Equilibrium quantum lattice systems

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Contents

CHAPTER 1

Spin systems

1.1. Spin operators

Let $S \in \frac{1}{2}\mathbb{N}$. On $\mathbb{C}^{2S+1}$, let $S^{(1)}, S^{(2)}, S^{(3)}$ be hermitian matrices that satisfy the following properties:

$$[S^{(1)}, S^{(2)}] = \mathrm{i}S^{(3)}, \quad [S^{(2)}, S^{(3)}] = \mathrm{i}S^{(1)}, \quad [S^{(3)}, S^{(1)}] = \mathrm{i}S^{(2)}, \tag{1.1}$$

$$[S^{(1)}]^{(2)} + [S^{(2)}]^{(2)} + [S^{(3)}]^{(2)} = S(S+1)\mathtt{Id}. \tag{1.2}$$

The existence of such matrices follows by construction: Let $|a\rangle$, $a \in \{-S, -S+1, \dots, S\}$ denote an orthonormal basis of $\mathbb{C}^{2S+1}$, and define $S^{(3)}|a\rangle = a|a\rangle$. Next, let $S^{(+)}, S^{(-)}$ be defined by

$$S^{(+)}|a\rangle = \sqrt{S(S+1) - a(a+1)}\ |a{+}1\rangle, \quad S^{(-)}|a\rangle = \sqrt{S(S+1) - (a-1)a}\ |a{-}1\rangle. \tag{1.3}$$

Then we set $S^{(1)} = \frac{1}{2}(S^{(+)} + S^{(-)})$ and $S^{(2)} = \frac{1}{2\mathrm{i}}(S^{(+)} - S^{(-)})$.

Lemma 1.1. *The operators $S^{(1)}, S^{(2)}, S^{(3)}$ constructed above satisfy the relations (1.1) and (1.2).*

Proof. One can check the following commutation relations:

$$[S^{(3)}, S^{(+)}] = S^{(+)}, \qquad [S^{(3)}, S^{(-)}] = -S^{(-)}, \qquad [S^{(+)}, S^{(-)}] = 2S^{(3)}. \tag{1.4}$$

The relations (1.1) follow. Finally,

$$[S^{(1)}]^2 + [S^{(2)}]^2 + [S^{(3)}]^2 = S^{(+)}S^{(-)} + [S^{(3)}]^2 - S^{(3)} = S(S+1)\mathtt{Id}. \tag{1.5}$$

□

For $S = \frac{1}{2}$, the choice above gives the Pauli matrices (multiplied by $\frac{1}{2}$):

$$S^{(1)} = \tfrac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad S^{(2)} = \tfrac{1}{2}\begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}, \qquad S^{(3)} = \tfrac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{1.6}$$

For $S = 1$, we get

$$S^{(1)} = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad S^{(2)} = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & -\mathrm{i} & 0 \\ \mathrm{i} & 0 & -\mathrm{i} \\ 0 & \mathrm{i} & 0 \end{pmatrix}, \quad S^{(3)} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}. \tag{1.7}$$

Notice that, for $S > 1$, the matrix of $S^{(1)}$ is not proportional to $\delta_{|i-j|,1}$. Spin operators are not unique, but their spectrum is uniquely determined by the commutation relations.

LEMMA 1.2. *Assume that $S^{(1)}, S^{(2)}, S^{(3)}$ are hermitian matrices in $\mathbb{C}^{2S+1}$ that satisfy the relations (1.1) and (1.2). Then each $S^{(i)}$ has eigenvalues $\{-S, -S+1, \dots, S\}$.*

PROOF. It is enough to prove the claim for $S^{(3)}$. Define $S^{(+)} = S^{(1)} + \mathrm{i}S^{(2)}$ and $S^{(-)} = S^{(1)} - \mathrm{i}S^{(2)}$. One can check that

$$\begin{aligned} S^{(+)}S^{(-)} &= S(S+1)\mathtt{Id} - [S^{(3)}]^2 + S^{(3)}, \\ S^{(-)}S^{(+)} &= S(S+1)\mathtt{Id} - [S^{(3)}]^2 - S^{(3)}. \end{aligned} \tag{1.8}$$

Let $|a\rangle$ be an eigenvector of $S^{(3)}$ with eigenvalue a. It follows from Eq. (1.8) that

$$\begin{aligned} \big\| S^{(+)}|a\rangle \big\|^2 &= \langle a|S^{(-)}S^{(+)}|a\rangle = S(S+1) - a^2 - a \geq 0, \\ \big\| S^{(-)}|a\rangle \big\|^2 &= \langle a|S^{(+)}S^{(-)}|a\rangle = S(S+1) - a^2 + a \geq 0. \end{aligned} \tag{1.9}$$

Then $|a| \leq S$, and $S^{(+)}|a\rangle \neq 0$ if $a \neq S$. Next, observe that $[S^{(3)}, S^{(+)}] = S^{(+)}$. Then

$$S^{(3)}S^{(+)}|a\rangle = (a+1)S^{(+)}|a\rangle. \tag{1.10}$$

Then if $a \neq S$ is an eigenvalue, $a+1$ is also an eigenvalue. There are similar relations with $S^{(-)}$, so that if $a \neq -S$ is an eigenvalue, $a-1$ is also an eigenvalue. It follows that $\{-S, -S+1, \dots S\}$ is the set of eigenvalues. □

Notice that the relations (1.3) always hold; this follows from (1.10) and (1.9). It follows from the parallelogram identity that $\|S^{\pm}\| = \sqrt{2}S$:

$$\begin{aligned} \|S^{(+)}\|^2 &= \tfrac14 (2\|S^{(+)}\|^2 + 2\|S^{(-)}\|^2) = \tfrac14 (\|S^{(+)} + S^{(-)}\|^2 + \|S^{(+)} - S^{(-)}\|^2) \\ &= \tfrac14 (4\|S^{(1)}\|^2 + 4\|S^{(2)}\|^2) = 2S^{(2)}. \end{aligned} \tag{1.11}$$

Spin operators are related to rotations in $\mathbb{R}^{(3)}$. Let $\vec{S} = (S^{(1)}, S^{(2)}, S^{(3)})$. Given $\vec{a} \in \mathbb{R}^{(3)}$, let

$$S^{\vec{a}} = \vec{a} \cdot \vec{S} = a_1 S^{(1)} + a_2 S^{(2)} + a_3 S^{(3)}. \tag{1.12}$$

By linearity, the commutation relations (1.1) generalize as

$$[S^{\vec{a}}, S^{\vec{b}}] = \mathrm{i}S^{\vec{a}\times\vec{b}}. \tag{1.13}$$

Finally, let $R_{\vec{a}}\vec{b}$ denote the vector $\vec{b}$ rotated around $\vec{a}$ by the angle $\|\vec{a}\|$.

LEMMA 1.3.

$$\mathrm{e}^{-\mathrm{i}S^{\vec{a}}}\, S^{\vec{b}}\, \mathrm{e}^{\mathrm{i}S^{\vec{a}}} = S^{R_{\vec{a}}\vec{b}}.$$

PROOF. We replace $\vec{a}$ by $s\vec{a}$, and we check that both sides of the identity satisfy the same differential equation. We find

$$\frac{\mathrm{d}}{\mathrm{d}s}\,\mathrm{e}^{-\mathrm{i}S^{s\vec{a}}}\,S^{\vec{b}}\,\mathrm{e}^{\mathrm{i}S^{s\vec{a}}} = -\mathrm{i}[S^{\vec{a}},\,\mathrm{e}^{-\mathrm{i}S^{s\vec{a}}}\,S^{\vec{b}}\,\mathrm{e}^{\mathrm{i}S^{s\vec{a}}}\,], \tag{1.14}$$

and

$$\frac{\mathrm{d}}{\mathrm{d}s}S^{R_{s\vec{a}}\vec{b}} = \Big(\frac{\mathrm{d}}{\mathrm{d}s}R_{s\vec{a}}\vec{b}\Big)\cdot\vec{S} = \Big(\vec{a}\times R_{s\vec{a}}\vec{b}\Big)\cdot\vec{S} = -\mathrm{i}[S^{\vec{a}}, S^{R_{s\vec{a}}\vec{b}}]. \tag{1.15}$$

We used (1.13) for the last identity. $\square$

It also follows from Lemmas 1.2 and 1.3 that any matrix $S^{\vec{a}}$, $\vec{a}\in\mathbb{R}^{(3)}$ with $\|\vec{a}\|=1$, has eigenvalues $\{-S,-S+1,\dots,S\}$.

COROLLARY 1.4. *Let $\psi_{\vec{b},c}$ be the eigenvector of $S^{\vec{b}}$ with eigenvalue c. Then $\mathrm{e}^{-\mathrm{i}S^{\vec{a}}}\,\psi_{\vec{b},c}$ is eigenvector of $S^{R_{\vec{a}}\vec{b}}$ with eigenvalue c.*

PROOF. Using Lemma 1.3,

$$S^{R_{\vec{a}}\vec{b}}\,\mathrm{e}^{-\mathrm{i}S^{\vec{a}}}\,\psi_{\vec{b},c} = \mathrm{e}^{-\mathrm{i}S^{\vec{a}}}\,S^{\vec{b}}\psi_{\vec{b},c} = c\,\mathrm{e}^{-\mathrm{i}S^{\vec{a}}}\,\psi_{\vec{b},c}. \tag{1.16}$$

$\square$

Finally, let us note the following useful relations:

$$\begin{aligned} \mathrm{e}^{-\mathrm{i}aS^{(3)}}\,S^{(+)}\,\mathrm{e}^{\mathrm{i}aS^{(3)}} &= \mathrm{e}^{-\mathrm{i}a}\,S^{(+)}, \\ \mathrm{e}^{-\mathrm{i}aS^{(3)}}\,S^{(-)}\,\mathrm{e}^{\mathrm{i}aS^{(3)}} &= \mathrm{e}^{\mathrm{i}a}\,S^{(-)}. \end{aligned} \tag{1.17}$$

1.2. Hamiltonians and Gibbs states

We consider this rather general "XYZ" hamiltonian, with two-body interactions in each spin directions, in the finite domain $\Lambda \Subset \mathbb{Z}^d$. The coupling constants are assumed to be symmetric, that is, $J^{(i)}_{xy} = J^{(i)}_{yx}$ for all $x,y\in\Lambda$ and all $i=1,2,3$.

$$H_{\Lambda,h} = -\tfrac12\sum_{x,y\in\Lambda}\Big(J^{(1)}_{xy}S^{(1)}_xS^{(1)}_y + J^{(2)}_{xy}S^{(2)}_xS^{(2)}_y + J^{(3)}_{xy}S^{(3)}_xS^{(3)}_y\Big) - h\sum_{x\in\Lambda}S^{(3)}_x. \tag{1.18}$$

With $Z_{\Lambda,h} = \operatorname{Tr}\mathrm{e}^{-\beta H_{\Lambda,h}}$ denoting the partition function, the finite volume Gibbs state at inverse temperature $\beta>0$ is the linear map

$$\begin{aligned} \langle\cdot\rangle_{\Lambda,\beta,h}:\quad &\mathcal{B}(\mathcal{H}_\Lambda)\to\mathbb{C} \\ &a\mapsto\langle a\rangle_{\Lambda,\beta,h} = \frac{1}{Z_{\Lambda,\beta,h}}\operatorname{Tr} a\,\mathrm{e}^{-\beta H_{\Lambda,h}}\,. \end{aligned} \tag{1.19}$$

The case $J^{(1)}_{xy} = J^{(2)}_{xy} = 0$, for all $x,y\in\Lambda$, corresponds to the Ising model, which is in fact a classical model. The case $J^{(3)}_{xy}=0$ and $J^{(1)}_{xy}=J^{(2)}_{xy}$, for all x,y, corresponds to the quantum XY model. And the symmetric case, $J^{(1)}_{xy} = J^{(2)}_{xy} = J^{(3)}_{xy}$, corresponds to the isotropic Heisenberg model. Positive values of the couplings correspond to ferromagnetic order, while negative values of the couplings correspond to antiferromagnetism.

1.3. Pressure, free energy, infinite volume limit

The statistical mechanics definition of the free energy, see Eq. (1.23) 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.

1.3.1. 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:

$$P(a) = \log \mathrm{Tr}\; \mathrm{e}^{-a}\,, \qquad a \in \mathcal{B}_{\mathrm{h}}(\mathcal{H}). \tag{1.20}$$

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

Proposition 1.5.

(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 $\langle a \rangle = \mathrm{Tr}\, a\, \mathrm{e}^{-H} / \mathrm{Tr}\; \mathrm{e}^{-H}$ 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 1.1 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 A.7) and then the Hölder inequality (Proposition A.1). For $s \in [0,1]$, we have

$$\begin{aligned} P(sa + (1-s)b) &= \log \mathrm{Tr}\; \mathrm{e}^{-sa-(1-s)b} \\ &\leq \log \mathrm{Tr}\; \mathrm{e}^{-sa}\; \mathrm{e}^{-(1-s)b} \\ &\leq \log \Big[\Big(\mathrm{Tr}\, \big(\mathrm{e}^{-sa} \big)^{\frac{1}{s}} \Big)^{s} \Big(\mathrm{Tr}\, \big(\mathrm{e}^{-(1-s)b} \big)^{\frac{1}{1-s}} \Big)^{1-s} \Big] \\ &= sP(a) + (1-s)P(b). \end{aligned} \tag{1.21}$$

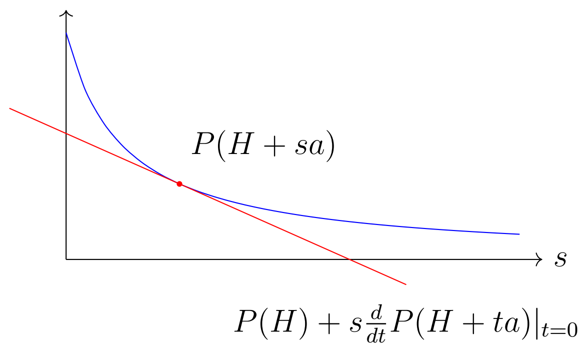

FIGURE 1.1. An illustration of tangents to the pressure: we have that $P(H+sa) \geq P(H) - s\langle a \rangle$ where $-\langle a \rangle = \frac{d}{dt}P(H+ta)|_{t=0}$. Note that $P(H+sa)$ is non-increasing in s for positive-definite a, which motivates the choice of sign in front of $\langle a \rangle$.

For the claim (b), let (φ_j) be an orthonormal basis of eigenvectors of a with eigenvalues (α_j). Starting with Peierls inequality (Proposition A.10) we have

$$\operatorname{Tr} \mathrm{e}^{-b} \geq \sum_j \mathrm{e}^{-\langle \varphi_j, b\varphi_j \rangle} \geq \mathrm{e}^{-\|a-b\|} \sum_j \mathrm{e}^{-\alpha_j} = \mathrm{e}^{-\|a-b\|} \operatorname{Tr} \mathrm{e}^{-a}. \tag{1.22}$$

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 $-\langle a \rangle$. □

1.3.2. The free energy and its infinite-volume limit. We define the (finite volume) free energy of the XYZ model to be

$$f_\Lambda(\beta, h) = -\frac{1}{\beta|\Lambda|} \log Z_{\Lambda,\beta,h}. \tag{1.23}$$

It follows from Proposition 1.5 that $\beta f_\Lambda(\beta, h)$ is a concave function of $(\beta, \beta h)$. We now check that we can take the limit of large volumes, along many sequences of increasing domains. 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 1.6. *Assume that the coupling constants satisfy:*

translation invariance: $J^{(i)}_{x+z,y+z} = J^{(i)}_{x,y}$ *for all* $x, y, z \in \mathbb{Z}^d, i = 1, 2, 3;$

summability: $\sum_{y \in \mathbb{Z}^d} |J^{(i)}_{x,y}| < \infty$ *for all* $x \in \mathbb{Z}^d, i = 1, 2, 3.$

Then there exists a function $f : \mathbb{R}_+ \times \mathbb{R} \to \mathbb{R}$ *such that*

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

where $\Lambda_n = \{1, \dots, n\}^d$.

PROOF. The proof of the existence of the infinite volume limit uses a superadditive 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 1.4).

$$\operatorname{Tr} \mathrm{e}^{a - \|b\|} \leq \operatorname{Tr} \mathrm{e}^{a+b} \leq \operatorname{Tr} \mathrm{e}^{a + \|b\|} . \tag{1.24}$$

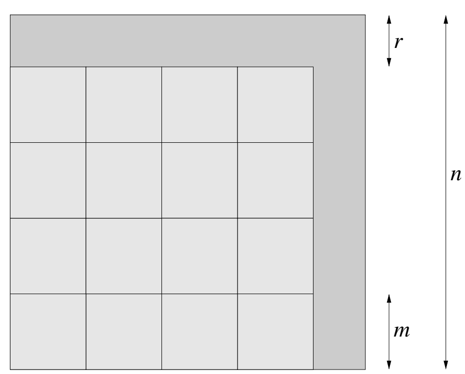

FIGURE 1.2. The large box of size n is decomposed in k^d boxes of size m; there are no more than drn^{d-1} remaining sites in the darker area.

Let m, n, k, r be integers such that $n = km + r$ and $0 \leq r < m$. The box Λ_n is the disjoint union of k^d boxes of size m and of some remaining sites, see Figure 1.2 for an illustration. Let C be the finite number

$$C = \sum_{y \in \mathbb{Z}^d} \sum_{i=1}^{3} |J^{(i)}_{x,y}|. \tag{1.25}$$

Notice that C does not depend on x by translation invariance. We get an inequality for the partition function in Λ_n by replacing all interactions that are not solely inside a single box of size m, by the bound βC. The boxes Λ_m become independent, and

$$\begin{aligned} Z_{\Lambda_n,\beta,h} &= \operatorname{Tr}_{\Lambda_n} \exp\Big(\beta \sum_{x,y\in\Lambda_n} \sum_{i=1}^{3} J^{(i)}_{x,y} S^{(i)}_x S^{(i)}_y + \beta h \sum_{x\in\Lambda_n} S^{(3)}_x\Big) \\ &\geq \Big[\operatorname{Tr}_{\mathcal{H}_{\Lambda_m}} \exp\Big(\beta \sum_{x,y\in\Lambda_m} \sum_{i=1}^{3} J^{(i)}_{x,y} S^{(i)}_x S^{(i)}_y + \beta h \sum_{x\in\Lambda_m} S^{(3)}_x\Big)\Big]^{k^d} \mathrm{e}^{-dk^d m^{d-1}\beta C + drn^{d-1})\beta C_h} \\ &= [Z_{\Lambda_m,\beta,h}]^{k^d} \, \mathrm{e}^{-dk^d m^{d-1}\beta C + drn^{d-1})\beta C_h}. \end{aligned} \tag{1.26}$$

Here we set $C_h = C + |h|S$. 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 Λ_n outside the small boxes. We then obtain a superadditive relation for the pressure:

$$f_{\Lambda_n}(\beta,h) \leq \frac{(km)^d}{n^d} f_{\Lambda_m}(\beta,h) + \frac{dk^d m^{d-1} C + drn^{d-1} C_h}{n^d}. \tag{1.27}$$

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

$$\limsup_{n\to\infty} f_{\Lambda_n}(\beta,h) \leq f_{\Lambda_m}(\beta,h) + \frac{d}{m} C. \tag{1.28}$$

Taking the lim inf over m in the right side, we see that it is greater or equal to the lim sup. It is not hard to verify that $f_\Lambda(\beta,h)$ is bounded uniformly in Λ, 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 $\Lambda_n^{\mathrm{per}} = (\mathbb{Z}/n\mathbb{Z})^d$ denote the periodic box of size n. Formally, elements of Λ_n^{per} are equivalence classes of sites where $x \sim y$ whenever $x_i - y_i = 0 \mod n$ for $i = 1, \dots, d$. The hamiltonian is as above but with coupling constants replaced by periodised ones:

$$J^{(i)}_{x,y,\mathrm{per}} = \sum_{z\in\mathbb{Z}^d} J^{(i)}_{x,y+nz}. \tag{1.29}$$

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

Corollary 1.7 (Thermodynamic limit with periodic boundary conditions). *Let $(\Lambda_n^{\mathrm{per}})$ be the sequence of cubes in $\mathbb{Z}^d$ of size n with periodic boundary conditions. Then $(f_{\Lambda_n^{\mathrm{per}}}(\beta,h))_{n\geq 1}$ converges pointwise to the same function $f(\beta,h)$ as in Theorem 1.9.*

This follows from $|f_{\Lambda_n^{\text{per}}}(\beta,h) - f_{\Lambda_n}(\beta,h)| \leq \frac{d}{n}\|C$, which is not too hard to prove, and Theorem 1.9.

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

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 1.9. *Assume that the coupling constants* $J^{(i)}_{x,y}$ *satisfy the conditions of Lemma 1.6. Then*

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

along all sequences of domains such that $\Lambda_n \Uparrow \mathbb{Z}^d$*. The function* f *is the same as in Lemma 1.6.*

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 Λ_n. Let

$$D = \Lambda_n \setminus \cup_{i=1}^k B_i. \tag{1.30}$$

We have the bounds

$$Z^k_{B,\beta,h}\,\mathrm{e}^{-(dkm^{d-1}+|D|)\beta C_h} \leq Z_{\Lambda_n,\beta,h} \leq Z^k_{B\beta,h}\,\mathrm{e}^{(dkm^{d-1}+|D|)\beta C_h}. \tag{1.31}$$

Then

$$\tfrac{km^d}{|\Lambda_n|} f_{B\beta,h} - \tfrac{dkm^{d-1}+|D|}{\Lambda_n|} C_h \geq f_{\Lambda_n,\beta,h} \geq \tfrac{km^d}{|\Lambda_n|} f_{B,\beta,h} + \tfrac{dkm^{d-1}+|D|}{\Lambda_n|} C_h. \tag{1.32}$$

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

$$1 - m^d \tfrac{|\partial\Lambda_n|}{|\Lambda_n|} \leq \tfrac{km^d}{|\Lambda_n|} \leq 1. \tag{1.33}$$

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

$$f_{B\beta,h} + \tfrac{d}{m} C_h \geq \liminf_{n\to\infty} f_{\Lambda_n\beta,h} \geq f_{B\beta,h} - \tfrac{d}{m} C_h. \tag{1.34}$$

(The inequalities hold with lim sup too.) Taking $m \to \infty$, both the left and right sides converge to the function $f(\beta, h)$ of Lemma 1.6. $\square$

1.4. Correlation functions and long-range order

The two-point correlation functions between sites 0 and x are given by

$$\langle S_0^{(i)} S_x^{(i)} \rangle_{\Lambda,\beta,h} = \frac{1}{Z_{\Lambda,\beta,h}} \mathrm{Tr}\, \big(S_0^{(i)} S_x^{(i)} \, \mathrm{e}^{-\beta H_{\Lambda,h}} \big). \tag{1.35}$$

We also consider the states $\langle \cdot \rangle_{\Lambda_\ell,\beta,h}^{\mathrm{per}}$ with periodic boundary conditions, where we use $H_{\Lambda_\ell,h}^{\mathrm{per}}$ instead of $H_{\Lambda_\ell,h}$. Often the system has *short range correlations* in the sense that

$$\langle S_0^{(i)} S_x^{(i)} \rangle_{\Lambda,\beta,h} \approx \langle S_0^{(i)} \rangle_{\Lambda,\beta,h} \langle S_0^{(i)} \rangle_{\Lambda,\beta,h} = 0, \tag{1.36}$$

as x is far from the origin. This happens e.g. at high temperatures, when β is small. At low temperatures the system may exhibit long-range correlations, or have the following property of long-range order.

DEFINITION 1.10 (Long-range order). *There exists a sequence of domains Λ_n, where either $\Lambda_n \Uparrow \mathbb{Z}^d$, or $\Lambda_n = \{1, \dots, m_n\}_{\mathrm{per}}^d$ with $m_n \to \infty$, such that*

$$\frac{1}{|\Lambda_n|^2} \sum_{x,y \in \Lambda_n} \langle S_x^{(3)} S_y^{(3)} \rangle_{\Lambda_n,\beta,0} \geq c > 0,$$

for all n.

In order to motivate the importance of this property, we show that it implies the occurrence of a first-order phase transition as h crosses 0. This also implies that there exist many distinct Gibbs states at $(\beta, 0)$, as we will see later.

THEOREM 1.11. *We assume that the system displays long-range order in the form of Eq. (1.10). Then*

$$\frac{\partial}{\partial h} f(\beta, h)\Big|_{h=0-} \; > \; 0 \; > \; \frac{\partial}{\partial h} f(\beta, h)\Big|_{h=0+}.$$

PROOF. We give a simplified proof in the case where $[H_{\Lambda,h}, M_\Lambda] = 0$, where M_Λ is the magnetisation operator

$$M_\Lambda = \sum_{x \in \Lambda} S_x^{(3)}. \tag{1.37}$$

For the general case, we refer to Koma and Tasaki [1993].

Let $|M_\Lambda|$ be the unique positive semi-definite square root of M_Λ^2. We have $|M_\Lambda| \leq |\Lambda| S \,\mathrm{Id}$, so that $M_\Lambda^2 \leq |\Lambda| S |M_\Lambda|$. Since Gibbs states are positive linear functionals, we get

$$\Big\langle \frac{M_\Lambda^2}{|\Lambda|^2} \Big\rangle_{\Lambda,\beta,0} \leq S \Big\langle \frac{|M_\Lambda|}{|\Lambda|} \Big\rangle_{\Lambda,\beta,0}. \tag{1.38}$$

Long-range order implies that $\frac{1}{|\Lambda|^2} \langle M_\Lambda^2 \rangle_{\Lambda,\beta,0} \geq c$, so the right side above is positive.

In order to get an inequality for the derivative of the free energy, let us introduce $\tilde{f}_\Lambda(\beta,h)$ to be the free energy of the model with Hamiltonian

$$\tilde{H}_{\Lambda,h} = -\sum_{i=1}^{3} \sum_{x,y\in\Lambda} J_{x-y}^{(i)} S_x^{(i)} S_y^{(i)} - h|M_\Lambda|. \tag{1.39}$$

We now check that $\tilde{f}_\Lambda(\beta,h)$ converges as $\Lambda \Uparrow \mathbb{Z}^d$ to the free energy $f(\beta,h)$ for $h \geq 0$. For this, notice that M_Λ (and $|M_\Lambda|$) commute with $H_{\Lambda,0} = \tilde{H}_{\Lambda,0}$. For $h \geq 0$ we have the inequalities (for the second one, observe that the spectrum of M_Λ is symmetric around 0)

$$\operatorname{Tr} \mathrm{e}^{-\beta H_{\Lambda,\beta,0} + \beta h M_\Lambda} \leq \operatorname{Tr} \mathrm{e}^{-\beta H_{\Lambda,\beta,0} + \beta h |M_\Lambda|} \leq 2 \operatorname{Tr} \mathrm{e}^{-\beta H_{\Lambda,\beta,0} + \beta h M_\Lambda}. \tag{1.40}$$

Taking the logarithm and dividing by $\beta|\Lambda|$, and taking the relevant limits, we get that f and $\tilde{f}$ are equal.

We now use the concavity in h of $\tilde{f}_\Lambda$ and the fact that $\sup_n(\liminf_m a_{m,n}) \leq \liminf_m(\sup_n a_{m,n})$ and we get

$$\begin{aligned}
\frac{\partial}{\partial h} f(\beta,h)\Big|_{h=0+} &= \sup_{h>0} \frac{f(\beta,h)-f(\beta,0)}{h} = \sup_{h>0} \liminf_{\Lambda\Uparrow\mathbb{Z}^d} \frac{\tilde{f}_\Lambda(\beta,h)-\tilde{f}_\Lambda(\beta,0)}{h} \\
&\leq \liminf_{\Lambda\Uparrow\mathbb{Z}^d} \sup_{h>0} \frac{\tilde{f}_\Lambda(\beta,h)-\tilde{f}_\Lambda(\beta,0)}{h} = \liminf_{\Lambda\Uparrow\mathbb{Z}^d} \frac{\partial}{\partial h} \tilde{f}_\Lambda(\beta,h)\Big|_{h=0} \\
&= \liminf_{\Lambda\Uparrow\mathbb{Z}^d} \Big\langle -\frac{|M_\Lambda|}{|\Lambda|} \Big\rangle_{\Lambda,\beta,0}.
\end{aligned} \tag{1.41}$$

The last expectation is with respect to the Gibbs state with Hamiltonian $\tilde{H}_{\Lambda,0} = H_{\Lambda,0}$. The right side is positive and $\frac{\partial}{\partial h} f(\beta,h)\big|_{h=0+}$ is indeed negative. Since f is even in h we get the other inequality as well.

When M_Λ does not commute with the Hamiltonian, it does not seem possible to show that f and $\tilde{f}$ are equal. But since right-derivatives of concave functions are right-continuous, we can proceed as above and get

$$\frac{\partial}{\partial h} f(\beta,h)\Big|_{h=0+} = \lim_{h'\to 0+} \frac{\partial}{\partial h} f(\beta,h)\Big|_{h=h'+} \leq \lim_{h'\to 0+} \liminf_{\Lambda\Uparrow\mathbb{Z}^d} \Big\langle -\frac{M_\Lambda}{|\Lambda|} \Big\rangle_{\Lambda,\beta,h'}. \tag{1.42}$$

Koma and Tasaki (1993) have proved that long-range order (in the sense of (1.10)) implies that the right side is strictly negative. □

1.5. Correlation inequalities

We now discuss some correlation inequalities for quantum spin systems. These are not as far-reaching as the GKS and FKG inequalities for classical spins.

THEOREM 1.12. *Assume that, for all $x, y \in \Lambda$, the couplings satisfy*

$$|J^{(2)}_{xy}| \leq J^{(1)}_{xy}.$$

Then we have that

$$\big|\langle S^{(2)}_0 S^{(2)}_x \rangle_{\Lambda,h}\big| \leq \langle S^{(1)}_0 S^{(1)}_x \rangle_{\Lambda,h},$$

for all $x \in \Lambda$. More generally, for all $x_1, \dots x_k \in \Lambda$ and $j_1, \dots, j_k \in \{1, 2\}$,

$$\big|\langle S^{(j_1)}_{x_1} \dots S^{(j_k)}_{x_k} \rangle_{\Lambda,h}\big| \leq \langle S^{(1)}_{x_1} \dots S^{(1)}_{x_k} \rangle_{\Lambda,h}.$$

Further inequalities can be generated using symmetries. Some inequalities hold for the staggered two-point function $(-1)^{|x|}\langle S^{(i)}_0 S^{(i)}_x \rangle_{\Lambda,h}$.

PROOF. Let $S \in \frac12\mathbb{N}$ such that $2S + 1 = N$, and let $|a\rangle$, $a \in \{-S, \dots, S\}$ denote basis elements of $\mathbb{C}^{2S+1}$. Let the operators $S^{(\pm)}$ be defined by

$$S^{(+)}|a\rangle = \sqrt{S(S+1) - a(a+1)}\;|a{+}1\rangle, \quad S^{(-)}|a\rangle = \sqrt{S(S+1) - (a-1)a}\;|a{-}1\rangle, \tag{1.43}$$

with the understanding that $S^{(+)}|S\rangle = S^{(-)}|-S\rangle = 0$. Then let $S^{(1)} = \frac12(S^{(+)} + S^{(-)})$, $S^{(2)} = \frac{1}{2\mathrm{i}}(S^{(+)} - S^{(-)})$, and $S^{(3)}|a\rangle = a|a\rangle$. It is well-known that these operators satisfy the spin commutation relations. Further, the matrix elements of $S^{(1)}, S^{(\pm)}$ are all nonnegative, and the matrix elements of $S^{(2)}$ are all less than or equal to those of $S^{(1)}$ in absolute values. Using the Trotter formula and multiple resolutions of the identity, we have

$$\begin{aligned}
\Big|\mathrm{Tr}\, S^{(2)}_0 S^{(2)}_x \,\mathrm{e}^{-\beta H_{\Lambda,h}}\,\Big| \leq \lim_{N\to\infty} \sum_{\sigma_0,\dots,\sigma_N \in \{-S,\dots,S\}^\Lambda} \Big| &\langle \sigma_0 | S^{(2)}_0 S^{(2)}_x | \sigma_1 \rangle \\
\langle \sigma_1 | \,\mathrm{e}^{\frac{\beta}{N}\sum J^{(3)}_{yz} S^{(3)}_y S^{(3)}_z + \frac{\beta h}{N}\sum S^{(3)}_x}\, | \sigma_1 \rangle \langle \sigma_1 | &\Big(1 + \frac{\beta}{N}\sum_{y,z\in\Lambda} (J^{(1)}_{yz} S^{(1)}_y S^{(1)}_z + J^{(2)}_{yz} S^{(2)}_y S^{(2)}_z)\Big) | \sigma_2 \rangle \\
\dots \langle \sigma_N | \,\mathrm{e}^{\frac{\beta}{N}\sum J^{(3)}_{yz} S^{(3)}_y S^{(3)}_z + \frac{\beta h}{N}\sum S^{(3)}_x}\, | \sigma_N \rangle \langle \sigma_N | &\Big(1 + \frac{\beta}{N}\sum_{y,z\in\Lambda} (J^{(1)}_{yz} S^{(1)}_y S^{(1)}_z + J^{(2)}_{yz} S^{(2)}_y S^{(2)}_z)\Big) | \sigma_0 \rangle \Big|.
\end{aligned} \tag{1.44}$$

Observe that the matrix elements of all operators are nonnegative, except for $S^{(2)}_0 S^{(2)}_x$. Indeed, this follows from

$$\begin{aligned}
J^{(1)}_{yz} S^{(1)}_y S^{(1)}_z + J^{(2)}_{yz} S^{(2)}_y S^{(2)}_z =& \tfrac14 (J^{(1)}_{yz} - J^{(2)}_{yz})(S^{(+)}_y S^{(+)}_z + S^{(-)}_y S^{(-)}_z) \\
&+ \tfrac14 (J^{(1)}_{yz} + J^{(2)}_{yz})(S^{(+)}_y S^{(-)}_z + S^{(-)}_y S^{(+)}_z).
\end{aligned} \tag{1.45}$$

We get an upper bound for the right side of (1.44) by replacing $|\langle\sigma_0|S_0^{(2)}S_x^{(2)}|\sigma_1\rangle|$ with $\langle\sigma_0|S_0^{(1)}S_x^{(1)}|\sigma_1\rangle$. We have obtained

$$\Big|\operatorname{Tr} S_0^{(2)}S_x^{(2)}\,\mathrm{e}^{-\beta H_{\Lambda,h}}\Big| \leq \operatorname{Tr} S_0^{(1)}S_x^{(1)}\,\mathrm{e}^{-\beta H_{\Lambda,h}}\,, \tag{1.46}$$

which proves the first claim. The second claim can be proved exactly the same way. □

COROLLARY 1.13. *Assume that for all $x, y \in \Lambda$, the couplings satisfy*

$$J_{xy}^{(1)} = J_{xy}^{(2)} \geq 0.$$

Then we have for all $x, y, z, u \in \Lambda$

$$\frac{\partial}{\partial J_{xy}^{(1)}}\langle S_z^{(2)}S_u^{(2)}\rangle_{\Lambda,h} \leq \frac{\partial}{\partial J_{xy}^{(1)}}\langle S_z^{(1)}S_u^{(1)}\rangle_{\Lambda,h}.$$

PROOF. For $i = 1, 2, 3$, we have

$$\frac{1}{\beta}\frac{\partial}{\partial J_{xy}^{(1)}}\langle S_z^{(i)}S_u^{(i)}\rangle_{\Lambda,h} = (S_x^{(1)}S_y^{(1)}, S_z^{(i)}S_u^{(i)}) - \langle S_x^{(1)}S_y^{(1)}\rangle_{\Lambda,h}\langle S_z^{(i)}S_u^{(i)}\rangle_{\Lambda,h}, \tag{1.47}$$

where (A, B) denotes the Duhamel two-point function,

$$(A, B) = \frac{1}{Z_{\Lambda,h}}\int_0^1 \operatorname{Tr} A\,\mathrm{e}^{-s\beta H_{\Lambda,h}}\,B\,\mathrm{e}^{-(1-s)\beta H_{\Lambda,h}}\,\mathrm{d}s. \tag{1.48}$$

It is not hard to extend the proof of Theorem 1.12 to the Duhamel function, so that

$$\big|(S_x^{(1)}S_y^{(1)}, S_z^{(2)}S_u^{(2)})\big| \leq (S_x^{(1)}S_y^{(1)}, S_z^{(1)}S_u^{(1)}). \tag{1.49}$$

Further, we have $\langle S_z^{(2)}S_u^{(2)}\rangle_{\Lambda,h} = \langle S_z^{(1)}S_u^{(1)}\rangle_{\Lambda,h}$ by symmetry. The result follows. □

EXERCISE 1.1. *For $S = 1$, check that the following matrices satisfy the spin relations.*

$$S^{(1)} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -\mathrm{i} \\ 0 & \mathrm{i} & 0 \end{pmatrix}, \qquad S^{(2)} = \begin{pmatrix} 0 & 0 & -\mathrm{i} \\ 0 & 0 & 0 \\ \mathrm{i} & 0 & 0 \end{pmatrix}, \qquad S^{(3)} = \begin{pmatrix} 0 & -\mathrm{i} & 0 \\ \mathrm{i} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

EXERCISE 1.2. *For $S = 1$, check that the following matrices do not satisfy the spin relations.*

$$S^{(1)} = \tfrac{1}{2}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \qquad S^{(2)} = \tfrac{1}{2}\begin{pmatrix} 0 & -\mathrm{i} & 0 \\ \mathrm{i} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \qquad S^{(3)} = \tfrac{1}{2}\begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

Exercise 1.3. *Let F be the linear operator for spin flips: If $|(\sigma_x)_{x\in\Lambda}\rangle$ denotes the ket associated with the classical configuration (σ_x), then $F|(\sigma_x)_{x\in\Lambda}\rangle = |(-\sigma_x)_{x\in\Lambda}\rangle$. Can F be written using spin operators?*

Exercise 1.4. *Prove the matrix inequality (1.24).*

CHAPTER 2

Two-dimensional systems with continuous symmetry

We consider a variant of the Mermin-Wagner theorem for systems that are effectively two-dimensional. The result is that the two-point function decays with the distance, at least like a power law. Logarithmic decay was first obtained by Fisher and Jasnow (1971). The decay is, however, expected to be power-law, and this was proven by McBryan and Spencer (1977) in a short and lucid article that exploits complex rotations. Power-law decay was proven for some quantum systems in Bonato, Fernando Perez, Klein (1982) and Ito (1982). The proofs use Fourier transform and the Bogolubov inequality, and they are limited to regular two-dimensional lattices. A much more general result was obtained by Koma and Tasaki (1992) using complex rotations. The present proof is slightly simpler and can be found in Fröhlich and Ueltschi (2015).

We assume that $J^1_{xy} = J^2_{xy}$ for all x, y. The decay of correlations is measured by the following expression:

$$\xi_\beta(x) = \sup_{\substack{(\phi_y)\in\mathbb{R}^\Lambda \\ \phi_x=0}} \Big[\phi_0 - 2\beta S^2 \sum_{y,z\in\Lambda} |J^1_{yz}| \big(\cosh(\phi_y - \phi_z) - 1\big) \Big]. \tag{2.1}$$

The solution of this variational problem is essentially a discrete harmonic function. We can estimate it explicitly in the case of "2D-like" graphs with nearest-neighbor couplings. Let Λ denote a graph, i.e. a finite set of vertices and a set of edges, and let $d(x,y)$ denote the graph distance, i.e. the length of the shortest path that connects x and y.

LEMMA 2.1. *Assume that $J^i_{xy} = 0$ whenever $d(x,y) \neq 1$ and let $J = \max |J^i_{xy}|$. Assume in addition that there exists a constant K such that, for any $\ell \geq 0$,*

$$\#\big\{\{x,y\} \subset \Lambda : d(0,x) = \ell, d(0,y) = \ell+1, \text{ and } d(x,y) = 1\big\} \leq K(\ell+1).$$

Then there exists $C = C(\beta, S, J, K)$, which does not depend on x, such that

$$\xi_\beta(x) \geq \frac{1}{16\beta J S^2 K} \log\big(d(0,x)+1\big) - C.$$

PROOF. With c to be chosen later, let

$$\phi_y = \begin{cases} c \log \frac{d(0,x)+1}{d(0,y)+1} & \text{if } d(0,y) \leq d(0,x), \\ 0 & \text{otherwise.} \end{cases} \tag{2.2}$$

Then

$$\xi_\beta(x) \geq c \log(d(0,x)+1) - 4\beta S^2 JK \sum_{\ell=0}^{d(0,x)-1} \Bigl(\cosh(c \log \tfrac{\ell+2}{\ell+1}) - 1\Bigr)(\ell+1). \tag{2.3}$$

From Taylor expansions of the logarithm and of the hyperbolic cosine, there exist C, C' such that

$$\begin{aligned} \xi_\beta(x) &\geq c \log(d(0,x)+1) - 4\beta S^2 JKc^2 \sum_{\ell=1}^{d(0,x)} \frac{1}{\ell} - C' \\ &\geq \Bigl[c - 4\beta S^2 JKc^2\Bigr] \log(d(0,x)+1) - C. \end{aligned} \tag{2.4}$$

The optimal choice is $c = (8\beta S^2 JK)^{-1}$. $\square$

THEOREM 2.2. *Assume that $J^1_{xy} = J^2_{xy}$ for all $x,y \in \Lambda$. Then, for $i = 1,2$, we have*

$$\bigl|\langle S^i_0 S^i_x \rangle\bigr| \leq S^2 \,\mathrm{e}^{-\xi_\beta(x)} \,.$$

In the case of 2D-like graphs, we can use Lemma 2.1 and we obtain algebraic decay with a power greater than $(8\beta JS^2K)^{-1}$.

PROOF. We use the method of complex rotations. Let

$$S^\pm_y = S^1_y \pm \mathrm{i} S^2_y. \tag{2.5}$$

One can check that for any $a \in \mathbb{C}$, we have

$$\mathrm{e}^{aS^3_y}\, S^\pm_y \,\mathrm{e}^{-aS^3_y} \;=\; \mathrm{e}^{\pm a}\, S^\pm_y. \tag{2.6}$$

We have $\langle S^+_0 S^-_x \rangle = 2\langle S^1_0 S^1_x \rangle$ and this is nonnegative by Theorem 1.12. The hamiltonian (1.18) can be rewritten as

$$H_\Lambda = -\tfrac12 \sum_{y,z\in\Lambda} \bigl(J^1_{yz} S^+_y S^-_z + J^3_{yz} S^3_y S^3_z \bigr) \tag{2.7}$$

Given numbers ϕ_y, let

$$A = \prod_{y\in\Lambda} \mathrm{e}^{\phi_y S^3_y} \,. \tag{2.8}$$

Then

$$\operatorname{Tr} S^+_0 S^-_x \,\mathrm{e}^{-\beta H_\Lambda} \;=\; \operatorname{Tr} A S^+_0 S^-_x A^{-1} \,\mathrm{e}^{-\beta A H_\Lambda A^{-1}} \,. \tag{2.9}$$

We now compute the rotated Hamiltonian.

$$\begin{aligned} AH_\Lambda A^{-1} &= -\tfrac12 \sum_{y,z\in\Lambda} \bigl(J^1_{yz}\, \mathrm{e}^{\phi_y - \phi_z}\, S^+_y S^-_z + J^3_{yz} S^3_y S^3_z \bigr) \\ &= H_\Lambda - \tfrac12 \sum_{y,z\in\Lambda} J^1_{yz} \bigl(\cosh(\phi_y - \phi_z) - 1\bigr)\; S^+_y S^-_z - \tfrac12 \sum_{y,z\in\Lambda} J^1_{yz} \sinh(\phi_y - \phi_z)\; S^+_y S^-_z \\ &\equiv H_\Lambda + B + C. \end{aligned} \tag{2.10}$$

Notice that $B^* = B$ and $C^* = -C$. We obtain

$$\operatorname{Tr} S_0^+ S_x^- \,\mathrm{e}^{-\beta H_\Lambda} \;=\; \mathrm{e}^{\phi_0 - \phi_x} \operatorname{Tr} S_0^+ S_x^- \,\mathrm{e}^{-\beta H_\Lambda - \beta B - \beta C}\,. \tag{2.11}$$

We now estimate the trace in the right side using the Trotter product formula and the Hölder inequality for traces. Recall that $\|B\|_s = (\operatorname{Tr}|B|^s)^{1/s}$, with $\|B\|_\infty = \|B\|$ being the usual operator norm.

$$\begin{aligned} \operatorname{Tr} S_0^+ S_x^- \,\mathrm{e}^{-\beta H_\Lambda - \beta B - \beta C} &= \lim_{N\to\infty} \operatorname{Tr} S_0^+ S_x^- \Big(\mathrm{e}^{-\frac{\beta}{N} H_\Lambda}\, \mathrm{e}^{-\frac{\beta}{N} B}\, \mathrm{e}^{-\frac{\beta}{N} C} \Big)^N \\ &\leq \lim_{N\to\infty} \|S_0^+ S_x^-\|_\infty \, \big\| \mathrm{e}^{-\frac{\beta}{N} H_\Lambda} \big\|_N^N \, \big\| \mathrm{e}^{-\frac{\beta}{N} B} \big\|_\infty^N \, \big\| \mathrm{e}^{-\frac{\beta}{N} C} \big\|_\infty^N. \end{aligned} \tag{2.12}$$

Observe now that $\|S_0^+ S_x^-\| = 2S^2$, $\| \mathrm{e}^{-\frac{\beta}{N} H_\Lambda} \|_N^N = Z_\Lambda$, $\| \mathrm{e}^{-\frac{\beta}{N} B} \|^N \leq \mathrm{e}^{\beta \|B\|}$, and $\| \mathrm{e}^{-\frac{\beta}{N} C} \| = 1$. The theorem then follows from

$$\|B\| \leq S^2 \sum_{y,z\in\Lambda} |J^1_{yz}| \big(\cosh(\phi_y - \phi_z) - 1 \big). \tag{2.13}$$

$\square$

CHAPTER 3

Long-range order via reflection positivity

We show that in the case of some quantum models with continuous symmetry, it is possible to prove long-range order, and hence non-differentiability of the infinite-volume pressure. The latter implies that the set of Gibbs states contains more than one element.

3.1. Long-range order

In what follows we need to consider periodic boundary conditions. Given $\ell \in \mathbb{N}$, let $\Lambda_\ell = \{0, 1, \dots, \ell - 1\}^d$, and let the hamiltonian $H^{\rm per}_{\Lambda_\ell, h}$ given by (1.18) but with coupling parameters $J^{(i)}_{xy} = J^{(i)}_{x-y}$ replaced by the following periodised ones:

$$J^{(i)}_{x,\rm per} = \sum_{z \in \mathbb{Z}^d} J^{(i)}_{x+\ell z}. \tag{3.1}$$

We can define the periodised partition function $Z^{\rm per}(\Lambda_\ell, \beta, h)$ accordingly, and the pressure

$$p^{\rm per}_{\Lambda_\ell}(\beta, h) = \frac{1}{\ell^d} \log Z^{\rm per}(\Lambda_\ell, \beta, h). \tag{3.2}$$

As $\ell \to \infty$, these pressures converge by Theorem 1.9. Recall the definition of finite-volume equilibrium states:

$$\langle \cdot \rangle_{\Lambda,\beta,h} = \frac{\operatorname{Tr}\left[\cdot \, \mathrm{e}^{-\beta H_{\Lambda,h}}\right]}{Z_{\Lambda,\beta,h}}. \tag{3.3}$$

We also consider the states $\langle \cdot \rangle^{\rm per}_{\Lambda_\ell,\beta,h}$ with periodic boundary conditions, where we use $H^{\rm per}_{\Lambda_\ell,h}$ instead of $H_{\Lambda_\ell,h}$. The concept of long-range order was introduced in Definition 1.10; it means that $\frac{1}{|\Lambda_n|^2} \sum_{x,y \in \Lambda_n} \langle S^{(3)}_x S^{(3)}_y \rangle_{\Lambda_n,\beta,0} \geq c > 0$, for a sequence of domains that tend to $\mathbb{Z}^d$.

We state two results about long-range order. The first theorem holds for a larger class of coupling constants and for S large enough. The second theorem is restricted to nearest-neighbour interactions, but it has the advantage of applying to more values of S and more dimensions. To briefly summarise the consequences of those results, we will see that long-range order (in the form of Definition 1.10) holds under the following conditions:

- for certain long-range interactions (specified below) if $\beta \geq \beta_0$ for some $\beta_0 < \infty$ provided $d \geq 3$ and S is large enough, or

- for nearest-neighbour interactions if $\beta \geq \beta_0$ for some $\beta_0 < \infty$ provided $d \geq 3$ and $S \geq \frac{1}{2}$, or
- for nearest-neighbour interactions in the ground-state $\beta = \infty$ provided $d \geq 2$ and either $S \geq 1$, or $S \geq \frac{1}{2}$ and $-J^{(2)}/J^{(1)} \leq 0.13$.

We consider the case of nearest-neighbour interactions, $J_x^{(i)} = 0$ unless $\|x\|_1 = 1$ (in which case it equals some constant $J^{(i)}$); and longer-range interactions that are given by a Fourier transform, $J_x^{(i)} = \int_{\mathbb{R}^d} \mathrm{d}\nu^{(i)}(k)\, \mathrm{e}^{ik\cdot x}$ where $\nu^{(i)}$ is a positive, finite measure on $\mathbb{R}^d$. The latter case allows us to include the following examples:

- $J_x^{(i)} = a^{(i)}\, \mathrm{e}^{-b^{(i)}\|x\|_p^p}$ for $p \in (0,2]$ and constants $a^{(i)} \in \mathbb{R}$, $b^{(i)} > 0$. Indeed, this follows from the fact that the characteristic function of a *stable distribution* in probability theory is of the form $\mathrm{e}^{-c|t|^p}$. (For $p > 2$ this is not possible as the positivity of ν would be violated.) See e.g. Durrett [2019].
- $J_x^{(i)} = a^{(i)}\|x\|_p^{-c^{(i)}}$ with $p \in (0,2]$, $a^{(i)} \in \mathbb{R}$ and $c^{(i)} > d$. Indeed, we can take linear combinations of the interactions above with non-negative coefficients, and we have
$$\int_0^\infty s^{(c-1)/p}\, \mathrm{e}^{-s\|x\|_p^p}\, \mathrm{d}s = C\|x\|_p^{-c}. \tag{3.4}$$
Here $c > d$ is required in order for the sum defining $J_{x,\mathrm{per}}^{(i)}$ to be convergent.
- Convex combinations of the above.

Let Λ_ℓ^* denote the dual of Λ_ℓ in Fourier theory, namely
$$\Lambda_\ell^* = \tfrac{2\pi}{\ell}\big\{-\tfrac{\ell}{2}+1, \dots, \tfrac{\ell}{2}\big\}^d \subset [-\pi,\pi]^d. \tag{3.5}$$

Theorem 3.1. *Assume that $J_x^{(i)}$ is one of the interactions above; we assume in addition that ℓ is even and that*
$$J_x^{(3)} \geq J_x^{(1)} \geq -J_x^{(2)} \geq 0, \qquad \textit{for all } x \in \mathbb{Z}^d.$$
Then
$$\frac{1}{\ell^d}\sum_{x\in\Lambda_\ell}\langle S_0^{(3)} S_x^{(3)}\rangle_{\Lambda_\ell,\beta,0}^{per} \geq \tfrac{1}{3}S(S+1) - \frac{1}{\ell^d}\sum_{k\in\Lambda_\ell^*\setminus\{0\}}\sqrt{\frac{e(k)}{2\varepsilon(k)}} - \frac{1}{2\beta\ell^d}\sum_{k\in\Lambda_\ell^*\setminus\{0\}}\frac{1}{\varepsilon(k)}. \tag{3.6}$$

Here we defined
$$\varepsilon(k) = \sum_{x\in\mathbb{Z}^d} J_{x,\mathrm{per}}^{(3)}(1-\cos kx) \tag{3.7}$$
while the function $e(k)$ is defined in (3.39). Notice that $\varepsilon(k)$ is bounded and that $\varepsilon(k) \sim k^2$ around $k=0$; it is positive for $k \neq 0$. It is worth pointing out

that $e(k) \leq \text{const}\, S^2$ around $k = 0$. Therefore the right-hand-side of (3.6) is necessarily positive when $d \geq 3$ and S, β are large enough.

We now assume that $J^{(i)}$ are nearest-neighbour couplings, that is,

$$J_x^{(i)} = \begin{cases} J^{(i)} & \text{if } \|x\| = 1, \\ 0 & \text{otherwise.} \end{cases} \tag{3.8}$$

We further normalise them so that $J^{(3)} = 1$. In this case we derive sharper lower bounds for long-range order. Let us introduce the following two sums:

$$\begin{aligned} I_\ell^{(d)} &= \frac{1}{\ell^d} \sum_{k \in \Lambda_\ell^* \setminus \{0\}} \sqrt{\frac{\varepsilon(k+\pi)}{\varepsilon(k)}}, \\ \tilde{I}_\ell^{(d)} &= \frac{1}{\ell^d} \sum_{k \in \Lambda_\ell^* \setminus \{0\}} \sqrt{\frac{\varepsilon(k+\pi)}{\varepsilon(k)}} \Big(\frac{1}{d} \sum_{i=1}^d \cos k_i \Big)_+ . \end{aligned} \tag{3.9}$$

Here, $\varepsilon(k) = 2\sum_{i=1}^d (1 - \cos k_i)$ and $\varepsilon(k+\pi) = 2\sum_{i=1}^d (1 + \cos k_i)$, and $(\cdot)_+$ denotes the positive part. Their infinite volume limits converge to the integrals

$$\begin{aligned} I^{(d)} &= \lim_{\ell \to \infty} I_\ell^{(d)} = \frac{1}{(2\pi)^d} \int_{[-\pi,\pi]^d} \sqrt{\frac{\varepsilon(k+\pi)}{\varepsilon(k)}} \mathrm{d}k, \\ \tilde{I}^{(d)} &= \lim_{\ell \to \infty} \tilde{I}_\ell^{(d)} = \frac{1}{(2\pi)^d} \int_{[-\pi,\pi]^d} \sqrt{\frac{\varepsilon(k+\pi)}{\varepsilon(k)}} \Big(\frac{1}{d} \sum_{i=1}^d \cos k_i \Big)_+ \mathrm{d}k. \end{aligned} \tag{3.10}$$

One can check that, as $d \to \infty$, these integrals satisfy $I^{(d)} \to 1$ (Dyson, Lieb, Simon [1978]) and $\tilde{I}^{(d)} \to 1$ (Kennedy, Lieb, Shastry [1988b]). We also introduce the expression

$$\alpha_\ell(\beta) = J^{(1)} \langle S_0^{(1)} S_{e_1}^{(1)} \rangle_{\Lambda_\ell, \beta, 0} + J^{(2)} \langle S_0^{(2)} S_{e_1}^{(2)} \rangle_{\Lambda_\ell, \beta, 0} \tag{3.11}$$

and $\alpha(\beta) = \liminf_{\ell \to \infty} \alpha_\ell(\beta)$. We also denote by $\alpha_\ell(\infty)$ the $\beta \to \infty$ limit.

THEOREM 3.2. *Assume that ℓ is even and that the nearest-neighbour coupling constants satisfy*

$$J^{(3)} = 1 \geq J^{(1)} \geq -J^{(2)} \geq 0.$$

Then we have the two lower bounds:

$$\frac{1}{\ell^d} \sum_{x \in \Lambda_\ell} \langle S_0^{(3)} S_x^{(3)} \rangle_{\Lambda_\ell, \beta, 0}^{per} \geq$$

$$\begin{cases} \frac{1}{3} S(S+1) - \frac{1}{2}\big(I_\ell^{(d)} + \frac{\sqrt{2}}{\ell^d}\big) \sqrt{\alpha_\ell(\beta)} - \frac{1}{2\beta\ell^d} \sum_{k \in \Lambda_\ell^* \setminus \{0\}} \frac{1}{\varepsilon(k)}, \\ \sqrt{\alpha_\ell(\beta)} \big[\frac{\sqrt{\alpha_\ell(\beta)}}{1 - J^{(2)}/J^{(1)}} - \frac{1}{2} \tilde{I}_\ell^{(d)} \big] - \frac{1}{2\beta\ell^d} \sum_{k \in \Lambda_\ell^* \setminus \{0\}} \frac{1}{\varepsilon(k)} \big(\frac{1}{d} \sum_{i=1}^d \cos k_i \big)_+ . \end{cases}$$

The theorem is proved at the end of Section 3.2.

We want to formulate sufficient conditions under which at least one of the lower bounds is positive, uniformly in ℓ. The terms involving $1/\beta$ converge as $\ell \to \infty$ if $d \geq 3$ and they can be made arbitrarily small by taking β sufficiently large. For $d = 2$ the bounds are useful in the ground state, i.e. when the limit $\beta \to \infty$ is taken before $\ell \to \infty$.

We get a uniform lower bound if either

$$\tfrac{1}{3}S(S+1) > \tfrac{1}{2}I^{(d)}\sqrt{\alpha(\beta)} \qquad \text{or} \qquad \frac{\sqrt{\alpha(\beta)}}{1 - J^{(2)}/J^{(1)}} > \tfrac{1}{2}\tilde{I}^{(d)}.$$

Irrespective of the value of $\alpha(\beta)$, at least one of the lower bound is positive if

$$\frac{\frac{1}{3}S(S+1)}{\frac{1}{2}I^{(d)}} > \tfrac{1}{2}\tilde{I}^{(d)}(1 - J^{(2)}/J^{(1)}) \quad \Longleftrightarrow \quad 1 - J^{(2)}/J^{(1)} < \frac{\frac{4}{3}S(S+1)}{I^{(d)}\tilde{I}^{(d)}}. \tag{3.12}$$

Values of $I^{(d)}$ and $\tilde{I}^{(d)}$ can be found numerically; they are listed in Table 1 for $d = 2, 3, 4$. This allows us to verify that the condition (3.12) holds for all values of $J^{(1)}, J^{(2)}$ such that $J^{(1)} \geq -J^{(2)} \geq 0$, all dimensions $d \geq 2$, and all spin values $S \in \frac{1}{2}\mathbb{N}$, with the *one exception* of the case $d = 2$ and $S = \frac{1}{2}$. In this case, (3.12) holds when $-J^{(2)}/J^{(1)} \in [0, 0.109]$.

d	$I^{(d)}$	$\tilde{I}^{(d)}$
2	1.393	0.6468
3	1.157	0.3499
4	1.094	0.2540

TABLE 1. Numerical values of the integrals $I^{(d)}$ and $\tilde{I}^{(d)}$ defined in (3.10).

Kubo and Kishi [1988] improved the interval to $[0, 0.13]$ and this is the current best result. To do this, they use the variational principle with the constant state $\otimes_{x \in \Lambda_\ell} |\frac{1}{2}\rangle$ to get a bound on the ground state energy. Combined with the correlation inequalities stated in Theorem 1.12, they get a lower bound for $\alpha(\infty) = \lim_{\beta \to \infty} \alpha(\beta)$, namely

$$\alpha(\infty) \geq \frac{1/4}{2 - J^{(2)}/J^{(1)}}. \tag{3.13}$$

(Kubo and Kishi considered the case $J^{(1)} = J^{(3)} = 1$ but it is easily extended.) This implies that the second bound of Theorem 3.2 is positive in the interval $[0, 0.13]$.

3.2. Infrared bounds

This section explores estimates of the Fourier transform of correlations and their consequences. Such estimates are particularly relevant at small Fourier parameters; this corresponds to large wavelengths, i.e. the infrared spectrum for light, hence the name given by physicists.

We need to introduce the conventions about the Fourier transform used in this survey. Recall that $\Lambda_\ell^* = \frac{2\pi}{\ell}\{-\frac{\ell}{2}+1,\dots,\frac{\ell}{2}\}^d$. The Fourier transform of a function $f:\Lambda_\ell \to \mathbb{C}$ is

$$\widehat{f}(k) = \sum_{x\in\Lambda_\ell} \mathrm{e}^{-\mathrm{i}kx}\, f(x), \qquad k \in \Lambda_\ell^*, \tag{3.14}$$

where we write kx for the usual inner product $\sum_{i=1}^d k_i x_i$. One can check that the inverse relation is then

$$f(x) = \frac{1}{\ell^d} \sum_{k\in\Lambda_\ell^*} \mathrm{e}^{\mathrm{i}kx}\, \widehat{f}(k). \tag{3.15}$$

Note that $\varepsilon(k) = \widehat{J}^{(3)}(0) - \widehat{J}^{(3)}(k)$.

The first infrared bound involves the Duhamel correlation function $\eta(x)$, defined by

$$\eta(x) = \frac{1}{\beta}\frac{1}{Z_{\rm per}(\Lambda_\ell,\beta,h)} \int_0^\beta \mathrm{d}s\ \mathrm{Tr}\, S_0^{(3)}\, \mathrm{e}^{-sH^{\rm per}_{\Lambda,h}}\, S_x^{(3)}\, \mathrm{e}^{-(\beta-s)H^{\rm per}_{\Lambda,h}}. \tag{3.16}$$

The method of reflection positivity allows us to establish the following infrared bound.

LEMMA 3.3. *Let $h=0$ and ℓ be even. Assume that the coupling constants $J^{(i)}$ satisfy the assumptions of Theorem 3.1. Then*

$$\widehat{\eta}(k) \le \frac{1}{2\beta\varepsilon(k)}, \qquad \text{for all } k \in \Lambda_\ell^* \setminus \{0\}.$$

The proof of this lemma can be found at the end of Section 3.3.

3.2.1. Falk–Bruch inequality.

We cannot use the infrared bound directly on the Duhamel function because of a lack of suitable lower bound for $\eta(0)$. The way out is to derive another bound on the ordinary correlation function. This can be done using the Falk–Bruch inequality, which was proposed independently in Falk, Bruch [1969] and Dyson, Lieb Simon [1978].

Let $\mathcal{H}$ be a separable Hilbert space, H a bounded hermitian operator such that $\mathrm{Tr}\,\mathrm{e}^{-H} < \infty$, and let $\mathcal{B}$ denote the space of bounded operators on $\mathcal{H}$. We define the *Duhamel inner product* in $\mathcal{B}$ by

$$(A,B) = \frac{1}{Z}\int_0^1 \mathrm{d}s\ \mathrm{Tr}\, \mathrm{e}^{-(1-s)H}\, A^*\, \mathrm{e}^{-sH}\, B, \qquad A,B\in\mathcal{B}, \tag{3.17}$$

with $Z = \mathrm{Tr}\ \mathrm{e}^{-H}$. We have

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}s}\mathrm{Tr}\ \mathrm{e}^{-(1-s)H}\,A^*\,\mathrm{e}^{-sH}\,B &= \mathrm{Tr}\ \mathrm{e}^{-(1-s)H}\,[H,A^*]\,\mathrm{e}^{-sH}\,B \\ &= \mathrm{Tr}\ \mathrm{e}^{-(1-s)H}\,A^*\,\mathrm{e}^{-sH}\,[B,H],\end{aligned} \tag{3.18}$$

and we obtain the useful identity

$$\big([A,H],B\big) = \big(A,[B,H]\big). \tag{3.19}$$

Further,

$$\big(A,[B,H]\big) = \frac{1}{Z}\int_0^1 \mathrm{d}s\,\frac{\mathrm{d}}{\mathrm{d}s}\mathrm{Tr}\ \mathrm{e}^{-(1-s)H}\,A^*\,\mathrm{e}^{-sH}\,B = \big\langle [B,A^*]\big\rangle \tag{3.20}$$

where

$$\langle\cdot\rangle = \frac{1}{Z}\mathrm{Tr}\ \cdot\ \mathrm{e}^{-H}. \tag{3.21}$$

For a given $A \in \mathcal{B}$, let us introduce the function $F(s) = \mathrm{Tr}\ \mathrm{e}^{-(1-s)H}\,A^*\,\mathrm{e}^{-sH}\,A$. We have

$$\frac{\mathrm{d}^2}{\mathrm{d}s^2}F(s) = \mathrm{Tr}\ \mathrm{e}^{-(1-s)H}\,[A,H]^*\,\mathrm{e}^{-sH}\,[A,H] \geq 0 \tag{3.22}$$

(positivity can be shown by casting the right side in the form $\mathrm{Tr}\,B^*B$). The function $F(s)$ is therefore convex. Then

$$\tfrac12\langle A^*A + AA^*\rangle = \frac{1}{2Z}\big(F(0)+F(1)\big) \geq \frac{1}{Z}\int_0^1 F(s)\mathrm{d}s = (A,A) \tag{3.23}$$

with equality if and only if $[A,H]=0$. The Cauchy–Schwarz inequality of the Duhamel inner product (3.17) gives

$$\big|\big(A,[B,H]\big)\big|^2 \leq (A,A)\ \big([B,H],[B,H]\big). \tag{3.24}$$

Using Eq. (3.20) to write the Duhamel inner product of commutators as expectations in the state $\langle\cdot\rangle$, and the inequalities (3.23) and (3.24) as well as cyclicity of the trace, we get *Bogolubov's inequality*

$$\big|\big\langle [B,A^*]\big\rangle\big|^2 \leq \tfrac12\langle A^*A + AA^*\rangle\ \big\langle\big[[B,H],B^*\big]\big\rangle. \tag{3.25}$$

Inequality (3.23) gives an upper bound for the Duhamel inner product, but we actually need a lower bound. For this, we consider the function

$$\Phi(s) = \sqrt{s}\coth\tfrac{1}{\sqrt{s}}. \tag{3.26}$$

This function is increasing, concave, and is depicted in Fig. 3.1. One can check that

$$\sqrt{s} \leq \Phi(s) \leq \sqrt{s} + s. \tag{3.27}$$

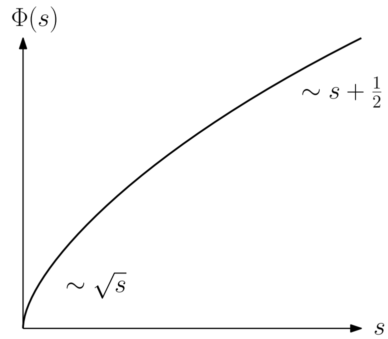

FIGURE 3.1. The function Φ of the Falk–Bruch inequality.

LEMMA 3.4 (Falk–Bruch inequality). *For all $A \in \mathcal{B}$ such that the denominators differ from zero, we have*

$$\frac{2\langle A^*A + AA^*\rangle}{\big\langle [A^*, [H, A]] \big\rangle} \leq \Phi\bigg(\frac{4(A, A)}{\big\langle [A^*, [H, A]] \big\rangle} \bigg).$$

It is worth noting that the double commutator is nonnegative, as can be seen from Eq. (3.20). Indeed, taking $A \mapsto [A^*, H]$ and $B \mapsto A^*$, we can express it using the Duhamel inner product as

$$\big\langle [A^*, [H, A]] \big\rangle = \big([A^*, H], [A^*, H] \big) \geq 0. \tag{3.28}$$

PROOF OF LEMMA 3.4. Recall the function $F(s)$ defined before (3.22). The Falk–Bruch inequality can be written as

$$2 \frac{F(0) + F(1)}{F'(1) - F'(0)} \leq \Phi\bigg(\frac{4 \int_0^1 F(s) \mathrm{d}s}{F'(1) - F'(0)} \bigg). \tag{3.29}$$

If $\{\varphi_j\}$ is an orthonormal set of eigenvectors of H with eigenvalues λ_j, we can write

$$F(s) = \sum_{i,j} \big| (\varphi_i, A\varphi_j) \big|^2 \, \mathrm{e}^{-\lambda_j} \, \mathrm{e}^{(\lambda_j - \lambda_i)s} = \int_{-\infty}^{\infty} \mathrm{e}^{st} \, \mathrm{d}\mu(t), \tag{3.30}$$

where μ is a positive measure. We have

$$\begin{aligned} F(0) + F(1) &= \int (\mathrm{e}^t + 1) \mathrm{d}\mu(t), \\ F'(1) - F'(0) &= \int t(\mathrm{e}^t - 1) \mathrm{d}\mu(t), \\ \int_0^1 F(s) \mathrm{d}s &= \int \frac{\mathrm{e}^t - 1}{t} \mathrm{d}\mu(t). \end{aligned} \tag{3.31}$$

Let us consider the probability measure $\mathrm{d}\nu(t) = (\int t(\mathrm{e}^t - 1)\mathrm{d}\mu(t))^{-1} t(\mathrm{e}^t - 1)\mathrm{d}\mu(t)$. We have

$$\begin{aligned} \frac{F(0)+F(1)}{F'(1)-F'(0)} &= \int \tfrac{1}{t} \coth \tfrac{t}{2} \, \mathrm{d}\nu(t), \\ \frac{\int F(s)\mathrm{d}s}{F'(1)-F'(0)} &= \int \tfrac{1}{t^2} \, \mathrm{d}\nu(t). \end{aligned} \tag{3.32}$$

Since Φ is concave we can use Jensen's inequality and we get (3.29):

$$\begin{aligned} \Phi\Bigl(\frac{4\int_0^1 F(s)\mathrm{d}s}{F'(1)-F'(0)}\Bigr) &= \Phi\Bigl(\int \tfrac{4}{t^2} \, \mathrm{d}\nu(t)\Bigr) \geq \int \Phi\bigl(\tfrac{4}{t^2}\bigr)\mathrm{d}\nu(t) \\ &= \int \tfrac{2}{t} \coth \tfrac{t}{2} \, \mathrm{d}\nu(t) = 2\frac{F(0)+F(1)}{F'(1)-F'(0)}. \end{aligned} \tag{3.33}$$

□

The Falk–Bruch inequality is saturated when the measure $\mathrm{d}\mu$ is a Dirac on a single value. This is the case if H is the hamiltonian of the harmonic oscillator, and A is the creation or annihilation operator.

The following inequality follows from Lemma 3.4 and the upper bound in Eq. (3.27).

Corollary 3.5. *We have*

$$\tfrac{1}{2}\langle A^* A + A A^* \rangle \leq \tfrac{1}{2}\sqrt{(A,A)\,\bigl\langle \bigl[A^*, [H,A]\bigr] \bigr\rangle} + (A,A).$$

For our purpose we have $H \sim \beta$ and $(A,A) \sim \frac{1}{\beta}$ with β large, so that this inequality is quite optimal. We use it below since it is simpler.

3.2.2. Infrared bound for the usual correlation function. In the rest of this section ℓ and β will be fixed, and we drop the subscripts on $\langle \cdot \rangle^{\mathrm{per}}_{\Lambda_\ell,\beta,0}$, writing simply $\langle \cdot \rangle$.

We introduce Fourier transforms of spin operators. This allows us to write the correlation functions in the form of Corollary 3.5. Accordingly, let

$$\widehat{S}^{(3)}_k = \sum_{x \in \Lambda_\ell} \mathrm{e}^{-\mathrm{i}kx} \, S^{(3)}_x, \qquad k \in \Lambda^*_\ell. \tag{3.34}$$

One easily checks the inverse identity

$$S^{(3)}_x = \frac{1}{\ell^d} \sum_{k \in \Lambda^*_\ell} \mathrm{e}^{\mathrm{i}kx} \, \widehat{S}^{(3)}_k, \qquad x \in \Lambda_\ell. \tag{3.35}$$

The Fourier transform of the usual correlation function is then equal to

$$\begin{aligned}\widehat{\langle S_0^{(3)} S_x^{(3)} \rangle}(k) &= \sum_{x\in\Lambda_\ell} \mathrm{e}^{-\mathrm{i}kx} \, \langle S_0^{(3)} S_x^{(3)} \rangle = \frac{1}{\ell^d} \sum_{x,y\in\Lambda_\ell} \mathrm{e}^{-\mathrm{i}k(x-y)} \, \langle S_x^{(3)} S_y^{(3)} \rangle \\ &= \frac{1}{\ell^d} \langle \widehat{S}_{-k}^{(3)} \widehat{S}_k^{(3)} \rangle.\end{aligned} \tag{3.36}$$

Notice that $(\widehat{S}_k^{(3)})^* = \widehat{S}_{-k}^{(3)}$, thus

$$\widehat{\langle S_0^{(3)} S_x^{(3)} \rangle}(k) \geq 0. \tag{3.37}$$

For the Duhamel correlation function we obtain

$$\widehat{\eta}(k) = \widehat{(S_0^{(3)}, S_x^{(3)})}(k) = \frac{1}{\ell^d} (\widehat{S}_k^{(3)}, \widehat{S}_k^{(3)}). \tag{3.38}$$

(There is no $-k$ because the Duhamel inner product involves taking the adjoint.) Let

$$e(k) = \tfrac{1}{2} \sum_{x\in\mathbb{Z}^d} \Big((J_{x,\mathrm{per}}^{(1)} - J_{x,\mathrm{per}}^{(2)} \cos kx) \langle S_0^{(1)} S_x^{(1)} \rangle + (J_{x,\mathrm{per}}^{(2)} - J_{x,\mathrm{per}}^{(1)} \cos kx) \langle S_0^{(2)} S_x^{(2)} \rangle \Big). \tag{3.39}$$

We will see in the proof of the next lemma that $e(k) \geq 0$, as it can be written as the expectation of a double commutator in the form of Eq. (3.28).

Lemma 3.6 (Infrared bound for the usual correlation function). *We have for all $k \in \Lambda_\ell^* \setminus \{0\}$ that*

$$\widehat{\langle S_0^{(3)} S_x^{(3)} \rangle}(k) \leq \sqrt{\frac{e(k)}{2\varepsilon(k)}} + \frac{1}{2\beta\varepsilon(k)}.$$

Proof. We take $A = \widehat{S}_k^{(3)}$ and $H = \beta H_{\Lambda,0}^{\mathrm{per}}$ in Corollary 3.5. We need to calculate the double commutator. First, we have

$$\begin{aligned}[H_{\Lambda,0}^{\mathrm{per}}, \widehat{S}_k^{(3)}] &= \sum_{x\in\Lambda_\ell} [H_{\Lambda,0}^{\mathrm{per}}, S_x^{(3)}] \, \mathrm{e}^{-\mathrm{i}kx} \\ &= -\sum_{i=1}^{3} \sum_{x,y,z\in\Lambda_\ell} \mathrm{e}^{-\mathrm{i}kx} \, J_{y-z,\mathrm{per}}^{(i)} [S_y^{(i)} S_z^{(i)}, S_x^{(3)}] \\ &= -2\mathrm{i} \sum_{x,y\in\Lambda_\ell} \mathrm{e}^{-\mathrm{i}kx} \Big(-J_{x-y,\mathrm{per}}^{(1)} S_x^{(2)} S_y^{(1)} + J_{x-y,\mathrm{per}}^{(2)} S_x^{(1)} S_y^{(2)} \Big).\end{aligned} \tag{3.40}$$

We used the fact that operators at different sites commute, and also that $J_x^{(i)} = J_{-x}^{(i)}$. Next,

$$\begin{aligned}\big[\widehat{S}_{-k}^{(3)}, [H_{\Lambda,0}^{\mathrm{per}}, \widehat{S}_k^{(3)}]\big] &= -2\mathrm{i} \sum_{x,y\in\Lambda_\ell} \mathrm{e}^{-\mathrm{i}kx} \Big[\mathrm{e}^{\mathrm{i}kx}\, S_x^{(3)} + \mathrm{e}^{\mathrm{i}ky}\, S_y^{(3)}, -J_{x-y,\mathrm{per}}^{(1)} S_x^{(2)} S_y^{(1)} \\ &\qquad\qquad + J_{x-y,\mathrm{per}}^{(2)} S_x^{(1)} S_y^{(2)} \Big] \\ &= 2 \sum_{x,y\in\Lambda_\ell} \Big(\big(J_{x-y,\mathrm{per}}^{(1)} - \cos(k(x-y)) J_{x-y,\mathrm{per}}^{(2)}\big) S_x^{(1)} S_y^{(1)} \\ &\qquad + \big(J_{x-y,\mathrm{per}}^{(2)} - \cos(k(x-y)) J_{x-y,\mathrm{per}}^{(1)}\big) S_x^{(2)} S_y^{(2)} \Big).\end{aligned} \tag{3.41}$$

Taking the expectation in the Gibbs state, we obtain

$$\big\langle \big[A^*, [H, A]\big] \big\rangle = \big\langle \big[\hat{S}_{-k}^{(3)}, [\beta H_{\Lambda,0}^{\mathrm{per}}, \hat{S}_k^{(3)}]\big] \big\rangle = 4\beta\ell^d e(k). \tag{3.42}$$

We also see that $e(k) \geq 0$ from Eq. (3.28). Lemma 3.6 follows from Corollary 3.5 and from the infrared bound on the Duhamel correlation function, Lemma 3.3. ☐

We can now prove the occurrence of long-range order.

Proof of Theorem 3.1. We have the inequality (see Theorem 1.12)

$$\langle S_0^{(3)} S_0^{(3)} \rangle \geq \tfrac{1}{3} \textstyle\sum_{i=1}^3 \langle S_0^{(i)} S_0^{(i)} \rangle = \tfrac{1}{3} S(S+1). \tag{3.43}$$

This is where we use that $J_x^{(3)} \geq J_x^{(1)} \geq -J_x^{(2)} \geq 0$.

We now use the inverse Fourier transform on the two-point correlation function, namely

$$\tfrac{1}{3} S(S+1) \leq \langle S_0^{(3)} S_0^{(3)} \rangle = \frac{1}{\ell^d} \widehat{\langle S_0^{(3)} S_x^{(3)} \rangle}(0) + \frac{1}{\ell^d} \sum_{k\in\Lambda_\ell^*\setminus\{0\}} \widehat{\langle S_0^{(3)} S_x^{(3)} \rangle}(k). \tag{3.44}$$

Notice that the first term of the right side is equal to the long-range order parameter. Then

$$\frac{1}{\ell^d} \sum_{x\in\Lambda_\ell} \langle S_0^{(3)} S_x^{(3)} \rangle = \frac{1}{\ell^d} \widehat{\langle S_0^{(3)} S_x^{(3)} \rangle}(0) \geq \tfrac{1}{3} S(S+1) - \frac{1}{\ell^d} \sum_{k\in\Lambda_\ell^*\setminus\{0\}} \widehat{\langle S_0^{(3)} S_x^{(3)} \rangle}(k). \tag{3.45}$$

We can bound the last term with the help of Lemma 3.6, which gives Theorem 3.1. ☐

Proof of Theorem 3.2. With nearest-neighbour interactions the function $e(k)$ can be written as

$$e(k) = \alpha_\ell(\beta) \sum_{i=1}^d (1 + r\cos k_i), \tag{3.46}$$

where

$$r = \frac{-J^{(2)}\langle S_0^{(1)} S_{e_1}^{(1)}\rangle - J^{(1)}\langle S_0^{(2)} S_{e_1}^{(2)}\rangle}{J^{(1)}\langle S_0^{(1)} S_{e_1}^{(1)}\rangle + J^{(2)}\langle S_0^{(2)} S_{e_1}^{(2)}\rangle}. \tag{3.47}$$

Here $e_1 = (1, 0, \dots, 0) \in \mathbb{Z}^d$ is the unit vector in the first direction. It follows from the fact that $e(k) \geq 0$ for all k, that $r \in [-1, 1]$. Let

$$I_\ell^{(d)}(r) = \frac{1}{\ell^d} \sum_{k \in \Lambda_\ell^* \setminus \{0,\pi\}} \sqrt{\frac{\sum_{i=1}^d (1 + r\cos k_i)}{\sum_{i=1}^d (1 - \cos k_i)}} \tag{3.48}$$

where we have omitted the term $\frac{1}{\ell^d}\sqrt{1-r}$ for $k = \pi = (\pi, \pi, \dots, \pi)$. Adding it back and bounding it by $\sqrt{2}/\ell^d$, the lower bound is

$$\frac{1}{\ell^d} \sum_{x \in \Lambda_\ell} \langle S_0^{(3)} S_x^{(3)}\rangle \geq \tfrac{1}{3}S(S+1) - \tfrac{1}{2}\sqrt{\alpha_\ell(\beta)}\,\big(I_\ell^{(d)}(r) + \tfrac{\sqrt{2}}{\ell^d}\big) - \frac{1}{2\beta\ell^d} \sum_{k \in \Lambda_\ell^* \setminus \{0\}} \frac{1}{\varepsilon(k)}. \tag{3.49}$$

Observe that $I_\ell^{(d)}(r)$ is concave with respect to r and that its derivative at $r = 1$ is equal to

$$\frac{\mathrm{d}}{\mathrm{d}r} I_\ell^{(d)}(r)\Big|_{r=1} = \frac{1}{\ell^d} \sum_{k \in \Lambda_\ell^* \setminus \{0,\pi\}} \frac{\sum_{i=1}^d \cos k_i}{\sqrt{\sum_{i=1}^d (1 - \cos k_i)\, \sum_{i=1}^d (1 + \cos k_i)}}. \tag{3.50}$$

This is equal to zero, as can be seen with the change of variables $k \mapsto k + (\pi, \dots, \pi)$. Then $I_\ell^{(d)}(r) \leq I_\ell^{(d)}(1) = I_\ell^{(d)}$. Using this with the lower bound of Theorem 3.1, we obtain the first bound of Theorem 3.2.

For the second bound, we follow Kennedy, Lieb, Shastry [1988a] and use the inverse Fourier transform. In what follows, x is the dummy variable summed over inside the Fourier transform. We have

$$\begin{aligned} \langle S_0^{(3)} S_{e_1}^{(3)}\rangle &= \frac{1}{d\ell^d} \sum_{k \in \Lambda_\ell^*} \sum_{i=1}^d \mathrm{e}^{\mathrm{i}k_i}\, \widehat{\langle S_0^{(3)} S_x^{(3)}\rangle}(k) \\ &= \frac{1}{\ell^d} \widehat{\langle S_0^{(3)} S_x^{(3)}\rangle}(0) + \frac{1}{\ell^d} \sum_{k \in \Lambda_\ell^* \setminus \{0\}} \widehat{\langle S_0^{(3)} S_x^{(3)}\rangle}(k) \Big(\frac{1}{d} \sum_{i=1}^d \cos k_i\Big). \end{aligned} \tag{3.51}$$

We used lattice symmetries and the fact that $\widehat{\langle S_0^{(3)} S_x^{(3)}\rangle} \geq 0$, see Eq. (3.37). We have

$$\begin{aligned} \frac{1}{\ell^d} \widehat{\langle S_0^{(3)} S_x^{(3)}\rangle}(0) &\geq \langle S_0^{(3)} S_{e_1}^{(3)}\rangle - \frac{1}{\ell^d} \sum_{k \in \Lambda_\ell^* \setminus \{0\}} \widehat{\langle S_0^{(3)} S_x^{(3)}\rangle}(k) \Big(\frac{1}{d} \sum_{i=1}^d \cos k_i\Big)_+ \\ &\geq \langle S_0^{(3)} S_{e_1}^{(3)}\rangle - \frac{1}{\ell^d} \sum_{k \in \Lambda_\ell^* \setminus \{0\}} \Big(\frac{1}{d} \sum_{i=1}^d \cos k_i\Big)_+ \Big[\sqrt{\frac{e(k)}{2\varepsilon(k)}} + \frac{1}{2\beta\varepsilon(k)}\Big]. \end{aligned} \tag{3.52}$$

Proceeding with $e(k)$ as we did with the first lower bound, we get

$$\frac{1}{\ell^d}\langle\widehat{S_0^{(3)}S_x^{(3)}}\rangle(0) \geq \langle S_0^{(3)}S_{e_1}^{(3)}\rangle - \tfrac{1}{2}\sqrt{\alpha_\ell(\beta)}\tilde{I}_\ell^{(d)}(r) - \frac{1}{2\beta\ell^d}\sum_{k\in\Lambda_\ell^*\setminus\{0\}}\frac{1}{\varepsilon(k)}, \tag{3.53}$$

where

$$\tilde{I}_\ell^{(d)}(r) = \frac{1}{\ell^d}\sum_{k\in\Lambda_\ell^*\setminus\{0\}}\sqrt{\frac{\sum_{i=1}^d(1+r\cos k_i)}{\sum_{i=1}^d(1-\cos k_i)}}\Big(\frac{1}{d}\sum_{i=1}^d\cos k_i\Big)_+. \tag{3.54}$$

One easily checks that the derivative of $\tilde{I}_\ell^{(d)}(r)$ is positive, so it is smaller than $\tilde{I}_\ell^{(d)}(1) = \tilde{I}_\ell^{(d)}$. Finally, using Theorem 1.12, we have

$$\langle S_0^{(3)}S_{e_1}^{(3)}\rangle \geq \frac{\alpha_\ell(\beta)}{1 - J^{(2)}/J^{(1)}}. \tag{3.55}$$

The second lower bound of Theorem 3.2 follows. $\square$

3.3. Reflection positivity

Let $\mathcal{H}$ be a separable Hilbert space, and let $\mathcal{B}_{\text{left}}$, resp. $\mathcal{B}_{\text{right}}$, denote the space of bounded operators on $\mathcal{H}\otimes\mathcal{H}$ that are of the form $a\otimes\mathbb{1}$, resp. $\mathbb{1}\otimes a$, for some $a\in\mathcal{B}(\mathcal{H})$. Let $\mathcal{R}$ denote the automorphism of $\mathcal{B}(\mathcal{H}\otimes\mathcal{H})$ such that

$$\begin{aligned}\mathcal{R}(a\otimes\mathbb{1}) &= \mathbb{1}\otimes a,\\ \mathcal{R}(\mathbb{1}\otimes a) &= a\otimes\mathbb{1}.\end{aligned} \tag{3.56}$$

Let us fix an orthonormal basis $\{e_i\}$ on $\mathcal{H}$, and define the complex conjugate $\overline{a}$ of a bounded operator a by

$$\langle e_i, \overline{a}e_j\rangle = \overline{\langle e_i, ae_j\rangle}. \tag{3.57}$$

In matrix notation, that means taking the complex conjugate of its elements, without transposing as for hermitian adjoints. The reason to use the complex conjugate is that for all $a,b\in\mathcal{B}(\mathcal{H})$, we have

$$\overline{a\,b} = \overline{a}\,\overline{b}. \tag{3.58}$$

Here is the key inequality that is closely related to reflection positivity. Let I be an index set and μ a positive, finite measure on I. We assume that $A, C_i\in\mathcal{B}_{\text{left}}$ and $B, D_i\in\mathcal{B}_{\text{right}}$ for all $i\in I$.

Lemma 3.7. *We have*

$$\Big|\operatorname{Tr}\,\mathrm{e}^{A+B+\int C_iD_i\mathrm{d}\mu(i)}\Big|^2 \leq \operatorname{Tr}\,\mathrm{e}^{A+\mathcal{R}\overline{A}+\int C_i\mathcal{R}\overline{C}_i\mathrm{d}\mu(i)}\cdot\operatorname{Tr}\,\mathrm{e}^{\mathcal{R}\overline{B}+B+\int\mathcal{R}\overline{D}_i\,D_i\mathrm{d}\mu(i)}.$$

PROOF. We use the Duhamel formula in the following form. If A, B are bounded operators, then

$$\mathrm{e}^{A+B} = \sum_{n\geq 0} \int_{0<t_1<\dots<t_n<1} \mathrm{d}t_1 \dots \mathrm{d}t_n \, \mathrm{e}^{t_1 A} \, B \, \mathrm{e}^{(t_2-t_1)A} \, B \dots B \, \mathrm{e}^{(1-t_n)A} \, . \tag{3.59}$$

In what follows, we use the shorthands

$$\int \mathrm{d}\boldsymbol{i} \equiv \int \mathrm{d}\mu(i_1) \cdots \int \mathrm{d}\mu(i_n) \qquad \text{and} \qquad \int \mathrm{d}\boldsymbol{t} \equiv \int_{0<t_1<\dots<t_n<1} \mathrm{d}t_1 \dots \mathrm{d}t_n. \tag{3.60}$$

We also write $A = a \otimes \mathbb{1}$, $B = \mathbb{1} \otimes b$, $C_i = c_i \otimes \mathbb{1}$, and $D_i = \mathbb{1} \otimes d_i$. Then

$$\begin{aligned}
&\Big| \mathrm{Tr}_{\,\mathcal{H}\otimes\mathcal{H}} \, \mathrm{e}^{A+B+\int C_i D_i \mathrm{d}\mu(i)} \Big|^2 \\
&= \Big| \sum_{n\geq 0} \int \mathrm{d}\boldsymbol{i} \int \mathrm{d}\boldsymbol{t} \, \mathrm{Tr}_{\,\mathcal{H}\otimes\mathcal{H}} \, \mathrm{e}^{t_1(A+B)} \, C_{i_1} D_{i_1} \dots C_{i_n} D_{i_n} \, \mathrm{e}^{(1-t_n)(A+B)} \Big|^2 \\
&= \Big| \sum_{n\geq 0} \int \mathrm{d}\boldsymbol{i} \int \mathrm{d}\boldsymbol{t} \, \mathrm{Tr}_{\,\mathcal{H}} \, \mathrm{e}^{t_1 a} \, c_{i_1} \dots c_{i_n} \, \mathrm{e}^{(1-t_n)a} \, \mathrm{Tr}_{\,\mathcal{H}} \, \mathrm{e}^{t_1 b} \, d_{i_1} \dots d_{i_n} \, \mathrm{e}^{(1-t_n)b} \Big|^2 \\
&\leq \sum_{n\geq 0} \int \mathrm{d}\boldsymbol{i} \int \mathrm{d}\boldsymbol{t} \, \mathrm{Tr}_{\,\mathcal{H}} \, \mathrm{e}^{t_1 a} \, c_{i_1} \dots c_{i_n} \, \mathrm{e}^{(1-t_n)a} \, \mathrm{Tr}_{\,\mathcal{H}} \, \mathrm{e}^{t_1 \overline{a}} \, \overline{c}_{i_1} \dots \overline{c}_{i_n} \, \mathrm{e}^{(1-t_n)\overline{a}} \\
&\qquad \cdot \sum_{n\geq 0} \int \mathrm{d}\boldsymbol{i} \int \mathrm{d}\boldsymbol{t} \, \mathrm{Tr}_{\,\mathcal{H}} \, \mathrm{e}^{t_1 \overline{b}} \, \overline{d}_{i_1} \dots \overline{d}_{i_n} \, \mathrm{e}^{(1-t_n)\overline{b}} \, \mathrm{Tr}_{\,\mathcal{H}} \, \mathrm{e}^{t_1 b} \, d_{i_1} \dots d_{i_n} \, \mathrm{e}^{(1-t_n)b} \\
&= \mathrm{Tr}_{\,\mathcal{H}\otimes\mathcal{H}} \, \mathrm{e}^{A+\mathcal{R}\overline{A}+\int C_i \mathcal{R}\overline{C}_i \mathrm{d}\mu(i)} \cdot \mathrm{Tr}_{\,\mathcal{H}\otimes\mathcal{H}} \, \mathrm{e}^{\mathcal{R}\overline{B}+B+\int \mathcal{R}\overline{D}_i \, D_i \mathrm{d}\mu(i)} \, .
\end{aligned} \tag{3.61}$$

We used the ordinary Cauchy–Schwarz inequality for functions, here with argument $(n, \boldsymbol{i}, \boldsymbol{t})$. The complex conjugate was written with the help of (3.58). $\square$

We now derive the infrared bound for the Duhamel correlation function, Lemma 3.3. In the rest of this Section, we fix an even integer ℓ and consider periodic couplings (3.1). Recall that $\Lambda_\ell = \{0, 1, \dots, \ell-1\}^d$. Let Δ denote the discrete Laplacian from the coupling constant $J^{(3)}_{\mathrm{per}}$, which acts on a field $v = (v_x) \in \mathbb{R}^\Lambda$ as

$$(\Delta v)_x = \sum_{y\in\Lambda_\ell} J^{(3)}_{x-y,\mathrm{per}} (v_y - v_x). \tag{3.62}$$

Notice the following identity, which is a discrete version of $\int f(-\Delta g) = \int \nabla f \nabla g$ for functions:

$$(u, -\Delta v) = \tfrac{1}{2} \sum_{x,y\in\Lambda_\ell} J^{(3)}_{x-y,\mathrm{per}} (u_x - u_y)(v_x - v_y). \tag{3.63}$$

In the left side, $(\cdot,\cdot)$ stands for the usual inner product on $\mathbb{R}^{\Lambda_\ell}$, i.e. $(u, v) = \sum_{x\in\Lambda_\ell} u_x v_x$. We introduce the following partition function that depends on a field v:

$$Z(v) = \mathrm{Tr}\; \mathrm{e}^{-\beta H(v)}, \tag{3.64}$$

with hamiltonian given by

$$H(v) = H^{\mathrm{per}}_{\Lambda_\ell,0} - \sum_{x\in\Lambda_\ell} h_x S^{(3)}_x, \tag{3.65}$$

where the local magnetic field is obtained from v by

$$h_x = (\Delta v)_x. \tag{3.66}$$

Let

$$\tilde Z(v) = \mathrm{e}^{\frac14 \beta (v,\Delta v)}\, Z(v). \tag{3.67}$$

We show that $\tilde Z(v)$ is maximised by the field $v \equiv 0$, which is the key to proving Lemma 3.3.

Let $\mathcal{R}$ denote a reflection across a plane cutting through edges. Namely, given a direction $i = 1,\dots,d$ and a half integer $\epsilon \in \{\frac12, \frac32, \dots, \frac{\ell-1}{2}\}$, let $\mathcal{R}$ be the bijection $\Lambda_\ell \to \Lambda_\ell$ such that

$$\mathcal{R}x = x + 2(\epsilon - x_i)e_i. \tag{3.68}$$

Let

$$\Lambda_{\mathrm{left}} = \{x \in \Lambda_\ell : \epsilon - \frac{\ell}{2} < x_i < \epsilon\}, \qquad \Lambda_{\mathrm{right}} = \{x \in \Lambda_\ell : \epsilon < x_i < \epsilon + \frac{\ell}{2}\}. \tag{3.69}$$

Given a field $v_1 \in \mathbb{R}^{\Lambda_{\mathrm{left}}}$, let $(\mathcal{R}v_1)_x = (v_1)_{\mathcal{R}x} \in \mathbb{R}^{\Lambda_{\mathrm{right}}}$.

Lemma 3.8. *Let the couplings $J^{(i)}$ satisfy the assumptions of Theorem 3.1. Then, for any $v_1 \in \mathbb{R}^{\Lambda_{left}}$ and $v_2 \in \mathbb{R}^{\Lambda_{right}}$, we have*

$$\tilde Z(v_1,v_2)^2 \le \tilde Z(v_1,\mathcal{R}v_1)\, \tilde Z(\mathcal{R}v_2, v_2).$$

We first prove the lemma in the case of nearest-neighbour couplings; we then consider long-range interactions.

PROOF OF LEMMA 3.8 FOR NEAREST-NEIGHBOUR COUPLINGS. We cast $\tilde{Z}(v_1, v_2)$ in the form of Lemma 3.7. Using (3.63), we get

$$\begin{aligned}\tilde{Z}(v) = \operatorname{Tr} \exp \beta \Big\{ \tfrac{1}{8} \sum_{x,y} J^{(3)}_{x-y} (v_y - v_x)^2 + \sum_{i=1}^{3} \sum_{x,y} J^{(i)}_{x-y} S^{(i)}_x S^{(i)}_y \\ + \sum_{x,y} J^{(3)}_{x-y} S^{(3)}_x (v_y - v_x) \Big\} \\ = \operatorname{Tr} \exp \beta \Big\{ \sum_{i=1}^{2} \sum_{x,y} J^{(i)}_{x-y} S^{(i)}_x S^{(i)}_y + \sum_{x,y} J^{(3)}_{x-y} \big(S^{(3)}_x + \tfrac{v_x}{2} \big) \big(S^{(3)}_y + \tfrac{v_y}{2} \big) \\ - \widehat{J}^{(3)}(0) \sum_x \big(S^{(3)}_x v_x + \tfrac{v_x^2}{4} \big) \Big\}.\end{aligned} \tag{3.70}$$

We used $J^{(i)}_x = J^{(i)}_{-x}$. This formula holds for general couplings and we will also use it in the long-range case (with $J^{(i)}_{x,\text{per}}$). We now assume that $J^{(i)}_x = 0$ except when $\|x\|_1 = 1$, in which case it equals a constant $J^{(i)}$. Then the above expression has the form of Lemma 3.7 by choosing

$$\begin{aligned} A &= \beta \sum_{x,y \in \Lambda_{\text{left}}} \Big[\sum_{i=1}^{2} J^{(i)}_{x-y} S^{(i)}_x S^{(i)}_y + J^{(3)}_{x-y} \big(S^{(3)}_x + \tfrac{v_x}{2} \big) \big(S^{(3)}_y + \tfrac{v_y}{2} \big) \Big] \\ &\qquad - \widehat{J}^{(3)}(0) \sum_{x \in \Lambda_{\text{left}}} \big(S^{(3)}_x v_x + \tfrac{v_x^2}{4} \big) \\ B &= \beta \sum_{x,y \in \Lambda_{\text{right}}} \Big[\sum_{i=1}^{2} J^{(i)}_{x-y} S^{(i)}_x S^{(i)}_y + J^{(3)}_{x-y} \big(S^{(3)}_x + \tfrac{v_x}{2} \big) \big(S^{(3)}_y + \tfrac{v_y}{2} \big) \Big] \\ &\qquad - \widehat{J}^{(3)}(0) \sum_{x \in \Lambda_{\text{right}}} \big(S^{(3)}_x v_x + \tfrac{v_x^2}{4} \big) \\ \int C_i D_i \mathrm{d}\mu(i) &= \beta \sum_{\substack{x \in \Lambda_{\text{left}} \\ y \in \Lambda_{\text{right}} \\ \|x-y\|=1}} \Big[J^{(1)} S^{(1)}_x S^{(1)}_y - J^{(2)} (\mathrm{i} S^{(2)}_x)(\mathrm{i} S^{(2)}_y) \\ &\qquad + J^{(3)} \big(S^{(3)}_x + \tfrac{v_x}{2} \big) \big(S^{(3)}_y + \tfrac{v_y}{2} \big) \Big]. \end{aligned} \tag{3.71}$$

In the usual basis where all $S^{(3)}_x$ are diagonal, we have $\overline{S^{(1)}_x} = S^{(1)}_x$, $\overline{\mathrm{i}S^{(2)}_x} = \mathrm{i}S^{(2)}_x$, $\overline{S^{(3)}_x} = S^{(3)}_x$. Then $\overline{A} = A$ and $\overline{B} = B$. We have multiplied $S^{(2)}_x$ by i, so taking the complex conjugate gives the operator back. Then $\overline{C_i} = C_i$ and $\overline{D_i} = D_i$. Moreover, when $x \in \Lambda_{\text{left}}$ and $y \in \Lambda_{\text{right}}$ with $\|x - y\| = 1$, the reflection interchanges x and y. In order to use Lemma 3.7 the measure μ needs to be positive, which is guaranteed by $J^{(1)}, J^{(3)} \geq 0$ and $J^{(2)} \leq 0$. $\square$

An important observation is that if certain interactions can be cast in the form above, then this can also be done with convex combinations of these interactions. We use this property below.

PROOF OF LEMMA 3.8 FOR LONG-RANGE COUPLINGS. We now consider the case when $J_x^{(i)} = \int_{\mathbb{R}^d} \mathrm{d}\nu^{(i)}(k)\, \mathrm{e}^{ik\cdot x}$ where $\nu^{(i)}$ is a positive, finite measure on $\mathbb{R}^d$. We see from (3.70) that it suffices to consider a fixed $i \in \{1, 2, 3\}$ and to simplify the notation we dispense with the superscript $^{(i)}$. We use the decomposition (3.71) but with $J_{x,\mathrm{per}}$ in place of J_x. It suffices to consider the cross-term

$$\sum_{\substack{x\in\Lambda_{\mathrm{left}}\\ y\in\Lambda_{\mathrm{right}}}} J_{x-y,\mathrm{per}} T_x T_y \tag{3.72}$$

where $T_x \in \{S_x^{(1)}, \mathrm{i}S_x^{(2)}, S_x^{(3)} + \frac{v_x}{2}\}$. We aim to write this in the form $\int_I C_i D_i \,\mathrm{d}\mu(i)$ in order to apply Lemma 3.7. We expand

$$J_{x-y,\mathrm{per}} = \sum_{z\in\mathbb{Z}^d} J_{x-y+\ell z} = \sum_{z\in\mathbb{Z}^d} \int_{\mathbb{R}^d} \mathrm{d}\nu(k)\, \mathrm{e}^{\mathrm{i}k\cdot(x-y+\ell z)} \tag{3.73}$$

to write

$$\sum_{\substack{x\in\Lambda_{\mathrm{left}}\\ y\in\Lambda_{\mathrm{right}}}} J_{x-y,\mathrm{per}} T_x T_y = \sum_{z\in\mathbb{Z}^d} \int_{\mathbb{R}^d} \mathrm{d}\nu(k) \Big(\sum_{x\in\Lambda_{\mathrm{left}}} \mathrm{e}^{\mathrm{i}k\cdot(x+\ell z/2)}\, T_x \Big) \Big(\sum_{y\in\Lambda_{\mathrm{right}}} \mathrm{e}^{-\mathrm{i}k\cdot(y-\ell z/2)}\, T_y \Big). \tag{3.74}$$

This is of the required form $\int_I C_i D_i \,\mathrm{d}\mu(i)$ with index set $I = \mathbb{Z}^d \times \mathbb{R}^d$, except that we need the measure μ to be finite. In order to achieve this, we may approximate the sum over $z \in \mathbb{Z}^d$ by a sum over $z \in \Lambda'$ and then let $\Lambda' \Uparrow \mathbb{Z}^d$. The rest of the argument follows as in the nearest-neighbour case. □

COROLLARY 3.9. *For all $v \in \mathbb{R}^{\Lambda_\ell}$, we have $\tilde{Z}(v) \le \tilde{Z}(0)$.*

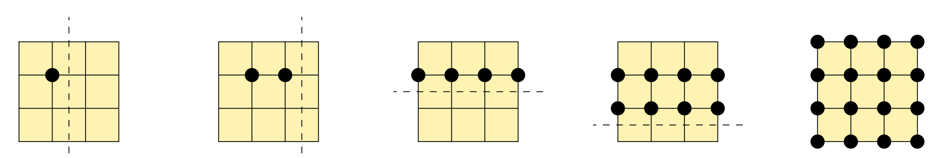

FIGURE 3.2. Starting with a maximiser, reflections yield further maximisers where more and more values are identical.

PROOF. Without loss of generality we can assume that $v_0 = 0$. We observe that $\tilde{Z}(\lambda v) \to 0$ as $|\lambda| \to \infty$, so that $\tilde{Z}(v)$ is maximised for finite v. Indeed, in the expression (3.67) we have $\mathrm{e}^{\frac{1}{4}\beta\lambda^2(v,\Delta v)} \sim \mathrm{e}^{-c\lambda^2}$ and $Z(\lambda v) \le \mathrm{e}^{C|\lambda|}$.

Then let (v_1, v_2) be a maximiser with $v_0 = 0$. Using Lemma 3.8 with a plane crossing the edge $(0, e_1)$, we have that $(v_1, \mathcal{R}v_1)$ is also a maximiser, with $v_0 = v_{e_1} = 0$. Using a plane crossing the edge $(e_1, 2e_1)$, we get a maximiser with more zeros. Iterating, we get a maximiser with a whole line of zeros. We then consider reflection planes in another direction to get a maximiser with a plane of zeros. We then consider reflection planes in further directions. See Fig. 3.2 for an illustration. $\square$

Proof of Lemma 3.3. From Corollary 3.9 and Eq. (3.67), we have the "Gaussian domination" bound

$$\frac{Z(sv)}{Z(0)} \leq \mathrm{e}^{-\frac{1}{4}s^2 \beta(v,\Delta v)}. \tag{3.75}$$

The derivative of $Z(sv)$ with respect to s is equal to 0 at $s = 0$ because of symmetries (for instance, a rotation around the 3rd spin axis by angle π, which takes $S_x^{(i)}$ to $-S_x^{(i)}$, $i = 1, 2$, and leaves $S_x^{(3)}$ invariant). The second derivative can be calculated e.g. using the Duhamel formula (3.59) and translation-invariance. Recalling the Duhamel correlation function η from (3.16), we get

$$\frac{1}{Z(0)} \frac{\mathrm{d}^2}{\mathrm{d}s^2} Z(sv) \Big|_{s=0} = \beta^2 \sum_{x,y \in \Lambda} h_x h_y \eta(x - y), \tag{3.76}$$

where we recall that $h_x = (\Delta v)_x$. We now choose the field v to be

$$v_x = \cos(kx), \qquad k \in \Lambda_\ell^*. \tag{3.77}$$

Observe that $\Delta v_x = -\varepsilon(k) v_x$. The order s^2 of the inequality (3.75) gives

$$\tfrac{1}{2}\beta^2 \varepsilon(k)^2 \sum_{x,y \in \Lambda_\ell} \cos(kx) \cos(ky) \eta(x - y) \leq \tfrac{1}{4}\beta\varepsilon(k) \sum_{x \in \Lambda_\ell} \cos(kx)^2. \tag{3.78}$$

Since $\eta(x)$ and $\widehat{\eta}(k)$ are both real, the left-hand-side satisfies

$$\begin{aligned}
\sum_{x,y \in \Lambda_\ell} \cos(kx) \cos(ky) \eta(x - y) &= \sum_{x \in \Lambda_\ell} \cos(kx) \sum_{y \in \Lambda_\ell} \mathrm{e}^{\mathrm{i}ky}\, \eta(x - y) \\
&= \sum_{x \in \Lambda_\ell} \cos(kx) \sum_{z \in \Lambda_\ell} \mathrm{e}^{\mathrm{i}k(x-z)}\, \eta(z) \\
&= \sum_{x \in \Lambda_\ell} \cos(kx)\, \mathrm{e}^{\mathrm{i}kx}\, \widehat{\eta}(k) \\
&= \widehat{\eta}(k) \sum_{x \in \Lambda_\ell} \cos(kx)^2.
\end{aligned} \tag{3.79}$$

Inserting this in Eq. (3.78) we obtain Lemma 3.3. $\square$

Bibliographical references

The first proof of continuous symmetry breaking is due to Fröhlich, Simon, and Spencer [1976]; they established that the classical Heisenberg model undergoes a phase transition in dimensions three and higher. Their work was inspired by ideas from quantum field field theory, specifically by the Källén–Lehmann representation of two-point Green functions in relativistic quantum field theory, which suggested the right form of infrared bounds, and by reflection positivity, as formulated in the works of Jost [1965], Osterwalder and Schrader [1973], and Glaser [1974]. (Furthermore, bounds in Glimm and Jaffe [1970] and Fröhlich [1974] inspired the exponential infrared bounds proved in Fröhlich, Simon, and Spencer [1976].)

The extension of these ideas to quantum spin systems was achieved in another groundbreaking article, by Dyson, Lieb, and Simon [1978]. The method was then further extended and streamlined in Fröhlich, Israel, Lieb, and Simon [1978] and [1980]. Further refinements include an extension to the ground states in two dimensions Neves, Perez [1986] and improved conditions that establish long-range order in the XY model in two dimensions (Kennedy, Lieb, Shastry [1988a] and [1988b]; Kubo, Kishi [1988]).

It should be pointed out that the method does not apply to models where all coupling constants are positive (Speers [1985]). An important problem, which remains open to this day, is to prove spontaneous magnetisation or long-range order in the Heisenberg ferromagnet.

A beautiful account of the method of reflection positivity in statistical mechanics (restricted to classical systems) has been written by Biskup [2009]. The handwritten notes of Tóth [1996] for his Prague lectures give a clear account of the method. And an extensive overview, which retraces the origin of the key ideas, can be found in the handwritten notes of Fröhlich [2011] for his Vienna lectures.

CHAPTER 4

Fermionic and bosonic systems

These systems are naturally defined in the continuum space but they also makes sense on lattices, where the setting is simpler and relevant for our purpose. Excellent introductory textbooks include Martin and Rothen [2004], ... A thorough description of systems in the continuum can be found in Bratteli and Robinson [1987].

4.1. Fock spaces

The Hilbert space for a single particle in $\Lambda \Subset \mathbb{Z}^d$ is $\ell^2(\Lambda)$. Recall that $\ell^2(\Lambda)$ is the vector space $\mathbb{C}^\Lambda$ with inner product

$$\langle \varphi | \psi \rangle = \sum_{x \in \Lambda} \overline{\varphi(x)}\, \psi(x), \qquad \varphi, \psi \in \ell^2(\Lambda). \tag{4.1}$$

A natural basis is $\{e_x\}_{x \in \Lambda}$ where these functions are defined by $e_x(y) = \delta_{x,y}$. The dimension of $\ell^2(\Lambda)$ is $|\Lambda|$.

The Hilbert space $\mathcal{H}_{\Lambda,n}$ for n *distinguishable* particles is the tensor product $\otimes_{i=1}^n \ell^2(\Lambda)$. Its dimension is $|\Lambda|^n$ and it can be identified with the linear space $\ell^2(\Lambda^n)$ of functions of n sites. Then

$$\mathcal{H}_{\Lambda,n} = \otimes_{i=1}^n \ell^2(\Lambda) \cong \ell^2(\Lambda^n). \tag{4.2}$$

A basis for $\otimes_{i=1}^n \ell^2(\Lambda)$ consists of the functions

$$\Big\{ \bigotimes_{i=1}^n e_{x_i} \Big\}_{x_1,\dots,x_n \in \Lambda}, \tag{4.3}$$

where the functions e_{x_i} are as above. A basis for $\ell^2(\Lambda^n)$ consists of the functions $e_{x_1,\dots,x_n}$ that satisfy

$$e_{x_1,\dots,x_n}(y_1,\dots,y_n) = \prod_{i=1}^n \delta_{x_i,y_i}. \tag{4.4}$$

As physicists have progressively understood in the early days of Quantum Mechanics, the Hilbert space for *indistinguishable* particles is different. Particles fall in two kinds of species: the symmetric **bosons** and the antisymmetric **fermions**. The latter include the electrons and are therefore very relevant to condensed matter physics. The former are also relevant in an indirect way, as they can describe composite particles (made of an even number of fermions) or virtual particles (such as the phonons that describe lattice vibrations). The correct Hilbert spaces are the symmetric and antisymmetric subspaces of $\mathcal{H}_{\Lambda,n}$. To define them we introduce the **symmetrisation operator** P_+ and the **antisymmetrisation operator** P_-. They can be defined both on $\otimes_{i=1}^n \ell^2(\Lambda)$ and $\ell^2(\Lambda^n)$. First, the action of P_+ is

$$\begin{aligned} \big(P_+\varphi\big)(x_1,\dots,x_n) &= \frac{1}{n!}\sum_{\sigma\in\mathfrak{S}_n}\varphi(x_{\sigma(1)},\dots,x_{\sigma(n)}), \qquad \varphi\in\ell^2(\Lambda^n) \\ P_+\bigotimes_{i=1}^n\varphi_i &= \frac{1}{n!}\sum_{\sigma\in\mathfrak{S}_n}\bigotimes_{i=1}^n\varphi_{\sigma(i)}, \qquad \varphi_i\in\ell^2(\Lambda) \text{ for } i=1,\dots,n. \end{aligned} \tag{4.5}$$

Here, $\mathfrak{S}_n$ denotes the symmetric group and the sum is over permutations of n elements. Second, the action of P_- is

$$\begin{aligned} \big(P_-\varphi\big)(x_1,\dots,x_n) &= \frac{1}{n!}\sum_{\sigma\in\mathfrak{S}_n}(-1)^\sigma\varphi(x_{\sigma(1)},\dots,x_{\sigma(n)}), \qquad \varphi\in\ell^2(\Lambda^n) \\ P_-\bigotimes_{i=1}^n\varphi_i &= \frac{1}{n!}\sum_{\sigma\in\mathfrak{S}_n}(-1)^\sigma\bigotimes_{i=1}^n\varphi_{\sigma(i)}, \qquad \varphi_i\in\ell^2(\Lambda) \text{ for } i=1,\dots,n, \end{aligned} \tag{4.6}$$

where $(-1)^\sigma$ is the signature of the permutation σ (it is equal to $+1$ if σ can be written as the product of an even number of transpositions; it is -1 if the number of transpositions is odd). Note that $P_\pm$ are Hermitian projection operators in the sense that

$$P_\pm^2 = P_\pm, \qquad P_\pm^* = P_\pm. \tag{4.7}$$

The symmetric subspace $\mathcal{H}_{\Lambda,n}^{(+)}$, resp. antisymmetric subspace $\mathcal{H}_{\Lambda,n}^{(-)}$, are then

$$\mathcal{H}_{\Lambda,n}^{(\pm)} \cong P_\pm\ell^2(\Lambda^n) \cong P_\pm\bigotimes_{i=1}^n\ell^2(\Lambda). \tag{4.8}$$

These spaces consist of symmetric or antisymmetric functions. We can identify

$$\begin{aligned} \mathcal{H}_{\Lambda,n}^{(+)} &= \Big\{\varphi\in\mathbb{C}^\Lambda : \varphi(x_{\sigma(1)},\dots,x_{\sigma(n)}) = \varphi(x_1,\dots,x_n)\ \forall\sigma\in\mathfrak{S}_n\Big\}; \\ \mathcal{H}_{\Lambda,n}^{(-)} &= \Big\{\varphi\in\mathbb{C}^\Lambda : \varphi(x_{\sigma(1)},\dots,x_{\sigma(n)}) = (-1)^\sigma\varphi(x_1,\dots,x_n)\ \forall\sigma\in\mathfrak{S}_n\Big\}. \end{aligned} \tag{4.9}$$

We now introduce the notion of **occupation numbers**. They are a convenient way to describe the spaces of symmetric and antisymmetric functions. Let

$$\begin{aligned} \mathcal{N}_{\Lambda,n}^{(+)} &= \big\{(n_x)_{x\in\Lambda} : n_x\in\mathbb{N} \text{ and } \sum_{x\in\Lambda}n_x = n\big\}; \\ \mathcal{N}_{\Lambda,n}^{(-)} &= \big\{(n_x)_{x\in\Lambda} : n_x\in\{0,1\} \text{ and } \sum_{x\in\Lambda}n_x = n\big\}. \end{aligned} \tag{4.10}$$

The set $\mathcal{N}^{(-)}_{\Lambda,n}$ is nonempty only if $n \leq |\Lambda|$. The goal now is to check that

$$\mathcal{H}^{(\pm)}_{\Lambda,n} \cong \ell^2(\mathcal{N}^{(\pm)}_{\Lambda,n}). \tag{4.11}$$

To see this, we define the vector $|\boldsymbol{n}\rangle$ in $\mathcal{H}^{\pm}_{\Lambda,n}$, for $\boldsymbol{n} = (n_x) \in \mathcal{N}^{(\pm)}_{\Lambda,n}$:

$$\begin{aligned} |\boldsymbol{n}\rangle &= \Big(\frac{n!}{\prod_x n_x!}\Big)^{1/2} P_+ e_{x_1,\dots,x_n} \qquad \text{in } \mathcal{H}^{(+)}_{\Lambda,n}; \\ |\boldsymbol{n}\rangle &= (n!)^{1/2} P_+ e_{x_1,\dots,x_n} \qquad \text{in } \mathcal{H}^{(-)}_{\Lambda,n}. \end{aligned} \tag{4.12}$$

The vectors $e_{x_1,\dots,x_n}$ above are the basis vectors defined in (4.4); the sites $x_1, \dots, x_n$ are chosen so that $\#\{i = 1, \dots, n : x_i = x\} = n_x$ for all $x \in \Lambda$. The order of $(x_1, \dots, x_n)$ does not matter for $P_+ e_{x_1,\dots,x_n}$. The order affects the sign for $P_- e_{x_1,\dots,x_n}$ so the sites should satisfy $x_1 \prec \cdots \prec x_n$ where $\prec$ is some fixed total order on Λ. One can check that the prefactors have been chosen so that $|\boldsymbol{n}\rangle$ is normalised, see Exercise 4.3. It is not too hard to check that $\langle \boldsymbol{n}' | \boldsymbol{n}\rangle = 0$ if $\boldsymbol{n}' \neq \boldsymbol{n}$. Since the vectors $e_{x_1,\dots,x_n}$ span $\mathcal{H}_{\Lambda,n}$, it follows that $\{|\boldsymbol{n}\rangle\}_{\boldsymbol{n} \in \mathcal{N}^{(\pm)}_{\Lambda,n}}$ is an orthonormal basis for $\mathcal{H}^{(\pm)}_{\Lambda,n}$. The dimensions of $\mathcal{H}^{(+)}_{\Lambda,n}$ and $\mathcal{H}^{(-)}_{\Lambda,n}$ are then equal to the cardinalities of $\mathcal{N}^{(\pm)}_{\Lambda,n}$; we get

$$\begin{aligned} \dim \mathcal{H}^{(+)}_{\Lambda,n} &= |\mathcal{N}^{(+)}_{\Lambda,n}| = \binom{n + |\Lambda| - 1}{|\Lambda| - 1}, \\ \dim \mathcal{H}^{(-)}_{\Lambda,n} &= |\mathcal{N}^{(-)}_{\Lambda,n}| = \binom{|\Lambda|}{n} \qquad \text{if } n \leq |\Lambda|; \end{aligned} \tag{4.13}$$

this is verified in Exercise 4.4.

Next we introduce the Fock spaces that describe systems with variable numbers of particles. Let

$$\mathcal{F}^{(+)}_{\Lambda} = \bigoplus_{n=0}^{\infty} \mathcal{H}^{(+)}_{\Lambda,n}, \qquad \mathcal{F}^{(-)}_{\Lambda} = \bigoplus_{n=0}^{|\Lambda|} \mathcal{H}^{(-)}_{\Lambda,n}. \tag{4.14}$$

Here $\mathcal{H}^{(\pm)}_{\Lambda,0} \cong \mathbb{C}$ by definition. An element of $\mathcal{F}^{(+)}_{\Lambda}$ is an ∞-tuple $(\varphi_0, \varphi_1, \dots)$ where each φ_n is a vector in $\mathcal{H}^{(+)}_{\Lambda,n}$. The inner product in $\mathcal{F}^{(+)}_{\Lambda}$ is defined by

$$\langle \varphi, \psi \rangle = \sum_{n \geq 0} \langle \varphi_n, \psi_n \rangle_{\mathcal{H}^{(+)}_{\Lambda,n}}. \tag{4.15}$$

The dimension of $\mathcal{F}^{(+)}_{\Lambda}$ is infinite. In terms of occupation numbers, we have

$$\mathcal{F}^{(+)}_{\Lambda} \cong \ell^2(\mathcal{N}^{(+)}_{\Lambda}) \tag{4.16}$$

where

$$\mathcal{N}^{(+)}_{\Lambda} = \bigcup_{n \geq 0} \mathcal{N}^{(+)}_{\Lambda,n} = \mathbb{N}^{\Lambda}. \tag{4.17}$$

An element of $\mathcal{F}_\Lambda^{(-)}$ is an $|\Lambda|$-tuple $(\varphi_0, \varphi_1, \dots, \varphi_{|\Lambda|})$ where φ_n is a vector in $\mathcal{H}_{\Lambda,n}^{(-)}$; the inner product is defined by

$$\langle \varphi, \psi \rangle = \sum_{n=0}^{|\Lambda|} \langle \varphi_n, \psi_n \rangle_{\mathcal{H}_{\Lambda,n}^{(-)}}. \tag{4.18}$$

The dimension of $\mathcal{F}_\Lambda^{(-)}$ is $2^{|\Lambda|}$. In terms of occupation numbers, we have

$$\mathcal{F}_\Lambda^{(-)} \cong \ell^2(\mathcal{N}_\Lambda^{(-)}) \tag{4.19}$$

where

$$\mathcal{N}_\Lambda^{(-)} = \bigcup_{n \geq 0} \mathcal{N}_{\Lambda,n}^{(+)} = \{0,1\}^\Lambda. \tag{4.20}$$

4.2. Creation and annihilation operators

We define annihilation operators a_x and creation operators a_x^* in $\ell^2(\mathcal{N}_{\Lambda,n}^{(\pm)})$ or $\ell^2(\mathcal{N}_\Lambda^{(\pm)})$; this immediately extends to $\mathcal{H}_{\Lambda,n}^{(\pm)}$ and $\mathcal{F}_\Lambda^{(\pm)}$.

$$\begin{aligned}
\text{Bosons:} \qquad & a_x : \ell^2(\mathcal{N}_{\Lambda,n}^{(+)}) \to \ell^2(\mathcal{N}_{\Lambda,n-1}^{(+)}) \\
& \quad a_x|\boldsymbol{n}\rangle = \begin{cases} \sqrt{n_x}\,|\boldsymbol{n} - \delta_x\rangle & \text{if } n_x \geq 1, \\ 0 & \text{if } n_x = 0. \end{cases} \\
& a_x^* : \ell^2(\mathcal{N}_{\Lambda,n}^{(+)}) \to \ell^2(\mathcal{N}_{\Lambda,n+1}^{(+)}) \\
& \quad a_x^*|\boldsymbol{n}\rangle = \sqrt{n_x + 1}\,|\boldsymbol{n} + \delta_x\rangle.
\end{aligned} \tag{4.21}$$

These definitions extend to $\ell^2(\mathcal{N}_\Lambda^{(+)})$ but we need to specify the domain since these are unbounded operators in an infinite-dimensional space. Consider $\ell^2_{\mathrm{f}}(\mathcal{N}_\Lambda^{(+)})$, the linear space of finite linear combinations of $\{|\boldsymbol{n}\rangle : \boldsymbol{n} \in \mathcal{N}_\Lambda^{(+)}\}$. This domain is dense in $\ell^2(\mathcal{N}_\Lambda^{(+)})$, and a_x, a_x^* can be defined as operators $\ell^2_{\mathrm{f}}(\mathcal{N}_\Lambda^{(+)}) \to \ell^2(\mathcal{N}_\Lambda^{(+)})$. The operators can be closed by taking the closure of their graphs.

In the exercises (Exercise 4.5) you can check that a_x^* is the adjoint of a_x (and conversely), and that these bosonic operators satisfy the commutation relations

$$[a_x, a_y] = 0; \qquad [a_x^*, a_y^*] = 0; \qquad [a_x, a_y^*] = \delta_{x,y}\mathbb{1}. \tag{4.22}$$

One can also check that

$$a_x^* a_x |\boldsymbol{n}\rangle = n_x\,|\boldsymbol{n}\rangle. \tag{4.23}$$

We now turn to fermions and recall the order $\prec$ on the sites of Λ.

$$\begin{aligned}
\text{Fermions:} \qquad & a_x : \ell^2(\mathcal{N}^{(-)}_{\Lambda,n}) \to \ell^2(\mathcal{N}^{(-)}_{\Lambda,n-1}) \\
& a_x|\boldsymbol{n}\rangle = \begin{cases} (-1)^{\sum_{y\prec x} n_y} \, |\boldsymbol{n} - \delta_x\rangle & \text{if } n_x = 1, \\ 0 & \text{if } n_x = 0. \end{cases} \\
& a^*_x : \ell^2(\mathcal{N}^{(-)}_{\Lambda,n}) \to \ell^2(\mathcal{N}^{(-)}_{\Lambda,n+1}) \\
& a^*_x|\boldsymbol{n}\rangle = \begin{cases} (-1)^{\sum_{y\prec x} n_y} \, |\boldsymbol{n} + \delta_x\rangle & \text{if } n_x = 0, \\ 0 & \text{if } n_x = 1. \end{cases}
\end{aligned} \tag{4.24}$$

The definitions extend to $\ell^2(\mathcal{N}^{(-)}_{\Lambda})$ and $\mathcal{F}^{(-)}_{\Lambda}$.

These operators are also adjoint of each other. They satisfy the anticommutation relations

$$\{a_x, a_y\} = 0; \qquad \{a^*_x, a^*_y\} = 0; \qquad \{a_x, a^*_y\} = \delta_{x,y} \mathbb{1}. \tag{4.25}$$

Here also we have that

$$a^*_x a_x|\boldsymbol{n}\rangle = n_x \, |\boldsymbol{n}\rangle. \tag{4.26}$$

One-body operators can be conveniently represented by creation and annihilation operators. Let $B = (b_{x,y})_{x,y\in\Lambda}$ be an operator on $\ell^2(\Lambda)$ (i.e. a $\Lambda \times \Lambda$ complex matrix). This yields the following operator on $\mathcal{H}_{\Lambda,n}$:

$$\boldsymbol{B} = \sum_{i=1}^{n} B_i, \tag{4.27}$$

where

$$B_i = \mathbb{1} \otimes \cdots \otimes \underbrace{B}_{i\text{th particle}} \otimes \cdots \otimes \mathbb{1}. \tag{4.28}$$

One easily checks that $[\boldsymbol{B}, P_\pm] = 0$ so $\boldsymbol{B}$ can also be viewed as an operator on $\mathcal{H}^{(+)}_{\Lambda,n}$ or $\mathcal{H}^{(-)}_{\Lambda,n}$.

Lemma 4.1. *On $\mathcal{H}^{(+)}_{\Lambda,n}$ or $\mathcal{H}^{(-)}_{\Lambda,n}$, we have*

$$\boldsymbol{B} = \sum_{x,y\in\Lambda} b_{x,y} a^*_x a_y.$$

Proof. Here we restrict to bosons, fermions are similar. Recalling that $\langle \boldsymbol{m}|a^*_x = \langle a_x \boldsymbol{m}|$, the matrix elements of the right side are

$$\langle \boldsymbol{m}|b_{x,y} a^*_x a_y|\boldsymbol{n}\rangle = \sqrt{m_x n_y} \, \delta_{\boldsymbol{m}-\delta_x, \boldsymbol{n}-\delta_y}. \tag{4.29}$$

Using that $P_+ = P_+^*$ commutes with $\boldsymbol{B}$ we get

$$\begin{aligned}\langle \boldsymbol{m}|\boldsymbol{B}|\boldsymbol{n}\rangle &= \frac{n!}{\sqrt{\prod_z m_z! n_z!}} \langle e_{x_1,\dots,x_n}|P_+^2 \boldsymbol{B}|e_{y_1,\dots,y_n}\rangle \\ &= \frac{n!}{\sqrt{\prod_z m_z! n_z!}} \sum_{i=1}^n \langle e_{x_1,\dots,x_n}|P_+^2 B_i|e_{y_1,\dots,y_n}\rangle.\end{aligned} \tag{4.30}$$

Here the sites $x_1, \dots, x_n$ are compatible with $\boldsymbol{m}$ and the sites $y_1, \dots, y_n$ are compatible with $\boldsymbol{n}$. It suffices to consider a matrix B with a single nonzero entry, $b_{x,y} = 1$ for some fixed $x, y \in \Lambda$. The general case follows by linearity. For this B, we have that

$$B_i|e_{y_1,\dots,y_n}\rangle = \delta_{y_i,y}|e_{y_1,\dots,x,\dots,y_n}\rangle \tag{4.31}$$

where the vector on the right has an x in position i. Thus

$$\begin{aligned}\langle \boldsymbol{m}|\boldsymbol{B}|\boldsymbol{n}\rangle &= \Big(\frac{n!}{\prod_z n_z!}\Big)^{1/2} \sum_{i=1}^n \delta_{y_i,y} \langle \boldsymbol{m}|P_+|e_{y_1,\dots,x,\dots,y_n}\rangle \\ &= \Big(\frac{n!}{\prod_z n_z!}\Big)^{1/2} n_y \Big(\frac{n!}{\prod_z (n_z - \delta_y + \delta_x)!}\Big)^{-1/2} \langle \boldsymbol{m}|\boldsymbol{n} - \delta_y + \delta_x\rangle \\ &= n_y \big(\tfrac{n_x+1}{n_y}\big)^{1/2} \, \delta_{\boldsymbol{m}-\delta_x, \boldsymbol{n}-\delta_y}.\end{aligned} \tag{4.32}$$

This agrees with (4.29). □

One can generalise this lemma to many-body operators. A natural hamiltonian for lattice particles with two-body interactions is

$$H_\Lambda = -\sum_{i=1}^n \Delta_i + \sum_{1 \le i < j \le n} V_{i,j}, \tag{4.33}$$

where $\Delta_i = \mathbb{1} \otimes \dots \otimes \Delta \otimes \dots \otimes \mathbb{1}$ and Δ is the discrete laplacian such that

$$(\Delta\varphi)(x) = \sum_{y \in \Lambda} t_{x,y} \varphi(y). \tag{4.34}$$

Here $t_{x,y} = t_{y,x} \in \mathbb{R}$ is finite-range or fast decaying (the standard case involves same sites and nearest-neighbours). The interactions are given by a multiplication operator

$$V_{i,j}\varphi(x_1, \dots, x_n) = W(x_i - x_j)\varphi(x_1, \dots, x_n). \tag{4.35}$$

Here $W(x)$ is a real function, of finite range or with fast decay. The hamiltonian above represents the energy of n particles, that consists of kinetic energy (the laplacians) and pair interactions (given by W). The hamiltonian above is both symmetric and antisymmetric, in the sense that $[H_\Lambda, P_\pm] = 0$, and its action on

$\mathcal{H}^{(\pm)}_{\Lambda,n}$ can be written as

$$H_\Lambda = -\sum_{x,y\in\Lambda} t_{x,y} a^*_x a_y + \tfrac{1}{2} W(0) \sum_{x\in\Lambda} a^*_x a_x (a^*_x a_x - 1) + \tfrac{1}{2} \sum_{\substack{x,y\in\Lambda \\ x\neq y}} W(x-y) a^*_x a_x a^*_y a_y. \quad (4.36)$$

As an operator in $\mathcal{F}^{(+)}_\Lambda$ it is unbounded. It is well defined on $\ell^2_{\rm f}(\mathcal{N}^{(+)}_\Lambda)$; it is symmetric, and its closure is self-adjoint.

One can take the limit $W(0) \to \infty$, which yields *hard-core bosons*, where at most one particle per site is allowed. The Hilbert space is then identical to that of $S = \frac{1}{2}$ quantum spins. One can identify $n_x = 0$ with $\sigma_x = -\frac{1}{2}$, and $n_x = 1$ with $\sigma_x = \frac{1}{2}$. As for operators we have

$$a_x \equiv S^{(-)}_x, \qquad a^*_x \equiv S^{(+)}_x, \qquad a^*_x a_x \equiv S^{(3)}_x + \tfrac{1}{2}. \quad (4.37)$$

4.3. Bose–Einstein condensation

We say that a two-body potential W is **stable** if there exists a constant B such for all $n \in \mathbb{N}$ and all $x_1, \dots, x_n \in \mathbb{Z}^d$, we have the lower bound

$$\sum_{1\leq i<j\leq n} W(x_i - x_j) \geq -Bn. \quad (4.38)$$

Typical examples are nonnegative (repulsive) potentials (the inequality is trivial, with $B = 0$) and potentials that are repulsive at short distance but attractive at longer distance. This condition guarantees that the particles of a large system spread everywhere, and do not collapse in a small region. This property is necessary for statistical mechanics to hold.

We define the **free energy** of a particle system by

$$\begin{aligned} f_{\Lambda,n}(\beta) &= -\frac{1}{\beta|\Lambda|} \log \operatorname{Tr}_{\mathcal{H}^{(\pm)}_{\Lambda,n}} \mathrm{e}^{-\beta H_\Lambda}. \\ f(\beta,\rho) &= \lim_{\Lambda \Uparrow \mathbb{Z}^d} f_{\Lambda,\lfloor \rho|\Lambda|\rfloor}(\beta). \end{aligned} \quad (4.39)$$

Here, the parameter ρ is the **density**. Existence of the limit can be proved in a similar fashion as for spin systems (the stability condition gives a lower bound for $f_{\Lambda,n}$ that is necessary for the subadditive argument). Introducing the number operator

$$N_\Lambda|\varphi\rangle = n|\varphi\rangle, \qquad \varphi \in \mathcal{H}^{(\pm)}_{\Lambda,n}, \quad (4.40)$$

we define the **pressure** by

$$\begin{aligned} p_\Lambda(\beta,\mu) &= \frac{1}{|\Lambda|} \log \operatorname{Tr}_{\mathcal{F}^{(\pm)}_\Lambda} \mathrm{e}^{-\beta(H_\Lambda - \mu N_\Lambda)}. \\ p(\beta,\mu) &= \lim_{\Lambda\Uparrow\mathbb{Z}^d} p_\Lambda(\beta,\mu). \end{aligned} \quad (4.41)$$

The functions $f(\beta,\rho)$ and $p(\beta,\mu)$ are related by Legendre transforms.

The hamiltonian commutes with the number of particles in the box, $[H_\Lambda, N_\Lambda] = 0$, which implies the presence of a continuous $U(1)$ symmetry:

$$H_\Lambda = \mathrm{e}^{\mathrm{i}\theta N_\Lambda}\, H_\Lambda\, \mathrm{e}^{-\mathrm{i}\theta N_\Lambda}\,, \qquad \theta \in [0, 2\pi). \tag{4.42}$$

The corresponding order parameter is the **off-diagonal long range order** proposed by Penrose and Onsager [1956]: the correlation function $\langle a_x^* a_y \rangle_{\Lambda,\beta}$ (in either the canonical or gran canonical ensemble). The question is whether it remains positive in the infinite volume limit, and as $\|x - y\| \to \infty$.

In the hard-core Bose, which is equivalent to the quantum XY model, off-diagonal long range order is equivalent to spontaneous magnetisation in the XY plane. The latter can be proved using reflection positivity (Dyson, Lieb, Simon [1978], see previous chapter). This is the only known proof of Bose–Einstein condensation in an interacting Bose gas, in the standard setting.

We conclude the chapter by describing the Bose–Einstein condensation of the ideal gas (no interactions) on the lattice.

Let $\Lambda_\ell^{\mathrm{per}} = \{1, \dots, \ell\}^d$ with periodic boundary conditions. We consider the model (4.36) with $W \equiv 0$.

Theorem 4.2.

$$\lim_{\ell \to \infty} \frac{1}{|\Lambda_\ell^{\mathrm{per}}|} \sum_{x \in \Lambda_\ell^{\mathrm{per}}} \langle a_0^* a_x \rangle_{\Lambda_\ell^{\mathrm{per}}, \beta, \lfloor \rho \ell^d \rfloor} = \max(0, \rho - \rho_{\mathrm{c}})$$

where the critical density is equal to

$$\rho_{\mathrm{c}} = \frac{1}{(2\pi)^d} \int_{[-\pi,\pi]^d} \frac{1}{\mathrm{e}^{\beta\varepsilon(k)} - 1} \mathrm{d}k.$$

Recall that $\varepsilon(k) = \sum_x t_{0,x}\, \mathrm{e}^{-\mathrm{i}kx}$. The critical density is finite when $d \geq 3$. In the continuum we have $\varepsilon(k) = k^2$; one can expand the fraction as geometric series, integrate the gaussians, and one gets the well-known formula of Einstein.

Proof. Let us introduce the creation and annihilation operators of the Fourier modes, namely

$$\hat{a}_k = \frac{1}{\ell^{d/2}} \sum_{x \in \Lambda_\ell^{\mathrm{per}}} \mathrm{e}^{-\mathrm{i}kx}\, a_x, \qquad k \in \Lambda_\ell^*. \tag{4.43}$$

Then we have

$$a_x = \frac{1}{\ell^{d/2}} \sum_{k \in \Lambda_\ell^*} \mathrm{e}^{\mathrm{i}kx}\, \hat{a}_k \tag{4.44}$$

and

$$\sum_{x,y \in \Lambda_\ell^{\mathrm{per}}} t_{x,y} a_x^* a_y = \sum_{k \in \Lambda_\ell^*} \varepsilon(k) \hat{a}_k^* \hat{a}_k. \tag{4.45}$$

One can also check that the eigenvalues of $\hat{a}_k^* \hat{a}_k$ are $0, 1, 2, \dots$. We also have

$$\frac{1}{\ell^d} \sum_{x \in \Lambda_\ell^{\text{per}}} \langle a_0^* a_x \rangle_{\Lambda_\ell^{\text{per}},\beta,n} = \frac{1}{\ell^{2d}} \sum_{x,y \in \Lambda_\ell^{\text{per}}} \langle a_x^* a_y \rangle_{\Lambda_\ell^{\text{per}},\beta,n} = \frac{1}{\ell^d} \langle \hat{a}_0^* \hat{a}_0 \rangle_{\Lambda_\ell^{\text{per}},\beta,n}. \tag{4.46}$$

The relevant expectation can then be written using random partitions $(n_k)_{k \in \Lambda_\ell^*}$ indexed by Λ_ℓ^* and satisfying $\sum_k n_k = n$. Namely,

$$\frac{1}{\ell^d} \sum_{x \in \Lambda_\ell^{\text{per}}} \langle a_0^* a_x \rangle_{\Lambda_\ell^{\text{per}},\beta,n} = \frac{1}{\ell^d} \langle \hat{a}_0^* \hat{a}_0 \rangle_{\Lambda_\ell^{\text{per}},\beta,n} = \frac{1}{Z_{\Lambda_\ell^{\text{per}},\beta,\rho}} \sum_{(n_k)_{k \in \Lambda_\ell^*} : \sum_k n_k = n} \frac{n_0}{\ell^k} \, \mathrm{e}^{-\beta \sum_k \varepsilon(k) n_k}. \tag{4.47}$$

We denote $\mathbb{P}, \mathbb{E}$ the corresponding probability and expectation where a partition (n_k) has probability proportional to $\mathrm{e}^{-\beta \sum_k \varepsilon(k) n_k}$. We have

$$\begin{aligned}
\frac{1}{\ell^d} \sum_{x \in \Lambda_\ell^{\text{per}}} \langle a_0^* a_x \rangle_{\Lambda_\ell^{\text{per}},\beta,n} &= \frac{1}{\ell^d} \mathbb{E}[n_0] = \frac{n}{\ell^d} - \frac{1}{\ell^d} \sum_{k \neq 0} \mathbb{E}[n_k] \\
&= \frac{n}{\ell^d} - \frac{1}{\ell^d} \sum_{k \neq 0} \sum_{i \geq 1} \mathbb{P}[n_k \geq i] \\
&= \frac{n}{\ell^d} - \frac{1}{\ell^d} \sum_{k \neq 0} \frac{1}{Z_{\Lambda_\ell^{\text{per}},\beta,n}} \sum_{i \geq 1} \sum_{(n_{k'}) : \sum_{k'} n_k = n, n_k \geq i} \mathrm{e}^{-\beta \sum_{k'} \varepsilon(k') n_{k'}} \\
&= \frac{n}{\ell^d} - \frac{1}{\ell^d} \sum_{k \neq 0} \sum_{i \geq 1} \mathrm{e}^{-\beta \varepsilon(k) i} \, \frac{Z_{\Lambda_\ell^{\text{per}},\beta,n-i}}{Z_{\Lambda_\ell^{\text{per}},\beta,n}} \\
&\geq \frac{n}{\ell^d} - \frac{1}{\ell^d} \sum_{k \neq 0} \frac{1}{\mathrm{e}^{\beta \varepsilon(k)} - 1}.
\end{aligned} \tag{4.48}$$

Notice that the ratio of partition functions is equal to $\mathbb{P}[n_0 \geq i]$ which is less than 1. As $\ell \to \infty$, the last term converges to $\rho - \rho_{\text{c}}$.

It is perhaps worth noting the infrared bound $\mathbb{E}[n_k] \leq (\mathrm{e}^{\beta \varepsilon(k)} - 1)^{-1}$, which implies long-range order as in the case of spin systems.

In order to prove the converse bound, let us observe that the pressure of the ideal Bose gas can be computed exactly, yielding (for $\mu < 0$)

$$p(\beta, \mu) = \lim_{\ell \to \infty} \frac{1}{\ell^d} \sum_{(n_k)} \mathrm{e}^{-\beta \sum_k (\varepsilon(k) - \mu) n_k} = -\frac{1}{(2\pi)^d} \int_{[-\pi,\pi]^d} \log\Big(1 - \mathrm{e}^{-\beta(\varepsilon(k) - \mu)}\Big) \mathrm{d}k. \tag{4.49}$$

The density is

$$\rho(\beta, \mu) = \frac{1}{\beta} \frac{\partial}{\partial \mu} p(\beta, \mu) = \frac{1}{(2\pi)^d} \int_{[-\pi,\pi]^d} \frac{1}{\mathrm{e}^{\beta(\varepsilon(k) - \mu)} - 1} \mathrm{d}k. \tag{4.50}$$

The critical density is equal to the limit $\mu \to 0-$ of $\rho(\beta,\mu)$. The free energy is given by the Legendre transform

$$f(\beta,\rho) = \sup_{\mu<0}\bigl(\rho\mu - \tfrac{1}{\beta}p(\beta,\mu)\bigr). \tag{4.51}$$

The plot of the pressure and its Legendre transform can be found in Fig. 4.1.

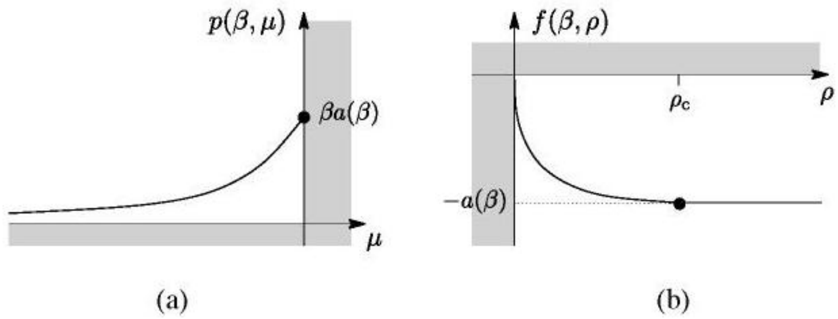

FIGURE 4.1. (a) The pressure of the ideal Bose gas; (b) its Legendre transform, the free energy.

For any $\eta \geq 0$, we have that

$$\lim_{\ell\to\infty}\frac{1}{\beta\ell^d}\log\mathbb{P}[n_0 \geq \ell^d\eta] = \lim_{\ell\to\infty}\frac{1}{\beta\ell^d}\log\frac{Z_{\Lambda_\ell^{\rm per},\beta,n-\ell^d\eta}}{Z_{\Lambda_\ell^{\rm per},\beta,n}} = f(\beta,\rho)-f(\beta,\rho-\eta). \tag{4.52}$$

If $\eta > \max(0,\rho-\rho_c)$, we have

$$\mathbb{P}[n_0 \geq \ell^d\eta] \leq \mathrm{e}^{-\ell^d\delta} \tag{4.53}$$

for some $\delta > 0$. It follows that $\frac{1}{\ell^d}\mathbb{E}[n_0] \leq \max(0,\rho-\rho_c)$, which completes the proof. $\square$

EXERCISE 4.1. *Verify that the operators $P_\pm$ defined in (4.5)–(4.6) are indeed projectors.*

EXERCISE 4.2. *Let $x_1,\dots,x_n \in \Lambda$ such that $x_i = x_j$ for some $i \neq j$. Check that $P_- e_{x_1,\dots,x_n} = 0$.*

EXERCISE 4.3. *Let $(n_x) \in \mathcal{N}^{(\pm)}_{\Lambda,n}$ and $(x_1,\dots,x_n)$ such that $\#\{i=1,\dots,n : x_i = x\} = n_x$ for all $x\in\Lambda$. Verify that*

$$\|P_\pm e_{x_1,\dots,x_n}\| = \Bigl(\frac{\prod_{x\in\Lambda} n_x!}{n!}\Bigr)^{1/2}.$$

EXERCISE 4.4. *Verify Eq. (4.13) about the dimensions of the symmetric and antisymmetric spaces.*

Exercise 4.5. *Verify that that a_x and a^*_x are adjoint of one another. In the bosonic case, this involves their domains.*

Exercise 4.6. *Verify the commutation relations (4.22) and (4.25).*

Exercise 4.7. *Give the proof of Lemma 4.1 in the fermionic case.*

Exercise 4.8. *In this exercise we outline a variant of the proof of Theorem 4.2, starting from the probabilistic representation in (4.47) and (4.48).*

(1) *Show that we can write*

$$\frac{1}{\ell^d}\sum_{k\neq 0}\mathbb{E}[n_k] = \mathbb{E}[X_\ell \mid X_\ell \leq \rho] \tag{4.54}$$

where

$$X_\ell = \frac{1}{\ell^d}\sum_{k\in\Lambda^*_\ell\setminus\{0\}} N_k \tag{4.55}$$

and the N_k are independent geometric random variables:

$$\mathbb{P}(N_k = r) = (\,\mathrm{e}^{-\beta\varepsilon(k)}\,)^r(1-\,\mathrm{e}^{-\beta\varepsilon(k)}\,), \qquad r\geq 0. \tag{4.56}$$

The goal is thus to show that

$$\lim_{\ell\to\infty}\mathbb{E}[X_\ell \mid X_\ell\leq\rho] = \begin{cases}\rho & \text{if } \rho\leq\rho_{\mathrm{c}},\\ \rho_{\mathrm{c}} & \text{if } \rho\geq\rho_{\mathrm{c}}.\end{cases} \tag{4.57}$$

(2) *Clearly $\lim_{\ell\to\infty}\mathbb{E}[X_\ell \mid X_\ell\leq\rho]\leq\rho$. Show that $\lim_{\ell\to\infty}\mathbb{E}[X_\ell] = \rho_{\mathrm{c}}$.*

(3) *Show that*

$$\mathbb{E}[(X_\ell-\rho_{\mathrm{c}})^2]\to 0, \qquad \text{as } \ell\to\infty. \tag{4.58}$$

(4) *Use Markov's inequality to deduce that*

$$\lim_{\ell\to\infty}\mathbb{E}[X_\ell \mid X_\ell\leq\rho] = \rho_{\mathrm{c}} \tag{4.59}$$

whenever $\rho > \rho_{\mathrm{c}}$.

(5) *It remains to show that $\lim_{\ell\to\infty}\mathbb{E}[X_\ell \mid X_\ell\leq\rho]\geq\rho$ when $\rho\leq\rho_{\mathrm{c}}$, and this is the hardest part. It uses ideas from large deviations theory.*

   (a) *Show that*

$$\Lambda(t) := \lim_{\ell\to\infty}\frac{1}{\ell^d}\log\mathbb{E}[\,\mathrm{e}^{t\ell^d X_\ell}\,] \tag{4.60}$$

   exists in $[-\infty,\infty]$ for all $t\in\mathbb{R}$.

   (b) *Deduce that for any $x<\rho_{\mathrm{c}}$*

$$\lim_{\ell\to\infty} -\frac{1}{\ell^d}\log\mathbb{P}(X_\ell\leq x) = \Lambda^*(x) := \sup_{t\in\mathbb{R}}\,(xt-\Lambda(t)) \tag{4.61}$$

   (c) *For any $\rho\leq\rho_{\mathrm{c}}$ and $\delta>0$,*

$$\mathbb{E}[X_\ell \mid X_\ell\leq\rho]\geq(\rho-\delta)\Big(1-\frac{\mathbb{P}(X_\ell\leq\rho-\delta)}{\mathbb{P}(X_\ell\leq\rho-\delta/2)}\Big). \tag{4.62}$$

(d) Deduce the result.

CHAPTER 5

Loop representation of the Heisenberg model

Feynman-Kac expansions of quantum statistical mechanical systems go back to Feynman [1953], Ginibre [1969], Kennedy [1985], and many others. Some models give rise to loops, see Tóth [1993], Aizenman and Nachtergaele [1994], Ueltschi [2013]. In $d \geq 3$ the joint distribution of the lengths of the loops is conjectured to be Poisson-Dirichlet (Goldschmidt, Ueltschi, Windridge [2011]); this is expected to be very general, occurring in any model involving one-dimensional loops that lives in space of dimensions three or higher. A proof for the random interchange model on the complete graph was proposed in Schramm [2005]. The model with "time reversals" was considered in Björnberg, Kotowski, Lees, and Miłoś [2019].

The goal of this section is first to derive the loop representation of the Heisenberg model. Then we calculate the "spin Laplace transform" of the symmetric Gibbs state in three different ways: 1) using the conjectured symmetry breaking; 2) exact calculations on the complete graph; 3) using the Poisson-Dirichlet distribution.

5.1. Bálint Tóth's loop representation

Let $\Lambda \Subset \mathbb{Z}^d$ and let $\mathcal{E}_\Lambda$ denote the set of nearest-neighbour sites. The Hilbert space $\mathcal{H}_\Lambda = \otimes_{x\in\Lambda}\mathbb{C}^2$. It is convenient to write the Heisenberg hamiltonian as

$$H_\Lambda = -2 \sum_{\{x,y\}\in\mathcal{E}_\Lambda} \big(\vec{S}_x \cdot \vec{S}_y - \tfrac{1}{2}\big). \tag{5.1}$$

We introduce the transposition operator $T_{x,y}$ whose action on $|(\sigma_z)\rangle$ is

$$T_{x,y}|(\sigma_z)\rangle = |(\sigma'_z)\rangle \qquad \text{where } \sigma'_z = \begin{cases} \sigma_y & \text{if } z = x, \\ \sigma_x & \text{if } z = y, \\ \sigma_z & \text{if } z \neq x, y. \end{cases} \tag{5.2}$$

Lemma 5.1.

$$T_{x,y} = 2\vec{S}_x \cdot \vec{S}_y + \tfrac{1}{2}.$$

Proof. This can be verified by looking at the action of these operators in the basis of spin configurations. But we can also remark that these operators commute, and that $T_{x,y}^2 = \mathbb{1}$. Since $\mathrm{Tr}_{\mathbb{C}^2\otimes\mathbb{C}^2} T_{x,y} = 2$, we see that the eigenvalues of $T_{x,y}$ are $(-1,1,1,1)$.

On the other hand, we have

$$2\vec{S}_x \cdot \vec{S}_y = (\vec{S}_x + \vec{S}_y)^2 - \vec{S}_x^2 - \vec{S}_y^2 = (\vec{S}_x + \vec{S}_y)^2 - \tfrac{3}{2}. \tag{5.3}$$

Applying Proposition A.11 with just two spins, we see that the eigenvalues of $(\vec{S}_x + \vec{S}_y)^2$ are $(0,2,2,2)$. The eigenvalues of $2\vec{S}_x \cdot \vec{S}_y$ are therefore $(-\frac{3}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ and we get $T_{x,y}$ by adding $\frac{1}{2}\mathbb{1}$. $\square$

The Heisenberg hamiltonian is then equal to

$$H_\Lambda = -\sum_{\{x,y\}\in\mathcal{E}_\Lambda} (T_{x,y} - 1). \tag{5.4}$$

This form is ideal for the loop expansion.

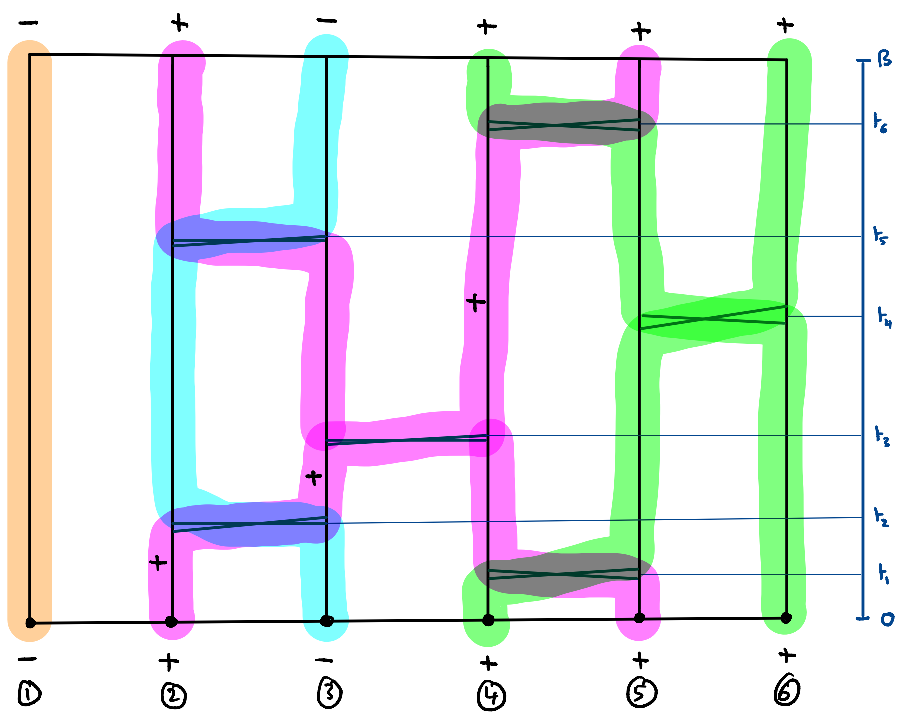

FIGURE 5.1. A realisation ω of the point point process on $\mathcal{E}_\Lambda \times [0,\beta]$. Here $|\omega| = 6$ and $|\mathcal{L}(\omega)| = 4$. The first transition occurs at the edge $(x_1, y_1) = (4,5)$. In order to get non-zero contribution, the initial spin configuration must have the same spin value at sites within the same loop.

We now describe the loop expansion, which is illustrated in Fig. 5.1. To each edge of Λ, we assign the "time" interval $[0,\beta]$. We consider independent Poisson processes (of intensity 1) on each interval. Let ρ denote the measure associated with these Poisson point processes. A realisation of ρ is a vector

$$\omega = \Big((\{x_1, y_1\}, t_1), \dots, (\{x_k, y_k\}, t_k) \Big), \tag{5.5}$$

where $\{x_i, y_i\} \in \mathcal{E}_\Lambda$; the times t_i satisfy $0 < t_1, \dots, t_k < \beta$; and the number of events $k \equiv |\omega|$ is random. Given a realisation ω, we denote by $\mathcal{L}(\omega)$ the set of loops, or close trajectories.

In order to get equivalence with the quantum system, we need to assign the weight $2^{|\mathcal{L}(\omega)|}$ to the realisation ω. We can now state the precise relation between the quantum spin system and the loop model.

THEOREM 5.2. *Let H_Λ be the hamiltonian of Eqs (5.1) or (5.4). We have*

(a) $Z_{\Lambda,\beta} = \mathrm{Tr}\, \mathrm{e}^{-\beta H_\Lambda} = \int \rho(\mathrm{d}\omega)\, 2^{|\mathcal{L}(\omega)|}$.

(b) $\langle S_x^{(3)} S_y^{(3)} \rangle_{\Lambda,\beta} = \frac{1}{4} \mathbb{P}[(x,0) \longleftrightarrow (y,0)]$.

(c) $\langle\, \mathrm{e}^{h \sum_{x\in\Lambda} S_x^{(3)}}\, \rangle_{\Lambda,\beta} = \mathbb{E}\Big[\prod_{\gamma \in \mathcal{L}(\omega)} \cosh\big(\frac{1}{2} h \ell(\gamma)\big) \Big]$.

For (c), we defined the length of the loop γ as the number of sites (at time 0) that belong to the loop.

PROOF. Given $N \in \mathbb{N}$, let I_N denote the discretised set $\{\frac{1}{N}, \frac{2}{N}, \dots, \frac{\beta}{N}\}$; we refer to its elements as "times". The partition function of the loop model is then

$$\int \rho(\mathrm{d}\omega)\, 2^{|\mathcal{L}(\omega)|} = \lim_{N\to\infty} \sum_{\omega \subset \mathcal{E}_\Lambda \times I_N} \Big(\frac{\beta}{N}\Big)^{|\omega|} \Big(1 - \frac{\beta}{N}\Big)^{N|\mathcal{E}_\Lambda| - |\omega|} 2^{|\mathcal{L}(\omega)|}. \tag{5.6}$$

We now expand the quantum spin system and show that we get the same expression. Using the limit formula for the exponential, we have

$$\begin{aligned} \mathrm{Tr}\, \mathrm{e}^{-\beta H_\Lambda} &= \lim_{N\to\infty} \mathrm{Tr} \Big(1 - \frac{\beta |\mathcal{E}_\Lambda|}{N} + \frac{\beta}{N} \sum_{\{x,y\} \in \mathcal{E}_\Lambda} T_{x,y} \Big)^N \\ &= \lim_{N\to\infty} \sum_{\omega \subset \mathcal{E}_\Lambda \times I_N} \Big(1 - \frac{\beta}{N}\Big)^{N|\mathcal{E}_\Lambda| - |\omega|} \Big(\frac{\beta}{N}\Big)^{|\omega|} \mathrm{Tr} \prod_{i=1}^{|\omega|} T_{x_i, y_i}. \end{aligned} \tag{5.7}$$

The sum over ω is restricted to configurations with at most one event at each "time". The last product must respect the order of occurrence of the operators T_{x_i,y_i}. In order to find the value of the trace, observe that

$$\langle \sigma | T_{x_1,y_1} \dots T_{x_k,y_k} = \langle \sigma' |, \tag{5.8}$$

where $\sigma'_x = \sigma_{\pi^{-1}(x)}$, where π is the permutation given by the product of transpositions of $(x_1, y_1), \dots, (x_k, y_k)$. We need $\sigma' = \sigma$ in order to contribute to the trace.

The restriction is then that the spin values must be the same in sites within the same permutation cycles. We then have

$$\operatorname{Tr} \prod_{i=1}^{|\omega|} T_{x_i,y_i} = 2^{|\mathcal{L}(\omega)|}. \tag{5.9}$$

We then get (5.6), which proves (a).

(b) is left as an exercise.

For (c), we expand

$$\operatorname{Tr} \mathrm{e}^{h \sum_{x\in\Lambda} S_x^{(3)}} \ \mathrm{e}^{-\beta H_\Lambda} = \lim_{N\to\infty} \sum_{\omega\subset\mathcal{E}_\Lambda\times I_N} \Big(1-\frac{\beta}{N}\Big)^{N|\mathcal{E}_\Lambda|-|\omega|} \Big(\frac{\beta}{N}\Big)^{|\omega|} \operatorname{Tr} \mathrm{e}^{h \sum_{x\in\Lambda} S_x^{(3)}} \prod_{i=1}^{|\omega|} T_{x_i,y_i}. \tag{5.10}$$

As before, the spin values must be the same in each permutation cycle (aka loop) in order to give non-zero contribution. Writing σ_γ the spin value for the sites of the loop γ, we have

$$\operatorname{Tr} \mathrm{e}^{h \sum_{x\in\Lambda} S_x^{(3)}} \prod_{i=1}^{|\omega|} T_{x_i,y_i} = \sum_{(\sigma_\gamma)_{\gamma\in\mathcal{L}(\omega)}} \mathrm{e}^{h\sum_{\gamma\in\mathcal{L}(\omega)} \sigma_\gamma \ell(\gamma)} = \prod_{\gamma\in\mathcal{L}(\omega)} 2\cosh\big(\tfrac12 h\ell(\gamma)\big). \tag{5.11}$$

The result follows. □

5.2. The spin-Laplace transform and symmetry breaking

Tom Spencer suggested that the following function of h is worth calculating, as it gives a partial characterisation of the Gibbs states:

$$\Phi(\beta,h) = \lim_{\Lambda\Uparrow\mathbb{Z}^d} \langle \, \mathrm{e}^{\frac{h}{|\Lambda|} \sum_{x\in\Lambda} S_x^{(3)}} \, \rangle_{\Lambda,\beta}. \tag{5.12}$$

Various models are discussed in Björnberg, Froöhlich, Ueltschi [2020]: the spin S Heisenberg and XY models, and the model of quantum transpositions.

The first calculation is **not rigorous**, but it is expected to be *exact*: it does not involve approximations. We expect that the infinite-volume, translation-invariant, extremal Gibbs states are

$$\langle\cdot\rangle_{\beta,\vec a} = \lim_{h\to0+} \lim_{\Lambda\Uparrow\mathbb{Z}^d} \frac{1}{Z_{\Lambda,\beta,\vec a}} \operatorname{Tr} \cdot \ \mathrm{e}^{-\beta H_\Lambda + h\sum_{x\in\Lambda} \vec a\cdot\vec S_x}. \tag{5.13}$$

The infinite-volume symmetric Gibbs state is then equal to

$$\langle\cdot\rangle_\beta = \int_{\mathbb{S}^2} \langle\cdot\rangle_{\beta,\vec a} \, \mathrm{d}\vec a. \tag{5.14}$$

Here, $\mathrm{d}\vec{a}$ denotes the uniform probability measure on the two-dimensional sphere $\mathbb{S}^2$. This decomposition allows to calculate the function $\Phi(\beta, h)$.

$$\begin{aligned}\Phi(\beta,h) &= \lim_{\Lambda\Uparrow\mathbb{Z}^d} \langle\, \mathrm{e}^{\frac{h}{|\Lambda|}\sum_{x\in\Lambda} S_x^{(3)}} \,\rangle_{\Lambda,\beta} = \lim_{\Lambda\Uparrow\mathbb{Z}^d} \lim_{\Lambda'\Uparrow\mathbb{Z}^d} \langle\, \mathrm{e}^{\frac{h}{|\Lambda|}\sum_{x\in\Lambda} S_x^{(3)}} \,\rangle_{\Lambda',\beta} \\ &= \lim_{\Lambda\Uparrow\mathbb{Z}^d} \int_{\mathbb{S}^2} \langle\, \mathrm{e}^{\frac{h}{|\Lambda|}\sum_{x\in\Lambda} S_x^{(3)}} \,\rangle_{\beta,\vec{a}}\, \mathrm{d}\vec{a} = \lim_{\Lambda\Uparrow\mathbb{Z}^d} \int_{\mathbb{S}^2} \langle\, \mathrm{e}^{\frac{h}{|\Lambda|}\sum_{x\in\Lambda} S_x^{(3)}} \,\rangle_{\beta,\vec{a}}\, \mathrm{d}\vec{a} \\ &= \lim_{\Lambda\Uparrow\mathbb{Z}^d} \int_{\mathbb{S}^2} \mathrm{e}^{\frac{h}{|\Lambda|}\langle\sum_{x\in\Lambda} S_x^{(3)}\rangle_{\beta,\vec{a}}}\, \mathrm{d}\vec{a} = \int_{\mathbb{S}^2} \mathrm{e}^{h\langle S_0^{(3)}\rangle_{\beta,\vec{a}}}\, \mathrm{d}\vec{a} \\ &= \int_{\mathbb{S}^2} \mathrm{e}^{h\langle \vec{a}\cdot\vec{S}_0\rangle_{\beta,\vec{e}_3}}\, \mathrm{d}\vec{a} = \int_{\mathbb{S}^2} \mathrm{e}^{ha_3\langle S_0^{(3)}\rangle_{\beta,\vec{e}_3}}\, \mathrm{d}\vec{a} = \frac{\sinh(hm(\beta))}{hm(\beta)}.\end{aligned} \tag{5.15}$$

In the last identity we defined the spontaneous magnetisation $m(\beta)$ by

$$m(\beta) = \langle S_0^{(3)} \rangle_{\beta,\vec{e}_3}. \tag{5.16}$$

We have found the function $\Phi(\beta, h)$. Notice that it is equal to 1 when the spontaneous magnetisation is 0.

5.3. The spin-Laplace transform on the complete graph

We consider the complete graph with n vertices. The hamiltonian is

$$H_n = -\frac{1}{n}\sum_{x,y=1}^{n} \vec{S}_x \cdot \vec{S}_y = -\frac{1}{n}\vec{R}^2, \tag{5.17}$$

where $\vec{R}$ is the total spin operator discussed in Section A.4. In order to formulate the result about the spin-Laplace transform, let us introduce the function $\phi(s)$ for $s \in [0, \frac{1}{2}]$ by

$$\phi(s) = \beta s^2 - (\tfrac{1}{2} - s)\log(\tfrac{1}{2} - s) - (\tfrac{1}{2} + s)\log(\tfrac{1}{2} + s). \tag{5.18}$$

A few calculations show that $\phi(0) = \log 2$, $\phi(\frac{1}{2}) = \frac{\beta}{4}$, $\phi'(0) = 0$, $\phi'(\frac{1}{2}) = -\infty$, $\phi''(0) = 2\beta - 4$. Let $m(\beta) \in [0, \frac{1}{2}]$ be the maximiser of ϕ. It is positive if and only if $\beta > 2$.

THEOREM 5.3. *We have*

$$\lim_{n\to\infty} \langle\, \mathrm{e}^{\frac{h}{n}R^{(3)}} \,\rangle_{n,\beta} = \frac{\sinh(hm(\beta))}{hm(\beta)}.$$

PROOF. We suppose that n is even for simplicity. We use Proposition A.11.

$$\begin{aligned}\operatorname{Tr} \mathrm{e}^{\frac{h}{n} R^{(3)}} \, \mathrm{e}^{\frac{\beta}{n} \vec{R}^2} &= \sum_{j=0}^{n/2} \sum_{m=-j}^{j} \binom{n}{\frac{n}{2}+j} \frac{2j+1}{\frac{n}{2}+j+1} \, \mathrm{e}^{\frac{h}{n} m + \frac{\beta}{n} j(j+1)} \\ &= \sum_{j=0}^{n/2} \mathrm{e}^{n\phi_n(j)} \, q_{n,j}(h)\end{aligned} \tag{5.19}$$

where

$$\begin{aligned}\phi_n(j) &= \tfrac{1}{n} \log \binom{n}{\frac{n}{2}+j} + \tfrac{1}{n} \log \frac{(2j+1)^2}{\frac{n}{2}+j+1} + \frac{\beta}{n^2} j(j+1), \\ q_{n,j}(h) &= \frac{1}{2j+1} \sum_{m=-j}^{j} \mathrm{e}^{h \frac{m}{n}} \, .\end{aligned} \tag{5.20}$$

From Stirling formula we get

$$\phi_n(j) = \beta(\tfrac{j}{n})^2 - (\tfrac{1}{2} - \tfrac{j}{n}) \log(\tfrac{1}{2} - \tfrac{j}{n}) - (\tfrac{1}{2} + \tfrac{j}{n}) \log(\tfrac{1}{2} + \tfrac{j}{n}) + o(1). \tag{5.21}$$

By Laplace's principle the ratio concentrates on the maximiser of $\phi_n \approx \phi$. Then

$$\begin{aligned}\lim_{n\to\infty} \langle \, \mathrm{e}^{\frac{h}{n} R^{(3)}} \, \rangle_{n,\beta} &= \lim_{n\to\infty} \frac{\sum_{j=0}^{n/2} \mathrm{e}^{n\phi_n(j)} \, q_{n,j}(h)}{\sum_{j=0}^{n/2} \mathrm{e}^{n\phi_n(j)}} \\ &= \lim_{n\to\infty} \tfrac{1}{2m(\beta)n+1} \sum_{m=-m(\beta)n}^{m(\beta)n} \mathrm{e}^{\frac{h}{n} m} \\ &= \frac{1}{2m(\beta)} \int_{-m(\beta)}^{m(\beta)} \mathrm{e}^{hs} \, \mathrm{d}s = \frac{\sinh(hm(\beta))}{hm(\beta}.\end{aligned} \tag{5.22}$$

□

5.4. The spin-Laplace transform and Poisson-Dirichlet

We now discuss a third way to calculate the spin-Laplace transform. This assumes that the joint distribution of long loops is a Poisson-Dirichlet distribution. For the random interchange model on the complete graph it was conjectured by Aldous and subsequently proved by Schramm [2005]. Then Goldschmidt, Ueltschi, and Windridge [2011] suggested that Poisson-Dirichlet is also present in spatial model of dimensions three and more, and also that it is a generic feature of loop models. The conjecture has been verified numerically for various models.

We look at the vector formed by the lengths of the loops in decreasing order, divided by the volume of the system:

$$\Big(\frac{\ell(\gamma_1)}{|\Lambda|}, \frac{\ell(\gamma_2)}{|\Lambda|}, \dots, \frac{\ell(\gamma_k)}{|\Lambda|} \Big). \tag{5.23}$$

This is a partition of $[0,1]$ by construction. The conjecture is that, as $\Lambda \Uparrow \mathbb{Z}^d$, the mass of macroscopic loops takes a typical value, denoted $\eta(\beta)$, which is positive for β large (it is zero for β small, something that can be proved). Further, the joint distribution of the lengths of macroscopic loops is Poisson-Dirichlet of parameter 2. This is illustrated in Fig. 5.2.

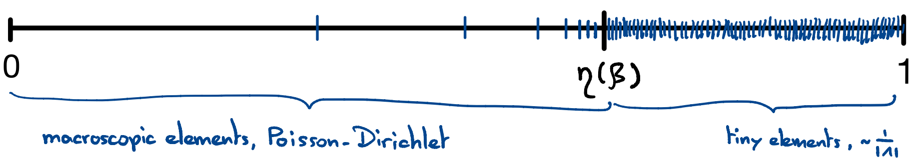

FIGURE 5.2. Expected partition formed by the lengths of the loops, divided by the volume. Macroscopic loops yield a Poisson-Dirichlet distribution. There is a density a small loops. The mass of long loops is related to spontaneous magnetisation.

The heuristics involves introducing a Glauber dynamics that leaves the loop measure invariant; when restricted to loop lengths, one can argue that it is an effective mean-field split-merge process, whose invariant measure is Poisson-Dirichlet. This is described in details in Ueltschi [2017].

We do not give a definition of the Poisson-Dirichlet distribution here. Rather we rely on this formula for the moments of Poisson-Dirichlet(θ), that first appeared in Nahum, Chalker, Serna, Ortuño, Somoza [2013]: For all ℓ and $n_1, \dots n_\ell \in \mathbb{N}$,

$$\mathbb{E}_{\mathrm{PD}(\theta)}\Big[\sum_{\substack{j_1,\dots,j_\ell\geq 1\\ \text{distinct}}} X_{j_1}^{n_1}\dots X_{j_\ell}^{n_\ell}\Big] = \frac{\theta^\ell \Gamma(\theta)\Gamma(n_1)\dots\Gamma(n_\ell)}{\Gamma(\theta+n_1+\dots+n_\ell)}. \tag{5.24}$$

Here $X_1, X_2, \dots$ denote the elements of the random partition. We use the formula below with $\theta = 2$.

We now compute the spin-Laplace transform. In the following equation, the first identity is Theorem 5.2 (c); the second identity is the Poisson-Dirichlet conjecture.

$$\Phi(\beta,h) = \mathbb{E}\Big[\prod_{\gamma\in\mathcal{L}(\omega)} \cosh\Big(\tfrac12 h \frac{\ell(\gamma)}{|\Lambda|}\Big)\Big] = \mathbb{E}_{\mathrm{PD}(2)}\Big[\prod_{i\geq 1}\cosh\big(\tfrac12 h\eta(\beta)X_i\big)\Big]. \tag{5.25}$$

The latter can be calculated explicitly using the moment formula (5.24). Expanding $\cosh(bX_i) = 1 + \sum_{k_i \geq 1} \frac{b^{2k_i} X_i^{2k_i}}{(2k_i)!}$, we get

$$\begin{aligned}\mathbb{E}_{\mathrm{PD}(2)}\Big[\prod_{i\geq 1} \cosh\big(bX_i\big)\Big] &= \mathbb{E}_{\mathrm{PD}(2)}\Big[\sum_{n\geq 0} \frac{1}{n!} \sum_{\substack{i_1,\dots,i_n\geq 1\\ \text{distinct}}} \sum_{k_1,\dots,k_n\geq 1} \frac{b^{2k_1+\dots+2k_n} X_{i_1}^{2k_1} \dots X_{i_n}^{2k_n}}{(2k_1)!\dots(2k_n)!}\Big] \\ &= \sum_{n\geq 0} \frac{1}{n!} \sum_{k_1,\dots,k_n\geq 1} \frac{b^{2k_1+\dots+2k_n}}{(2k_1)!\dots(2k_n)!} \frac{2^n (2k_1-1)!\dots(2k_n-1)!}{(2(k_1+\dots+k_n)+1)!} \\ &= \sum_{n\geq 0} \frac{1}{n!} \sum_{r\geq 1} \frac{b^{2r}}{(2r+1)!} \sum_{\substack{k_1,\dots,k_n\geq 1\\ k_1+\dots+k_n=r}} \frac{1}{k_1\dots k_n}.\end{aligned} \tag{5.26}$$

As can be verified using a generating function, we have the curious identity

$$\sum_{n\geq 0} \frac{1}{n!} \sum_{\substack{k_1,\dots,k_n\geq 1\\ k_1+\dots+k_n=r}} \frac{1}{k_1\dots k_n} = 1. \tag{5.27}$$

It follows that

$$\Phi(\beta,h) = \frac{1}{b} \sum_{r\geq 1} \frac{b^{2r+1}}{(2r+1)!} = \frac{\sinh b}{b}. \tag{5.28}$$

We have obtained the spin-Laplace transform, namely

$$\Phi(\beta,h) = \lim_{\Lambda\Uparrow\mathbb{Z}^d} \langle\, \mathrm{e}^{\frac{h}{|\Lambda|}\sum_x S_x^{(3)}} \,\rangle_{\Lambda,\beta} = \frac{\sinh(\frac{1}{2}h\eta(\beta))}{\frac{1}{2}h\eta(\beta)}. \tag{5.29}$$

This agrees with Eq. (5.15) with $m(\beta) = \frac{1}{2}\eta(\beta)$. This confirms the conjecture that the extremal states of the Heisenberg model are indexed by $\vec{a} \in \mathbb{S}^2$.

There is an $S = 1$ spin system that displays "nematic order" and whose extremal states were not immediate to guess. Indeed, they turn out to be "planar nematic" rather than "axis nematic". The Poisson-Dirichlet conjecture was key to understanding this; see Caci, Mühlbacher, Ueltschi, Wessel [2023] for more details.

APPENDIX A

Mathematical supplement

A.1. Hölder inequality for traces

PROPOSITION A.1 (**Hölder inequality for matrices**). *If* $1 \leq p, q, r \leq \infty$ *with* $\frac{1}{p} + \frac{1}{q} = \frac{1}{r}$, *we have*

$$\|ab\|_r \leq \|a\|_p \|b\|_q.$$

It follows from a simple induction that

$$\Big\| \prod_{j=1}^{n} a_j \Big\|_r \leq \prod_{j=1}^{n} \|a_j\|_{p_j} \tag{A.1}$$

whenever $1 \leq r, p_1, \dots, p_n$ with $\sum_{j=1}^{n} \frac{1}{p_j} = \frac{1}{r}$. The proof of Proposition A.1 can be found in the appendix.

There are no short proofs in the case of matrices. The proof here is due to Fröhlich [1978] and it uses chessboard estimates. The proof of Proposition A.1 can be found after that of Lemma A.4.

LEMMA A.2 (Chessboard estimate). *For any* $n \in \mathbb{N}$ *and any matrices* $a_1, \dots, a_{2n}$, *we have*

$$\big|\mathrm{Tr}\, a_1 \dots a_{2n}\big| \leq \prod_{i=1}^{2n} \Big(\mathrm{Tr}\, (a_i a_i^*)^n\Big)^{1/2n}.$$

PROOF. Since $(a, b) \mapsto \mathrm{Tr}\, a^* b$ is an inner product, we have the Cauchy–Schwarz inequality: $||trab|^2 \leq \mathrm{Tr}\, a^* a \mathrm{Tr}\, b^* b$. The following inequality follows:

$$\big|\mathrm{Tr}\, a_1 \dots a_{2n}\big|^2 \leq \mathrm{Tr}\, \big(a_1 \dots a_n a_n^* \dots a_1^*\big)\ \mathrm{Tr}\, \big(a_{2n}^* \dots a_{n+1}^* a_{n+1} \dots a_{2n}\big). \tag{A.2}$$

This allows to use a reflection positivity argument. By replacing a_i with $a_i / \sqrt{\mathrm{Tr}\, (a_i a_i^*)^n}$ it is enough to prove the inequality for matrices that satisfy $\mathrm{Tr}\, (a_i a_i^*)^n = 1$; the general result follows from scaling. Note that the set of such matrices is compact.

Let $a_1, \dots, a_{2n}$ be matrices that maximise $|\mathrm{Tr}\, a_1 \dots a_{2n}|$, with maximum number of matching neighbours $a_{i+1} = a_i^*$. Suppose there exists an index j such that $a_{j+1} \neq a_j^*$. Using cyclicity, we can assume that $j = n$. By the inequality (A.2), $a_1, \dots, a_n, a_n^*, \dots, a_1^*$ and $a_{2n}^*, \dots, a_{n+1}^*, a_{n+1}, \dots, a_{2n}$ are also maximisers.

At least one has strictly more matching neighbours, hence a contradiction. The maximum is then $\mathrm{Tr}\,(aa^*)^n$ for some matrix $a \in \{a_1, \dots, a_n\}$, which is equal to 1. $\square$

Chessboard estimates allow to prove what is essentially the case $r = 1$ of Hölder's inequality.

Corollary A.3. *We have*

$$|\mathrm{Tr}\, a_1 \dots a_n| \leq \prod_{i=1}^n \|a_i\|_{p_i}$$

for all n and all $p_i \geq 1$ such that $\sum_{i=1}^n \frac{1}{p_i} = 1$.

Proof. It suffices to consider rational p_i, by continuity. Let ℓ be a positive integer such that $2\ell/p_i$ is integer for all i. Let $a_i = U_i|a_i|$ be the polar decomposition of a_i, and let

$$b_i = |a_i|^{p_i/2\ell}, \qquad \hat{b}_i = U_i|a_i|^{p_i/2\ell}. \tag{A.3}$$

Then $a_i = \hat{b}_i b_i^{(2\ell/p_i)-1}$, and we have

$$\begin{aligned} \big|\mathrm{Tr}\, a_1 \dots a_n\big| &= \big|\mathrm{Tr}\, \hat{b}_1 \underbrace{b_1 \dots b_1}_{(2\ell/p_1)-1} \dots \hat{b}_n \underbrace{b_n \dots b_n}_{(2\ell/p_n)-1}\big| \\ &\leq \prod_{i=1}^n (\mathrm{Tr}\, |a_i|^{p_i})^{1/p_i} \qquad \text{(A.4)} \\ &= \prod_{i=1}^n \|a_i\|_{p_i}. \end{aligned}$$

The inequality follows from Lemma A.2 and from the identities

$$\mathrm{Tr}\, (b_i b_i^*)^\ell = \mathrm{Tr}\, (\hat{b}_i \hat{b}_i^*)^\ell = \mathrm{Tr}\, |a_i|^{p_i}. \tag{A.5}$$

$\square$

Lemma A.4. *Let $r, r' \in [1, \infty]$ such that $\frac{1}{r} + \frac{1}{r'} = 1$. Then for any square matrix a, we have*

$$\|a\|_r = \max_{\|c\|_{r'}=1} \mathrm{Tr}\, c^* a.$$

Proof. The right side is smaller by Corollary A.3:

$$\big|\mathrm{Tr}\, c^* a\big| \leq \|c\|_{r'} \|a\|_r = \|a\|_r. \tag{A.6}$$

In order to check that this inequality is saturated, let $a = U|a|$ be the polar decomposition of a, and choose $c = \|a\|_r^{1-r} U|a|^{r-1}$. Then $\|c\|_{r'} = 1$ and $\mathrm{Tr}\, c^* a = \|a\|_r$. $\square$

Proof of Proposition A.1. Starting with Lemma A.4 and then using Corollary A.3 with $a_1 = c^*$, $a_2 = a$, $a_3 = b$ and $p_1 = r$, $p_2 = p$, $p_3 = q$, we have

$$\begin{aligned} \|ab\|_r &= \sup_{\|c\|_{r'}=1} \operatorname{Tr} c^* ab \\ &\leq \sup_{\|c\|_{r'}=1} \|c\|_{r'} \|a\|_p \|b\|_q. \end{aligned} \tag{A.7}$$

□

A.2. Trotter and Duhamel

We now review a ueful expansion for the exponential of a sum of two non-commuting operators, namely the Duhamel formula.

Proposition A.5 (Lie–Trotter formula). *Let a, b be $n \times n$ matrices. Then*

$$\mathrm{e}^{a+b} = \lim_{N\to\infty} \Big(\mathrm{e}^{\frac{1}{N}a}\, \mathrm{e}^{\frac{1}{N}b} \Big)^N = \lim_{N\to\infty} \Big[\mathrm{e}^{\frac{1}{N}a} \big(1 + \tfrac{1}{N} b\big) \Big]^N.$$

Proof. We prove the second formula — the mild changes for the other formula are straightforward. Let K_N be the matrix such that

$$\mathrm{e}^{\frac{1}{N}a} \big(1 + \tfrac{1}{N} b\big) = 1 + \tfrac{1}{N}(a+b) + K_N. \tag{A.8}$$

It is clear that $\|K_N\| = O(\frac{1}{N^2})$. We have

$$\Big[\mathrm{e}^{\frac{1}{N}a} \big(1 + \tfrac{1}{N} b\big) \Big]^N = \Big(1 + \tfrac{1}{N}(a+b)\Big)^N + R_N, \tag{A.9}$$

where R_N is a matrix whose norm satisfies

$$\|R_N\| \leq \sum_{k=0}^{N-1} \binom{N}{k} \|1 + \tfrac{1}{N}(a+b)\|^k \, \|K_N\|^{N-k} = O(\tfrac{1}{N}). \tag{A.10}$$

The first term in the right side of (A.9) converges to e^{a+b}. □

Proposition A.6 (Duhamel formula). *Let a, b be $n \times n$ matrices. Then*

$$\begin{aligned} \mathrm{e}^{a+b} &= \mathrm{e}^{a} + \int_0^1 \mathrm{e}^{ta}\, b\, \mathrm{e}^{(1-t)(a+b)}\, \mathrm{d}t \\ &= \sum_{k\geq 0} \int_{0<t_1<\dots<t_k<1} \mathrm{d}t_1 \dots \mathrm{d}t_k\, \mathrm{e}^{t_1 a}\, b\, \mathrm{e}^{(t_2-t_1)a}\, b \dots b\, \mathrm{e}^{(1-t_k)a}. \end{aligned}$$

Proof. Let $F(s)$ be the matrix-valued function

$$F(s) = e^{sa} + \int_0^s e^{ta}\, b\, e^{(s-t)(a+b)}\, dt. \tag{A.11}$$

We show that, for all s,

$$e^{s(a+b)} = F(s). \tag{A.12}$$

The derivative of $F(s)$ is

$$F'(s) = e^{sa}\, a + e^{sa}\, b + \int_0^s e^{ta}\, b\, e^{(s-t)(a+b)}\, (a+b) dt = F(s)(a+b). \tag{A.13}$$

On the other hand, the derivative of $e^{s(a+b)}$ is $e^{s(a+b)}\,(a+b)$. The identity (A.12) clearly holds for $s=0$ and, since both sides satisfy the same differential equation, they must be equal for all s.

We can iterate Duhamel's formula N times so as to get

$$\begin{aligned} e^{a+b} &= \sum_{k=0}^{N} \int_{0<t_1<\dots<t_k<1} dt_1 \dots dt_k\, e^{t_1 a}\, b\, e^{(t_2-t_1)a}\, b \dots b\, e^{(1-t_k)a} \\ &+ \int_{0<t_1<\dots<t_N<1} dt_1 \dots dt_k\, e^{t_1 a}\, b\, e^{(t_2-t_1)a}\, b \dots b \Big[e^{(1-t_N)(a+b)} - e^{(1-t_N)a} \Big]. \end{aligned} \tag{A.14}$$

Using $\| e^{ta} \| \leq e^{t\|a\|}$, the last line is less than $2\, e^{\|a\|+\|b\|}\, \frac{\|b\|^N}{N!}$ and so it vanishes in the limit $N \to \infty$. The summand is less than $e^{\|a\|}\, \frac{\|b\|^k}{k!}$, so that the sum is absolutely convergent. □

A.3. Further matrix inequalities

Proposition A.7 (**Golden–Thompson inequality**). *Let a, b be hermitian matrices. Then*

$$\mathrm{Tr}\left(e^{a+b} \right) \leq \mathrm{Tr}\left(e^{a}\, e^{b} \right).$$

Proof. Hölder's inequality, in the form (A.1) with $r=1$, $p_j = n$ and $a_j = ab$, implies that $|\mathrm{Tr}\,(ab)^n| \leq \|ab\|_n^n$. The latter is equal to $\mathrm{Tr}\,(a^2b^2)^{n/2}$ since a, b are hermitian. Letting n be a power of 2, we can iterate and we get

$$\mathrm{Tr}\,(ab)^n \leq \mathrm{Tr}\, a^n b^n. \tag{A.15}$$

We use this inequality with $a \mapsto e^{\frac{1}{n}a}$ and $b \mapsto e^{\frac{1}{n}b}$, which gives

$$\mathrm{Tr}\left(e^{\frac{1}{n}a}\, e^{\frac{1}{n}b} \right)^n \leq \mathrm{Tr}\, e^{a}\, e^{b}. \tag{A.16}$$

The left side converges to $\mathrm{Tr}\, e^{a+b}$ as $n \to \infty$ by the Trotter formula (Proposition A.5). □

PROPOSITION A.8 (**Klein inequality**). *Let f be a convex differentiable function, and a, b be hermitian matrices with eigenvalues in the domain of f. Then*

$$\operatorname{Tr}\big[f(a) - f(b) - (a-b)f'(b)\big] \geq 0.$$

With $f(s) = \mathrm{e}^{s}$, exchanging a and b, we get

$$\operatorname{Tr}\big(\mathrm{e}^{a} - \mathrm{e}^{b}\big) \leq \operatorname{Tr}(a-b)\,\mathrm{e}^{a}. \tag{A.17}$$

PROOF. Let (ϕ_i) and (ψ_i) be orthonormal bases of eigenvectors of a and b, and let (α_i) and (β_i) the eigenvalues. Let $c_{ij} = \langle \phi_i, \psi_j \rangle$. Then

$$\begin{aligned}\big\langle \phi_i, \big[f(a) - f(b) - &(a-b)f'(b)\big]\phi_i \big\rangle \\ &= f(\alpha_i) - \sum_j |c_{ij}|^2 f(\beta_j) - \sum_j |c_{ij}|^2 (\alpha_i - \beta_j) f'(\beta_j) \\ &= \sum_j |c_{ij}|^2 \big[f(\alpha_i) - f(\beta_j) - (\alpha_i - \beta_j) f'(\beta_j)\big] \\ &\geq 0.\end{aligned} \tag{A.18}$$

□

PROPOSITION A.9 (**Peierls–Bogolubov inequality**). *Let f be convex on $\mathbb{R}$ and a, h be hermitian matrices such that $\operatorname{Tr}\mathrm{e}^{-h} = 1$. Then*

$$f\big(\operatorname{Tr} a\,\mathrm{e}^{-h}\big) \leq \operatorname{Tr} f(a)\,\mathrm{e}^{-h}.$$

PROOF. Let (ϕ_i) and (η_i) be the eigenvectors and eigenvalues of h. Using Jensen's inequality twice,

$$\begin{aligned} f\big(\operatorname{Tr} a\,\mathrm{e}^{-h}\big) &= f\Big(\sum_i \langle \phi_i, a\phi_i \rangle\,\mathrm{e}^{-\eta_i}\Big) \leq \sum_i f\big(\langle \phi_i, a\phi_i \rangle\big)\,\mathrm{e}^{-\eta_i} \\ &\leq \sum_i \langle \phi_i, f(a)\phi_i \rangle\,\mathrm{e}^{-\eta_i} = \operatorname{Tr} f(a)\,\mathrm{e}^{-h}. \end{aligned} \tag{A.19}$$

□

PROPOSITION A.10 (**Peierls inequality**). *Let a be a hermitian matrix and (ϕ_i) an orthonormal set of vectors. Then*

$$\sum_i \mathrm{e}^{\langle \phi_i, a\phi_i \rangle} \leq \operatorname{Tr}\mathrm{e}^{a}.$$

PROOF. Let α_j, ψ_j be the eigenvalues and eigenvectors of a. Then

$$\mathrm{e}^{\langle \phi_i, a\phi_i\rangle} = \exp\Big\{\sum_j \alpha_j |\langle \phi_i, \psi_j\rangle|^2\Big\} \leq \sum_j |\langle \phi_i, \psi_j\rangle|^2 \, \mathrm{e}^{\alpha_j} . \tag{A.20}$$

We used Jensen's inequality. The claim then follows by summing over i, using $\sum_i |\langle \phi_i, \psi_j\rangle|^2 \leq 1$ (Bessel inequality). ☐

A.4. Addition of spins

Let $\mathcal{H}_n = \otimes_{x=1}^n \mathbb{C}^2$ and $S_x^{(i)}$, $x \in \{1, \dots, n\}$, $i = 1, 2, 3$, be the usual spin operators. Let $R^{(i)}$ denote the total spin, namely

$$R^{(i)} = \sum_{x=1}^n S_x^{(i)}. \tag{A.21}$$

We also write $\vec{R}^2$ for the operator $(R^{(1)})^2 + (R^{(2)})^2 + (R^{(3)})^2$. Notice that $[\vec{R}^2, R^{(i)}] = 0$.

PROPOSITION A.11.

(a) *The set of eigenvalues of* $R^{(i)}$ *is* $\mathfrak{E}(R^{(i)}) = \{-\frac{n}{2}, -\frac{n}{2}+1, \dots, \frac{n}{2}\}$. *The multiplicity of* $m \in \mathfrak{E}(R^{(i)})$ *is* $\binom{n}{\frac{n}{2}+m}$.

(b) *The set of eigenvalues of* $\vec{R}^2$ *is*

$$\mathfrak{E}(\vec{R}^2) = \begin{cases} \{j(j+1) : j = 0, 1, \dots, \frac{n}{2}\} & \text{if } n \text{ is even,} \\ \{j(j+1) : j = \frac{1}{2}, \frac{3}{2}, \dots, \frac{n}{2}\} & \text{if } n \text{ is odd.} \end{cases}$$

(c) *Let* $\mathcal{H}_n^{(j)}$ *the eigensubspace for the eigenvalue* $j(j+1)$ *of* $\vec{R}^2$ *and* $\mathcal{H}_n^{(j,m)}$ *the eigensubspace where* $\vec{R}^2$ *has eigenvalue* $j(j+1)$ *and* $R^{(3)}$ *has eigenvalue* m. *Then for* $|m| \leq j$,

$$\tfrac{1}{2j+1} \dim \mathcal{H}_n^{(j)} = \dim \mathcal{H}_n^{(j,m)} = \binom{n}{\frac{n}{2}+j} \tfrac{2j+1}{\frac{n}{2}+j+1}.$$

PROOF. (a) is easy since $\mathcal{H}_n = \operatorname{span}\{(\sigma_x)_{x=1}^n, \sigma_x = \pm\frac{1}{2}\}$, and $R^{(3)}|(\sigma_x)\rangle = \sum_{x=1}^n \sigma_x |(\sigma_x)\rangle$. Notice that $\frac{n}{2} + m$ is the number of $-\frac{1}{2}$ in (σ_x).

For (b) we introduce $R^{(\pm)} = R^{(1)} \pm \mathrm{i} R^{(2)}$. One chan check that

$$[R^{(3)}, R^{(\pm)}] = \pm R^{(\pm)}, \qquad [R^{(+)}, R^{(-)}] = 2R^{(3)}, \tag{A.22}$$

and

$$R^{(\pm)} R^{(\mp)} = \pm R^{(\pm)} - (R^{(3)})^2 \pm R^{(3)}. \tag{A.23}$$

The left side is nonnegative, which implies that $|m| \leq j$. If $|m\rangle$ is eigenvector of $R^{(3)}$ with eigenvalue m, then

$$R^{(3)} R^{(\pm)} |m\rangle = (R^{(\pm)} R^{(3)} \pm R^{(\pm)}) |m\rangle = (m \pm 1) R^{(\pm)} |m\rangle. \tag{A.24}$$

Further, if $|m\rangle \in \mathcal{H}_n^{(j)}$, we have

$$\|R^{(\pm)}|m\rangle\|^2 = j(j+1) - m(m \pm 1). \tag{A.25}$$

Then $R^{(\pm)}|m\rangle$ is eigenvector of $R^{(3)}$ with eigenvalue $m \pm 1$, unless $m = \pm j$, in which case $R^{(\pm)}|m\rangle$ is zero. It follows that the eigenvalues of $R^{(3)}$ in the subspace $\mathcal{H}_n^{(j)}$ are $-j, -j+1, \ldots, j$. Combined with (a), this gives (b).

For (c), let $|j, m, \alpha\rangle$ denote the eigenvectors in $\mathcal{H}_n^{(j,m)}$ of eigenvalues $j(j+1)$ for $\vec{R}^2$ and m for $R^{(3)}$; the third index α runs from 1 to $\dim\mathcal{H}_n^{(j,m)}$. Since $[\vec{R}^2, R^{(\pm)}] = 0$, we have that $R^{(\pm)}|j, m, \alpha\rangle \in \mathcal{H}_n^{(j,m\pm1)}$. Invoking (A.24) we find that $R^{(\pm)}|j, m, \alpha\rangle$ is perpendicular $R^{(\pm)}|j, m, \alpha'\rangle$ when $\alpha \neq \alpha'$. It follows that $\dim\mathcal{H}_n^{(j,m)}$ depends on j but not on m. We have

$$\binom{n}{\frac{n}{2} + m} = \sum_{j=|m|}^{n/2} \dim\mathcal{H}_n^{(j)}. \tag{A.26}$$

Then $\dim\mathcal{H}_n^{(j)} = \binom{n}{\frac{n}{2}+j} - \binom{n}{\frac{n}{2}+j+1}$, which gives (c). $\square$

APPENDIX B

Solutions to some exercises

EXERCISE 1.3: The answer is yes. Notice that $F = F^* = F^{-1}$. In the representation given by Eq. (1.3) we have $FS_x^{(1)}F = S_x^{(1)}$, $FS_x^{(2)}F = -S_x^{(2)}$, and $FS_x^{(3)}F = -S_x^{(3)}$. Then $F = \mathrm{e}^{\mathrm{i}\pi \sum_x S_x^{(1)}}$. In the case of spin $S = \frac{1}{2}$ we also have $F = \prod_{x\in\Lambda} 2S_x^{(1)}$.

EXERCISE 1.4: Both bounds follow from Peierls inequality (Proposition A.10). Use a basis of eigenvectors of a for the lower bound, and a basis of eigenvectors of $a+b$ for the upper bound.

EXERCISE 4.2: Recall that

$$P_- e_{x_1,\dots,x_n} = \frac{1}{n!} \sum_{\sigma\in\mathfrak{S}_n} (-1)^\sigma e_{x_{\sigma(1)},\dots,x_{\sigma(n)}}.$$

We use the change of variables $\sigma \mapsto \sigma'$ where $\sigma' = \sigma \circ \tau_{i,j}$ with $\tau_{i,j}$ the transposition of i and j. The sum over σ can be replaced by a sum over σ'. We have $(-1)^\sigma = -(-1)^{\sigma'}$ and $e_{x_{\sigma(1)},\dots,x_{\sigma(n)}} = e_{x_{\sigma'(1)},\dots,x_{\sigma'(n)}}$. We obtain

$$P_- e_{x_1,\dots,x_n} = \frac{1}{n!} \sum_{\sigma'\in\mathfrak{S}_n} -(-1)^{\sigma'} e_{x_{\sigma'(1)},\dots,x_{\sigma'(n)}} = -P_- e_{x_1,\dots,x_n},$$

so that $P_- e_{x_1,\dots,x_n} = 0$.

EXERCISE 4.3: We have

$$\begin{aligned}\|P_+ e_{x_1,\dots,x_n}\|^2 = \langle P_+ e_{x_1,\dots,x_n} | P_+ e_{x_1,\dots,x_n}\rangle &= \frac{1}{n!} \sum_{\sigma\in\mathfrak{S}_n} \langle e_{x_{\sigma(1)},\dots,x_{\sigma(n)}} | e_{x_1,\dots,x_n}\rangle \\ &= \frac{1}{n!} \#\big\{\sigma \in \mathfrak{S}_n : (x_{\sigma(1)},\dots,x_{\sigma(n)}) = (x_1,\dots,x_n)\big\} = \frac{1}{n!} \prod_{x\in\Lambda} n_x!.\end{aligned}$$

The case of $P_- e_{x_1,\dots,x_n}$ is similar and actually simpler. Since all the sites x_i are distinct (otherwise the vector is 0 by the previous exercise), the permutation must be the identity.

EXERCISE 4.4: The cardinality of $\mathcal{N}_{\Lambda,n}^{(+)}$ is equal to the number of integer partitions with $|\Lambda|$ elements and total length n. Such partitions can be obtained by selecting $|\Lambda| - 1$ separations in the interval $\{1, 2, \dots, n + |\Lambda|\}$, so we get $\binom{n+|\Lambda|-1}{|\Lambda|-1}$.

The case of $\mathcal{N}_{\Lambda,n}$ is immediate.

EXERCISE 4.8: The first two parts are straightforward. For the third part, use that

$$\mathbb{E}\big((X_\ell-\rho_{\rm c})^2\big)=\mathbb{E}\big((X_\ell-\mathbb{E}(X_\ell))^2\big)+(\mathbb{E}(X_\ell^2)-\rho_{\rm c}^2), \tag{B.1}$$

where the second term goes to zero and the first term is the variance of X_ℓ. By properties of the variance of geometric random variables we get

$$\mathbb{E}\big((X_\ell-\mathbb{E}(X_\ell))^2\big)=\frac{1}{\ell^{2d}}\sum_{k\in\Lambda^*\setminus\{0\}}\frac{{\rm e}^{-\beta\varepsilon(k)}}{(1-{\rm e}^{-\beta\varepsilon(k)})}. \tag{B.2}$$

Here

$$\frac{1}{\ell^d}\sum_{k\in\Lambda^*\setminus\{0\}}\frac{{\rm e}^{-\beta\varepsilon(k)}}{(1-{\rm e}^{-\beta\varepsilon(k)})} \tag{B.3}$$

converges to a Riemann integral, so due to the additional factor $1/\ell^d$ in front, we see that $\mathbb{E}\big((X_\ell-\mathbb{E}(X_\ell))^2\big)\to 0$.

For the next part, Markov's inequality gives, for any $\delta>0$,

$$\mathbb{P}(X_\ell\le\rho_{\rm c}+\delta)\ge 1-\frac{\mathbb{E}[(X_\ell-\rho_{\rm c})^2]}{\delta^2}\to 1. \tag{B.4}$$

We have

$$\mathbb{E}[X_\ell\mid X_\ell\le\rho_{\rm c}+\delta]-\rho_{\rm c}=\frac{\mathbb{E}[X_\ell-\rho_{\rm c}]}{\mathbb{P}(X_\ell\le\rho_{\rm c}+\delta)}-\frac{\mathbb{E}[(X_\ell-\rho_{\rm c})1\!\!1\{X_\ell>\rho_{\rm c}+\delta\}]}{\mathbb{P}(X_\ell\le\rho_{\rm c}+\delta)}. \tag{B.5}$$

The first term goes to zero. The second term satisfies

$$\begin{aligned}0\le\frac{\mathbb{E}[(X_\ell-\rho_{\rm c})1\!\!1\{X_\ell>\rho_{\rm c}+\delta\}]}{\mathbb{P}(X_\ell\le\rho_{\rm c}+\delta)}&\le\frac{\mathbb{E}[(X_\ell-\rho_{\rm c})^2]^{1/2}\mathbb{P}(X_\ell>\rho_{\rm c}+\delta)^{1/2}}{\mathbb{P}(X_\ell\le\rho_{\rm c}+\delta)}\\ &\le\frac{\mathbb{E}[(X_\ell-\rho_{\rm c})^2]^{1/2}}{\mathbb{P}(X_\ell\le\rho_{\rm c}+\delta)}\to 0,\end{aligned} \tag{B.6}$$

by the Cauchy–Schwarz inequality. Thus $\mathbb{E}[X_\ell\mid X_\ell\le\rho]\to\rho_{\rm c}$ whenever $\rho>\rho_{\rm c}$.

The computation of $\Lambda(t)$ is similar to the convergence of the pressure (4.49): we get

$$\Lambda(t)=\begin{cases}\int_{[-\pi,\pi]^d}dk\ \log\frac{1-{\rm e}^{t-\beta\varepsilon(k)}}{1-{\rm e}^{-\beta\varepsilon(k)}}, & \text{if } t\le 0,\\ -\infty & \text{otherwise.}\end{cases} \tag{B.7}$$

The resulting formula for $\lim_{\ell\to\infty}-\frac{1}{\ell^d}\log\mathbb{P}(X_\ell\le x)$ is a version of Cramér's Theorem, see e.g. [**8**]. We then get for any $\rho\le\rho_{\rm c}$ and any $\delta>0$ that

$$\begin{aligned}\mathbb{E}[X_\ell\mid X_\ell\le\rho]\ge\mathbb{E}[X_\ell 1\!\!1\{X_\ell\ge\rho-\delta\}\mid X_\ell\le\rho]&\ge(\rho-\delta)\mathbb{P}(X_\ell\ge\rho-\delta\mid X_\ell\le\rho)\\ &=(\rho-\delta)(1-\mathbb{P}(X_\ell<\rho-\delta\mid X_\ell\le\rho))\\ &=(\rho-\delta)\Big(1-\frac{\mathbb{P}(X_\ell<\rho-\delta)}{\mathbb{P}(X_\ell\le\rho)}\Big)\\ &\ge(\rho-\delta)\Big(1-\frac{\mathbb{P}(X_\ell<\rho-\delta)}{\mathbb{P}(X_\ell<\rho-\delta/2)}\Big).\end{aligned} \tag{B.8}$$

Now

$$-\lim_{\ell\to\infty}\frac{1}{\ell^d}\log\frac{\mathbb{P}(X_\ell<\rho-\delta)}{\mathbb{P}(X_\ell<\rho-\delta/2)}=\Lambda^*(\rho-\delta)-\Lambda^*(\rho-\delta/2)>0, \tag{B.9}$$

the last inequality holding since $\Lambda^*(x)$ is strictly monotone for $x < \rho_c$. We conclude that

$$\frac{\mathbb{P}(X_\ell < \rho - \delta)}{\mathbb{P}(X_\ell < \rho - \delta/2)} \to 0. \tag{B.10}$$

Thus $\lim_{\ell\to\infty} \mathbb{E}[X_\ell \mid X_\ell \le \rho] \ge \rho - \delta$ whenever $\rho \le \rho_c$. Since $\delta > 0$ was arbitrary, $\lim_{\ell\to\infty} \mathbb{E}[X_\ell \mid X_\ell \le \rho] \ge \rho$ whenever $\rho \le \rho_c$.

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