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 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

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

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 ρ_0 is in the interior of the set of density operators. For any operator η 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 ρ_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 ρ_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 ρ_Λ. 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_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. □

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 (3.18) of a_Φ. 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*

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

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