsilon)\rho + \varepsilon\rho') = (1 - \varepsilon)F(\rho) + \varepsilon F(\rho') + (1 - \varepsilon) \log(1 - \varepsilon) + \varepsilon \log \varepsilon. \quad (4.3)$$

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 ρ_0 is in the interior of the set of density operators. For any operator η such that $\text{Tr } \eta = 0$, we have

$$0 = \left. \frac{d}{ds} F(\rho_0 + s\eta) \right|_{s=0} = \text{Tr } \eta(H + \log \rho_0). \quad (4.4)$$

It follows that $H + \log \rho_0$ is proportional to the identity, so that $\rho_0 = \text{const } e^{-H}$ is the only solution. The constant is $1/\text{Tr } e^{-H}$ in order for ρ_0 to be a density operator.

Although this is redundant, one can check that

$$\left. \frac{d^2}{ds^2} F(\rho_0 + s\eta) \right|_{s=0} = \text{Tr } \eta \rho_0^{-1} \eta \geq 0, \quad (4.5)$$

which confirms that ρ_0 is a minimiser. \square

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}_Λ is represented by the density matrix ρ_Λ . This allows to define

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

(We dropped the reference to the state in the notation for S_Λ .) 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. \square

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

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

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. \square

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_Φ . The pressure is then equal to

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

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

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

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

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

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

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