CHAPTER 5

Mean-field systems

Mean-field systems are models where the geometry of $\mathbb{Z}^d$ is drastically simplified in order to increase the amount of symmetry: instead of just translations, we allow *all* permutations. This allows for more explicit calculations, in particular we can fully describe the set of Gibbs states in many examples. Such calculations are valuable as a guide, since it is expected that features of mean-field systems hold also in $\mathbb{Z}^d$ for all d greater than the *upper critical dimension*, which is expected to be equal to 4 in our spin models.

5.1. Permutation-invariant states

We consider Gibbs states which are invariant under all (finite) permutations. Since the geometric structure of the lattice $\mathbb{Z}^d$ is not relevant, we instead take $\mathbb{N}^+ = \{1, 2, 3, \dots\}$ as our indexing set.

Recall that $\mathcal{H}_n$ denotes $\mathbb{C}^n$ with associated spin matrics (i.e. an irreducible representation of $\mathfrak{su}(2)$). We use the following notation:

$$\mathcal{A}_N = \mathcal{A}_{\{1,2,\dots,N\}} = \mathcal{B}(\mathcal{H}_n^{\otimes\{1,2,\dots,N\}}), \qquad \mathcal{A}_{\mathrm{loc}} = \bigcup_{N\geq 1} \mathcal{A}_N, \qquad \mathcal{A} = \overline{\mathcal{A}_{\mathrm{loc}}}. \tag{5.1}$$

Permutations $\tau \in \mathcal{S}_N$, the symmetric group, act on $\mathcal{A}_{\mathrm{loc}}$ and $\mathcal{A}$ in the natural way:

$$\begin{aligned} &\tau|\varphi_1, \varphi_2, \cdots \varphi_N\rangle = |\varphi_{\tau(1)}, \varphi_{\tau(2)}, \cdots \varphi_{\tau(N)}\rangle, \qquad |\varphi_1, \varphi_2, \cdots \varphi_N\rangle \in \mathcal{H}_n^{\otimes\{1,2,\dots,N\}}, \\ &(\tau A)|\varphi\rangle = \tau A \tau^{-1}|\varphi\rangle, \qquad A \in \mathcal{A}_{\mathrm{loc}}. \end{aligned} \tag{5.2}$$

Definition 5.1. *A state $\boldsymbol{\rho}$ on $\mathcal{A}$ is called* permutation-invariant *or* exchangeable *if for all $N \geq 1$, all $A \in \mathcal{A}_N$ and all $\tau \in \mathcal{S}_N$, we have that $\boldsymbol{\rho}(\tau A) = \boldsymbol{\rho}(A)$. We write $\mathfrak{E}_{\mathrm{p.i.}}$ for the set of such states.*

Permutation-invariant states arise from *mean-field* models in statistical physics. We consider models defined by Hamiltonians of the form

$$H_N = \sum_{k=1}^{K} \sum_{\substack{L \subseteq \{1,\dots,N\} \\ |L|=k}} \frac{N}{\binom{N}{k}} \Phi_L, \tag{5.3}$$

where the (finite-range) interaction $\Phi = (\Phi_L)_{L\subseteq\mathbb{N}^+, |L|\leq K}$ is assumed to be permutation-invariant in the sense that $\tau\Phi_L = \Phi_{\tau L}$ for all $L \Subset \mathbb{N}^+$ and permutations τ. Here Φ_L represents the interaction between the spins in the set L, and our assumptions mean that any set of k spins interact equally. We may thus view (5.3) as defining a model on the *complete graph* rather than the lattice, where the complete graph K_N consists of N vertices and an edge between any pair of vertices.

EXAMPLE 5.1. *The mean-field XYZ-model is obtained by taking the 2-body interaction*

$$-\Phi_L = \begin{cases} (J_1 S_x^{(1)} S_y^{(1)} + J_2 S_x^{(2)} S_y^{(2)} + J_3 S_x^{(3)} S_y^{(3)}), & \text{if } L = \{x, y\}, x \neq y, \\ 0, & \text{otherwise.} \end{cases}$$

Gibbs-states for the models (5.3) can be defined using tangent functionals, entropy, KMS- or RAS-condition, as in the case of $\mathbb{Z}^d$. Most convenient in this setting is the variational definition through entropy. We define

$$A_\Phi = \sum_{k=1}^{K} \Phi_{\{1,\dots,k\}}, \qquad s(\boldsymbol{\rho}) = \lim_{N\to\infty} \tfrac{1}{N}(-\mathrm{tr}\,\rho_N \log \rho_N),$$

where ρ_N is the density matrix, with respect to the normalized trace $\mathrm{tr}\,(\cdot) = \frac{1}{n^N}\mathrm{Tr}\,(\cdot)$, for the restriction of the state $\boldsymbol{\rho}$ to $\mathcal{A}_N$. Existence of the specific entropy $s(\cdot)$ is proved as for $\mathbb{Z}^d$ and it has the same properties, in particular it is affine.

DEFINITION 5.2. *A* permutation-invariant Gibbs state *for the model (5.3) is a permutation-invariant state $\boldsymbol{\rho}$ on $\mathcal{A}$ which minimizes the free energy functional*

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

The set of permutation-invariant Gibbs states for the interaction Φ, at inverse temperature β, is written $\mathcal{G}^{\beta\Phi}_{\text{p.i.}}$.

We note that $f^{\beta,\Phi}(\cdot)$ is affine and $\mathcal{G}^{\beta\Phi}_{\text{p.i.}}$ convex.

We now focus on the extremal elements of $\mathcal{G}^{\beta\Phi}_{\text{p.i.}}$. An analog of Theorem 3.28 (equivalent properties of extremal states) holds in the permutation-invariant setting, with an important strengthening of the notions of mixing and short-range correlations. As an analogue of a translation, we introduce the permutation

$$\tau_m := (1, m)(2, m+1)\cdots(m-1, 2m-1). \tag{5.4}$$

We say that a state $\boldsymbol{\rho} \in \mathfrak{E}_{\text{p.i.}}$ is *mixing* if for all $A, B \in \mathcal{A}_{\text{loc}}$ we have

$$\lim_{m\to\infty} \boldsymbol{\rho}(A\,\tau_m B) = \boldsymbol{\rho}(A)\boldsymbol{\rho}(B). \tag{5.5}$$

DEFINITION 5.3 (Product state). *A state $\boldsymbol{\rho}$ on $\mathcal{A}$ is called a* product state *if there is a density matrix $\rho \in \mathcal{B}(\mathcal{H}_n)$ such that for all $N \geq 1$ and all $A \in \mathcal{A}_N$ we have that $\boldsymbol{\rho}(A) = \mathrm{tr}\,(\rho^{\otimes N} A)$. (Equivalently, $\rho_N = \rho^{\otimes N}$ for all N.)*

PROPOSITION 5.4. *Let $\boldsymbol{\rho}$ be a permutation-invariant state on $\mathcal{A}$. Then it is mixing if and only if it is a product state.*

PROOF. All product-states are mixing, because if m is large enough then A and $\tau_m B$ act on disjoint tensor factors (for local A, B), so $\boldsymbol{\rho}(A\tau_m B) = \boldsymbol{\rho}(A)\boldsymbol{\rho}(B)$ for all large enough m.

Fore the converse, assume that $\boldsymbol{\rho}$ is mixing. Set $\rho = \rho_1$, i.e. for all $A \in \mathcal{A}_1 = \mathcal{B}(\mathcal{H}_n)$ we have

$$\boldsymbol{\rho}(A) = \mathrm{tr}\,(\rho A). \tag{5.6}$$

It suffices to show that for any $A_1, \ldots, A_N \in \mathcal{B}(\mathcal{H}_n)$ the operator $A = \bigotimes_{j=1}^N A_j$ satisfies

$$\boldsymbol{\rho}(A) = \prod_{j=1}^N \mathrm{tr}\,(\rho A_j). \tag{5.7}$$

For any $m > N$, we can find a permutation fixing $1, 2, \ldots, N-1$ and sending N to m. Thus, by permutation-invariance of $\boldsymbol{\rho}$,

$$\boldsymbol{\rho}(A) = \boldsymbol{\rho}\Big(\bigotimes_{j=1}^{N-1} A_j \cdot \tau_m A_N.\Big) \tag{5.8}$$

Taking the limit $m \to \infty$ and using that $\boldsymbol{\rho}$ is mixing, we conclude that

$$\boldsymbol{\rho}(A) = \boldsymbol{\rho}\Big(\bigotimes_{j=1}^{N-1} A_j\Big)\boldsymbol{\rho}(A_N) = \boldsymbol{\rho}\Big(\bigotimes_{j=1}^{N-1} A_j\Big)\mathrm{tr}\,(\rho A_N). \tag{5.9}$$

Then (5.7) follows by induction. □

The following is the analog of Theorem 3.28 for permutation-invariant states.

THEOREM 5.5. *Assume that $\boldsymbol{\rho} \in \mathfrak{E}_{\mathrm{p.i.}}$. The following are equivalent:*

(a) $\boldsymbol{\rho}$ is extremal in $\mathfrak{E}_{\mathrm{p.i.}}$
(b) $\boldsymbol{\rho}$ is mixing
(c) $\boldsymbol{\rho}$ is a product state.

Furthermore, if $\boldsymbol{\rho} \in \mathcal{G}^{\beta\Phi}_{\mathrm{p.i.}}$, then the above are all equivalent to:

(d) $\boldsymbol{\rho}$ is extremal in $\mathcal{G}^{\beta\Phi}_{\mathrm{p.i.}}$

REMARK 5.1. *The fact that the extremal elements of $\mathfrak{E}_{\mathrm{p.i.}}$ are precisely the product states is (essentially) the* quantum de Finetti theorem*.*

PROOF. Let us start with the equivalence of (a), (b) and (c). We already established the equivalence of (b) and (c) in Proposition 5.4. We prove that (a) $\Rightarrow$ (b) and then that (c) $\Rightarrow$ (a).

For (a) $\Rightarrow$ (b), assume that (b) fails (we will show that (a) then fails). There are then $A, B \in \mathcal{A}_{\mathrm{loc}}$ such that $\boldsymbol{\rho}(A\tau_m B) \not\to \boldsymbol{\rho}(A)\boldsymbol{\rho}(B)$. By modifying B, if necessary, we can assume that $B \geq 0$ and $\theta := \boldsymbol{\rho}(B) \in (0,1)$. Define, using subsequences if necessary,

$$\boldsymbol{\rho}_1(\cdot) := \lim_{m\to\infty} \frac{\boldsymbol{\rho}(\cdot\,\tau_m B)}{\boldsymbol{\rho}(B)}, \qquad \boldsymbol{\rho}_2(\cdot) := \lim_{m\to\infty} \frac{\boldsymbol{\rho}(\cdot\,\tau_m(\mathbb{1} - B))}{1 - \boldsymbol{\rho}(B)}. \tag{5.10}$$

One may check that $\boldsymbol{\rho}_1, \boldsymbol{\rho}_2$ are states and they satisfy

$$\boldsymbol{\rho} = \theta\boldsymbol{\rho}_1 + (1-\theta)\boldsymbol{\rho}_2. \tag{5.11}$$

Furthermore, $\boldsymbol{\rho}_1, \boldsymbol{\rho}_2$ are permutation-invariant: given any N and any permutation of $1, \dots, N$, when m is large enough the permutation does not affect $\tau_m B$. Thus we found a non-trivial decomposition of $\boldsymbol{\rho}$ in $\mathfrak{E}_{\text{p.i}}$, i.e. (a) fails.

For (c) $\Rightarrow$ (a), assume that $\boldsymbol{\rho}$ is a product state but not extremal. Then there is a non-trivial decomposition (5.11) with $\boldsymbol{\rho}_1, \boldsymbol{\rho}_2 \in \mathfrak{E}_{\text{p.i.}}$. Moreover, we can assume $\boldsymbol{\rho}_1, \boldsymbol{\rho}_2$ to be extremal (by the Krein–Milman theorem $\mathfrak{E}_{\text{p.i.}}$ is the convex hull of its extreme points). Using the implications we already proved, this means that $\boldsymbol{\rho}_1, \boldsymbol{\rho}_2$ are product states. Let ρ, ρ_1, ρ_2 denote the (single-site) density matrices for $\boldsymbol{\rho}, \boldsymbol{\rho}_1, \boldsymbol{\rho}_2$ respectively:

$$\operatorname{tr}(\rho^{\otimes N}\cdot) = \theta \operatorname{tr}(\rho_1^{\otimes N}\cdot) + (1-\theta)\operatorname{tr}(\rho_2^{\otimes N}\cdot). \tag{5.12}$$

Since $\boldsymbol{\rho}_1 \neq \boldsymbol{\rho}_2$ we have $\rho_1 \neq \rho_2$, so there exits $A \in \mathcal{A}_1$ such that $\operatorname{tr}\rho_1 A \neq \operatorname{tr}\rho_2 A$. We may further assume that A is positive-definite and satisfies $\operatorname{tr}\rho A = 1$. Then (5.12) applied to $A^{\otimes N}$ gives

$$1 = \theta(\operatorname{tr}\rho_1 A)^N + (1-\theta)(\operatorname{tr}\rho_2 A)^N. \tag{5.13}$$

Not both of $\operatorname{tr}\rho_1 A$ and $\operatorname{tr}\rho_2 A$ can equal 1, so the right-hand-side of (5.13) goes either to 0 or to ∞, a contradiction.

Now assume that $\boldsymbol{\rho}$ is a Gibbs state. Clearly (a) implies (d) in this case. We prove that (d) $\Rightarrow$ (b), which then links up to the chain of equivalences already proved. As above, assume that (b) fails, and use the same decomposition (5.10) and (5.11). We only need to check that $\boldsymbol{\rho}_1$ and $\boldsymbol{\rho}_2$ are in fact Gibbs states. Since $\boldsymbol{\rho}$ is a Gibbs state, it minimizes $f^{\beta,\Phi}(\cdot)$ over $\mathfrak{E}_{\text{p.i.}}$ (Definition 5.2). Moreover, $f^{\beta,\Phi}(\cdot)$ is affine, so we have

$$f^{\beta,\Phi}(\boldsymbol{\rho}) = \theta f^{\beta,\Phi}(\boldsymbol{\rho}_1) + (1-\theta) f^{\beta,\Phi}(\boldsymbol{\rho}_2). \tag{5.14}$$

Since $\boldsymbol{\rho}_1, \boldsymbol{\rho}_2 \in \mathfrak{E}_{\text{p.i.}}$, we have $f^{\beta,\Phi}(\boldsymbol{\rho}_1), f^{\beta,\Phi}(\boldsymbol{\rho}_2) \geq f^{\beta,\Phi}(\boldsymbol{\rho})$ and if either of them was $> f^{\beta,\Phi}(\boldsymbol{\rho})$ we would get a contradiction from (5.14). Hence, both $\boldsymbol{\rho}_1, \boldsymbol{\rho}_2$ are minimizers and therefore Gibbs states. □

5.2. The mean-field equation

We now restrict to the case of two-body interactions, meaning that $\Phi_L = 0$ unless $|L| = 2$. The results and arguments are easily extended to many-body interactions. Write $\Phi_{x,y}$ for $\Phi_{\{x,y\}}$.

In what follows we will mostly work with Hilbert spaces of fixed dimension and therefore find it more convenient to work the 'big trace' Tr rather than the 'little trace' tr . Recall the partial trace $\operatorname{Tr}_2 : \mathcal{B}(\mathcal{H} \otimes \mathcal{H}) \to \mathcal{B}(\mathcal{H})$ defined to satisfy $\operatorname{Tr}_2(A \otimes B) = A\operatorname{Tr}(B)$ (and linearity). Given a density matrix $\rho \in \mathcal{B}(\mathcal{H})$, with respect to Tr i.e. satisfying $\operatorname{Tr}\rho = 1$, define the 'on-site Hamiltonian'

$$H_\rho = \operatorname{Tr}_2\big((\mathbb{1} \otimes \rho)\Phi_{1,2}\big). \tag{5.15}$$

THEOREM 5.6 (Fannes–Spohn–Verbeure). *Let Φ be a permutation-invariant two-body interaction. Then the extremal elements of $\mathcal{G}^{\Phi}_{\mathrm{p.i.}}(\beta)$ are those product states whose density matrix ρ (with $\mathrm{Tr}\,\rho = 1$) minimizes the function*

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

PROOF. The fact that all extremal permutation-invariant states are product states was shown in Theorem 5.5. By the variational principle, Definition 5.2, the product state $\boldsymbol{\rho}$ minimizes

$$\boldsymbol{\rho}(A_\Phi) - \tfrac{1}{\beta}s(\boldsymbol{\rho}) = \mathrm{tr}\,(\rho^{\otimes 2}\Phi_{1,2}) + \tfrac{1}{\beta}\mathrm{tr}\,\rho\log\rho. \tag{5.16}$$

We used that $\mathrm{tr}\,\rho^{\otimes N}\log\rho^{\otimes N} = N\mathrm{tr}\,\rho\log\rho$. Here $\mathrm{tr}\,\rho = 1$, that is $\mathrm{Tr}\,\rho = n$. We now rewrite (5.16) in terms of Tr. We have

$$\mathrm{tr}\,(\rho^{\otimes 2}\Phi_{1,2}) = \mathrm{Tr}\,((\tfrac{\rho}{n})^{\otimes 2}\Phi_{1,2}), \quad \mathrm{tr}\,\rho\log\rho = \mathrm{Tr}\,\tfrac{\rho}{n}\log\tfrac{\rho}{n} + \log n,$$

where $\mathrm{Tr}\,\frac{\rho}{n} = 1$. Letting $\tilde\rho = \frac{\rho}{n}$ we get

$$\boldsymbol{\rho}(A_\Phi) - \tfrac{1}{\beta}s(\boldsymbol{\rho}) = \mathrm{Tr}\,\tilde\rho^{\otimes 2}\Phi_{1,2} + \tfrac{1}{\beta}(\mathrm{Tr}\,\tilde\rho\log\tilde\rho + \log n).$$

Since $\mathrm{Tr}\,\tilde\rho^{\otimes 2}\Phi_{1,2} = \mathrm{Tr}\,\tilde\rho H_{\tilde\rho}$, the claim follows. □

The first-order condition for a minimizer leads to the following non-linear equation for ρ.

PROPOSITION 5.7 (Mean-field equation). *Let ρ be a density matrix ($\mathrm{Tr}\,\rho = 1$) which minimizes the function $\mathcal{F}(\rho)$ in Theorem 5.6. Then ρ satisfies*

$$\rho = \frac{\mathrm{e}^{-2\beta H_\rho}}{\mathrm{Tr}\;\mathrm{e}^{-2\beta H_\rho}}.$$

The mean-field equation is a necessary, but not sufficient, condition for a minimiser of $f(\rho)$.

PROOF. We first check that any minimiser of $\mathcal{F}(\cdot)$ is in the interior of the set of density matrices. Indeed, let ρ belong to its boundary. Then has at least one eigenvalue $= 0$ and there exists a density matrix ρ' that is positive precisely on the zero-eigenvectors for ρ. Concretely, we can find an orthonormal eigenbasis $\phi_1, \ldots, \phi_n$ for ρ such that in this basis

$$\rho = \sum_{i=1}^{k}\lambda_i|\phi_i\rangle\langle\phi_i|, \qquad \rho' = \sum_{i=k+1}^{n}\mu_i|\phi_i\rangle\langle\phi_i|, \tag{5.17}$$

where $k < n$ and $\phi_{k+1}, \ldots, \phi_n$ are eigenvectors for ρ with eigenvalue 0. Using this expansion we can check that

$$\mathcal{F}\big((1-\varepsilon)\rho + \varepsilon\rho'\big) = (1-\varepsilon)\mathcal{F}(\rho) + \varepsilon\mathcal{F}(\rho') + \tfrac{1}{\beta}(1-\varepsilon)\log(1-\varepsilon) + \tfrac{1}{\beta}\varepsilon\log\varepsilon. \tag{5.18}$$

It is clear that $\varepsilon = 0$ is not a minimum, as the last term is negative and stronger than linear.

Knowing that minimizers are in the interior, assume that ρ is a minimizer and let $\eta = \eta^*$ have trace 0 and let $\varepsilon > 0$ be small enough that $\rho + \varepsilon\eta$ is a density matrix. We will compute the derivative of $\mathcal{F}(\rho + \varepsilon\eta)$ at $\varepsilon = 0$, and use that this is $= 0$ to derive the equation for ρ. We have that

$$\begin{aligned}\mathcal{F}(\rho+\varepsilon\eta) - \mathcal{F}(\rho) = \varepsilon\big(\mathrm{Tr}\,\eta H_\rho + \mathrm{Tr}\,\rho H_\eta + \tfrac{1}{\beta}\mathrm{Tr}\,\eta\log\rho\big) \\ + \tfrac{1}{\beta}\mathrm{Tr}\,(\rho+\varepsilon\eta)(\log(\rho+\varepsilon\eta) - \log\rho) + O(\varepsilon^2).\end{aligned} \tag{5.19}$$

Here, by non-negativity of the relative entropy, Proposition **??**,

$$\begin{aligned}0 &\le \mathrm{Tr}\,(\rho+\varepsilon\eta)(\log(\rho+\varepsilon\eta) - \log\rho) \\ &= \mathrm{Tr}\,\rho(\log(\rho+\varepsilon\eta) - \log\rho) + \varepsilon\mathrm{Tr}\,\eta(\log(\rho+\varepsilon\eta) - \log\rho) \\ &\le \varepsilon\mathrm{Tr}\,\eta(\log(\rho+\varepsilon\eta) - \log\rho).\end{aligned} \tag{5.20}$$

The right-hand-side is $o(\varepsilon)$. Moreover, since Φ is symmetric we have

$$\mathrm{Tr}\,\rho H_\eta = \mathrm{Tr}\,\eta H_\rho. \tag{5.21}$$

It follows that for all traceless $\eta = \eta^*$ we have

$$0 = \tfrac{\mathrm{d}}{\mathrm{d}\varepsilon}\mathcal{F}(\rho+\varepsilon\eta)|_{\varepsilon=0} = \mathrm{Tr}\,\eta(2H_\rho + \tfrac{1}{\beta}\log\rho). \tag{5.22}$$

Then $2H_\rho + \frac{1}{\beta}\log\rho$ is a multiple of the identity, which gives the claim. □

5.3. Gibbs states of some mean-field models

We use the theory above to characterize the permutation-invariant Gibbs states of some mean-field systems based on the XYZ-model (Example 5.1).

5.3.1. The spin-$\frac{1}{2}$ Heisenberg model. Consider the fully isotropic model for spin $\frac{1}{2}$, that is we take $n = 2$ and $J_1 = J_2 = J_3 = 1$. Thus we have the interaction

$$\Phi_L = \begin{cases} -\vec{S}_x \cdot \vec{S}_y, & \text{if } L = \{x,y\}, x \neq y, \\ 0, & \text{otherwise.}\end{cases} \tag{5.23}$$

We identify the density matrices ρ corresponding to extremal states. From Exercise 1.7 we know that $\Phi_{1,2} = -(\frac{1}{2}T_{1,2} - \frac{1}{4})$ where $T_{1,2}$ is the transposition operator. Thus

$$(\mathbb{1}\otimes\rho)\Phi_{1,2} = -(\mathbb{1}\otimes\rho)(\tfrac{1}{2}T_{1,2} - \tfrac{1}{4}) = -\tfrac{1}{2}\rho\otimes\mathbb{1} + \tfrac{1}{4}\mathbb{1}\otimes\rho. \tag{5.24}$$

Taking the partial trace we get

$$H_\rho = -\rho + \tfrac{1}{4}\mathbb{1}. \tag{5.25}$$

Any 2×2 density matrix can be written (compare Exercise 3.4) in the form

$$\rho = \tfrac{1}{2}\mathbb{1} + \vec{a}\cdot\vec{S}, \qquad \vec{a} = (a_1, a_2, a_3) \in \mathbb{R}^3. \tag{5.26}$$

With this parameterization,

$$H_\rho = -\vec{a}\cdot\vec{S} - \tfrac{1}{4}\mathbb{1}. \tag{5.27}$$

We need to compute $\frac{\mathrm{e}^{-2\beta H_\rho}}{\mathrm{Tr}\,\mathrm{e}^{-2\beta H_\rho}}$, and we see that the scalar term $-\frac{1}{4}\mathbb{1}$ in H_ρ cancels. To compute $\mathrm{e}^{2\beta\vec{a}\cdot\vec{S}}$, note that $(\vec{a}\cdot\vec{S})^2 = \frac{1}{4}\|\vec{a}\|^2$, so from the power series expansion of the exponential we get

$$\mathrm{e}^{2\beta\vec{a}\cdot\vec{S}} = \cosh\big(\beta\|\vec{a}\|\big)\mathbb{1} + \frac{\sinh\big(\beta\|\vec{a}\|\big)}{\frac{1}{2}\|\vec{a}\|}(\vec{a}\cdot\vec{S}). \tag{5.28}$$

Then $\mathrm{Tr}\ \mathrm{e}^{2\beta\vec{a}\cdot\vec{S}} = 2\cosh\big(\frac{\beta}{2}\|\vec{a}\|\big)$, so

$$\frac{\mathrm{e}^{-2\beta H_\rho}}{\mathrm{Tr}\ \mathrm{e}^{-2\beta H_\rho}} = \tfrac{1}{2}\mathbb{1} + (\vec{a}\cdot\vec{S})\frac{\tanh\big(\beta\|\vec{a}\|\big)}{\|\vec{a}\|}. \tag{5.29}$$

The mean-field equation reduces to

$$(\vec{a}\cdot\vec{S})\Big(\frac{\tanh\big(\beta\|\vec{a}\|\big)}{\|\vec{a}\|} - 1\Big) = 0. \tag{5.30}$$

One solution is always $\vec{a} = 0$. If $\beta > 1 =: \beta_\mathrm{c}$ then the equation $\tanh(\beta x) = x$ has a (unique) positive solution $x = x^\star(\beta)$. Any $\vec{a}$ with $\|\vec{a}\| = x^\star$ thus solves the mean-field equation. One may check that all such $\vec{a}$ give the same value of the free energy, and that it is smaller than for $\vec{a} = 0$ (see Exercise 5.1). It follows that the extremal permutation-invariant Gibbs states for the spin-$\frac{1}{2}$ Heisenberg XXX-model are indexed by the points on a sphere, that is by SO(3).

5.3.2. Higher spin Heisenberg model. Next, we consider the higher spin case $n \geq 2$, still with $J_1 = J_2 = J_3 = 1$. Thus we have (5.23), but now with the spin matrices defined in (1.9):

$$S^{(1)} = \tfrac{1}{2}(S^{(+)} + S^{(-)}), \qquad S^{(2)} = \tfrac{1}{2\mathrm{i}}(S^{(+)} - S^{(-)}), \qquad S^{(3)}|a\rangle = a|a\rangle. \tag{5.31}$$

where

$$S^{(+)}|a\rangle = \sqrt{J(J+1) - a(a+1)}\ |a+1\rangle, \quad S^{(-)}|a\rangle = \sqrt{J(J+1) - (a-1)a}\ |a-1\rangle. \tag{5.32}$$

The set of Hermitian $n\times n$ matrices forms a real vector space. On this space we use the (Hilbert–Schmidt) inner product $\langle A, B\rangle_{\mathrm{HS}} = \mathrm{Tr}\, A^* B$. The spin matrices (5.31) are orthogonal with respect to this inner product, indeed $\mathrm{Tr}\, S^{(j)}S^{(k)} = -\mathrm{Tr}\, S^{(j)}S^{(k)}$ for any $j \neq k$, as can be seen by performing a rotation which fixes $S^{(j)}$ while mapping $S^{(k)}$ to its negative. Moreover $S^{(1)}, S^{(2)}, S^{(3)}$ are orthogonal to $\mathbb{1}$ since they are traceless. Write $\mathcal{S} = \mathrm{Span}(\mathbb{1}, S^{(1)}, S^{(2)}, S^{(3)})$ and $\mathcal{T} = \mathcal{S}^\perp$, the orthogonal complement of $\mathcal{S}$ in the real vector space of Hermitian $n\times n$ matrices. It follows that we can write any $n\times n$ density matrix ρ in the form

$$\rho = \tfrac{1}{n}\mathbb{1} + \vec{a}\cdot\vec{S} + T, \qquad \vec{a}\in\mathbb{R}^3, \quad T\in\mathcal{T}. \tag{5.33}$$

Note that for any $j \in \{1,2,3\}$ we have (with $J = (n-1)/2$ the spin)

$$\begin{aligned}\mathrm{Tr}\,(S^{(j)})^2 &= \tfrac{1}{3}\mathrm{Tr}\,\big((S^{(1)})^2 + (S^{(2)})^2 + (S^{(3)})^2\big) = \tfrac{1}{3}J(J+1)(2J+1)\\ &= \tfrac{1}{12}n(n^2-1) =: c_n.\end{aligned} \tag{5.34}$$

Thus, expanding the expression $(\mathbb{1}\otimes\rho)\Phi_{1,2}$ and taking the partial trace (using orthogonality of T to all spin matrices), we get

$$H_\rho = -c_n\vec{a}\cdot\vec{S}. \tag{5.35}$$

The mean-field equation becomes

$$\tfrac{1}{n}\mathbb{1} + \vec{a}\cdot\vec{S} + T = \frac{\mathrm{e}^{2c_n\beta\vec{a}\cdot\vec{S}}}{\mathrm{Tr}\ \mathrm{e}^{2c_n\beta\vec{a}\cdot\vec{S}}} \tag{5.36}$$

At this point we already see the SO(3)-symmetry: if $\vec{a}$ is a solution, then any rotation of $\vec{a}$ is a solution. Thus it suffices to look for solutions of the form $\vec{a} = x\mathbf{e}_3$ where $x = \|\vec{a}\|$. Then

$$\tfrac{1}{n}\mathbb{1} + xS^{(3)} + T = \frac{\mathrm{e}^{2c_n\beta x S^{(3)}}}{\mathrm{Tr}\ \mathrm{e}^{2c_n\beta S^{(3)}}}, \tag{5.37}$$

and since the right-hand-side is diagonal it follows that T is diagonal. Let us index the diagonal entries of T using $m \in \{-J, -J+1, \ldots, J\}$, i.e. $T = \mathrm{diag}\,(t_J, t_{J-1}, \ldots, t_{-J})$. Multiplying both sides of (5.37) by $S^{(3)}$ and taking the trace, we conclude that x should satisfy

$$xc_n = \frac{\sum_{m=-J}^{J} m\, \mathrm{e}^{2c_n\beta x m}}{\sum_{m=-J}^{J} \mathrm{e}^{2c_n\beta x m}}. \tag{5.38}$$

One may check that the righ-hand-side is an increasing, concave function of $x > 0$, and there is a (unique) positive solution x if and only if $\beta > n/2c_n = 6/(n^2-1)$.

5.4. Exercises

EXERCISE 5.1. *Complete the calculation after (5.30) as follows. Let* $\rho = \frac{1}{2}\mathbb{1} + \vec{a}\cdot\vec{S}$ *be a density-matrix such that* $x = \|\vec{a}\|$ *is a solution to* $x = \tanh(\frac{\beta}{2}x)$*. Calculate the free energy*

$$f(\rho) = \mathrm{Tr}\,[\rho H_\rho] + \tfrac{1}{\beta}\mathrm{Tr}\,[\rho\log\rho].$$

Deduce that the set of extremal permutation-invariant Gibbs states is in one-to-one correspondence with the 2-sphere when $\beta > 2$.

EXERCISE 5.2. *Now consider the XXZ-case* $J_1 = J_2 = 1$, $J_3 = \Delta > 1$. *Calculate all density matrices* ρ *satisfying the mean-field equation*

$$\rho = \frac{\mathrm{e}^{-\beta H_\rho}}{\mathrm{Tr}\ \mathrm{e}^{-\beta H_\rho}}$$

Which of these minimize the free energy? Use your conclusions to explicitly describe the set of extremal permutation-invariant Gibbs states.