Analysis of Heisenberg Ferromagnets

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1 Coupled Spin-S Particles

1.1 A single particle

Let $S \in \{n/2 \mid n = 1, 2, 3 \ldots\}$ be positive half-integer. The state of a single spin-S particle is represented by a normalised vector in the Hilbert space $\mathbb{C}^{2S+1}$. We define three Hermitian operators S^1, S^2 and S^3 on $\mathbb{C}^{2S+1}$ as follows. Over the natural orthonormal basis on $\mathbb{C}^{2S+1}$, the actions of $S^i, i = 1, 2, 3$ are given by the following matrices.

$$S^1 = \frac{\hbar}{2} \begin{pmatrix} 0 & \sqrt{2S} & 0 & \cdots & 0 & 0 & 0 \\ \sqrt{2S} & 0 & \sqrt{2(2S-1)} & \cdots & 0 & 0 & 0 \\ 0 & \sqrt{2(2S-1)} & 0 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & \sqrt{(2S-1)2} & 0 \\ 0 & 0 & 0 & \cdots & \sqrt{(2S-1)2} & 0 & \sqrt{2S} \\ 0 & 0 & 0 & \cdots & 0 & \sqrt{2S} & 0 \end{pmatrix}$$

$$S^2 = \frac{\hbar}{2} \begin{pmatrix} 0 & i\sqrt{2S} & 0 & \cdots & 0 & 0 & 0 \\ -i\sqrt{2S} & 0 & i\sqrt{2(2S-1)} & \cdots & 0 & 0 & 0 \\ 0 & -i\sqrt{2(2S-1)} & 0 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & i\sqrt{(2S-1)2} & 0 \\ 0 & 0 & 0 & \cdots & -i\sqrt{(2S-1)2} & 0 & i\sqrt{2S} \\ 0 & 0 & 0 & \cdots & 0 & -i\sqrt{2S} & 0 \end{pmatrix}$$

$$S^3 = \hbar \begin{pmatrix} -S & 0 & 0 & \cdots & 0 & 0 & 0 \\ 0 & -S+1 & 0 & \cdots & 0 & 0 & 0 \\ 0 & 0 & -S+2 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & S-2 & 0 & 0 \\ 0 & 0 & 0 & \cdots & 0 & S-1 & 0 \\ 0 & 0 & 0 & \cdots & 0 & 0 & S \end{pmatrix}$$

In the abstract theory of Lie algebras, the space $\mathbb{C}^{2S+1}$ carries an irreducible representation of $\mathfrak{sl}_2(\mathbb{C})$. The matrices above are the actions of the Pauli matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \quad \in \mathfrak{sl}_2(\mathbb{C})$$

respectively. The operator $\vec{S}^2 = (S^1)^2 + (S^2)^2 + (S^3)^2$ is diagonal and the $(m+1)$-th diagonal entry is $\hbar^2(S-m)^2 + \frac{\hbar^2}{2}((m+1)(2S-m) + m(2S-(m-1))) = \hbar^2 S(S+1)$ for all $0 \leq m \leq 2S$. In the following, we shall assume $\hbar = 1$.

1.2 Multiple particles

The states of a composite system consisting of L particles each of spin-S are described by elements in the tensor product

$$\mathbb{C}^{2S+1} \otimes \mathbb{C}^{2S+1} \otimes \mathbb{C}^{2S+1} \otimes \cdots \otimes \mathbb{C}^{2S+1}.$$

For $x = 1, 2, \ldots, L$ and $j = 1, 2, 3$, let $S_x^j = \mathrm{id} \otimes \cdots \otimes S^j \otimes \cdots \otimes \mathrm{id}$ be the operator acting on the x-th component by S^j.

Define the total angular momentum operators to be

$$S_{tot}^j = \sum_{x \in V} S_x^j, \quad j = 1, 2, 3. \tag{1.1}$$

The number operator n_x is defined to be $n_x = S_x^3 + S$. For a state vector $|m_1, m_2, \ldots, m_L\rangle$ satisfying

$$S_x^3 |m_1, m_2, \ldots, m_L\rangle = m_x |m_1, m_2, \ldots, m_L\rangle,$$

we can think of it as a state having $m_x + S \geq 0$ many particles at the site $x = 1, 2, \ldots, L$. Define the so-called ladder (raising and lowering) operators to be

$$\vec{S}_{tot}^{\pm} = S_{tot}^1 \pm i S_{tot}^2. \tag{1.2}$$

The triple of operators $\{S_{tot}^1, S_{tot}^2, S_{tot}^3\}$ gives a representation of $\mathfrak{sl}_2(\mathbb{C})$ on the space $\bigotimes_{x \in V} \mathbb{C}^{2S+1}$, although this representation is not irreducible in general. By standard facts on semisimple Lie algebras, we can decompose the representation $\bigotimes_{x \in V} \mathbb{C}^{2S+1}$ into a direct sum of irreducible representations of $\mathfrak{sl}_2(\mathbb{C})$ as follows.

$$\begin{aligned} \bigotimes_{x \in V} \mathbb{C}^{2S+1} =& \mathbb{C}^{2SL+1} \oplus \mathbb{C}^{2(SL-1)+1} \oplus \cdots \oplus \mathbb{C}^{2(SL-1)+1} \\ & \oplus \mathbb{C}^{2(SL-2)+1} \oplus \cdots \oplus \mathbb{C}^{2(SL-2)+1} \\ & \oplus \mathbb{C}^{2(SL-3)+1} \oplus \cdots \oplus \mathbb{C}^{2(SL-3)+1} \\ & \oplus \cdots \\ & \oplus \mathbb{C}^{2(SL-\lfloor SL \rfloor)+1} \oplus \cdots \oplus \mathbb{C}^{2(SL-\lfloor SL \rfloor)+1}. \end{aligned} \tag{1.3}$$

On each component $\mathbb{C}^{2(SL-n)+1}$ of (1.3), the Casimir operator $(\vec{S}_{tot})^2$ acts as a scalar $(SL-n)(SL-n+1)$. Let us define an operator T which acts on each component $\mathbb{C}^{2(SL-n)+1}$ as the scalar $SL-n$ so that $(\vec{S}_{tot})^2 = T(T+1)$. The integer n is the

'minimal number of particles' for the states in $\mathbb{C}^{2(SL-n)+1}$, i.e. the smallest eigenvalue of the operator $\sum_x n_x$ is n when restricted onto the subspace $\mathbb{C}^{2(SL-n)+1}$. Generally, the number of irreducible representations in the direct sum

$$\mathbb{C}^{2SL+1} \oplus \cdots \oplus \mathbb{C}^{2(SL-n)+1}, \quad 0 \leq n \leq \lfloor SL \rfloor, \tag{1.4}$$

i.e. the direct sum of the eigenspaces of T corresponding to eigenvalues $\leq n$, is equal to the number of ways to distribute n identical particles into L distinct bins *subject to the condition that each bin contains* $\leq 2S$ *particles*. When $n \leq 2S$, this number is $\binom{L+n-1}{n}$.

1.3 Two coupled particles

Consider a quantum system consisting of two spin-S particles, or more generally a spin-J_1 particle and a spin-J_2 particle. Let the system's Hamiltonian be given by

$$H = -\vec{S}_1 \cdot \vec{S}_2 = -\sum_{j=1}^{3} S_1^j S_2^j.$$

To be precise, the symbol $S_1^j S_2^j$ is the shorthand for the operator $S_1^j \circ S_2^j = (S^j \otimes \mathrm{id}) \circ (\mathrm{id} \otimes S^j) = S^j \otimes S^j$.

Recall the ladder operators are defined as

$$S_k^{\pm} := S_k^1 \pm i S_k^2, \quad k = 1, 2$$

By a simple manipulation, we can recast H as

$$H = \frac{1}{2}(S_1^+ S_2^- + S_1^- S_2^+) + S_1^3 S_2^3.$$

For $|\psi\rangle = |m_1, m_2\rangle$,

$$\langle \psi | S_1^+ S_2^- + S_1^- S_2^+ | \psi \rangle = 0$$

since $|m_1\rangle \otimes |m_2\rangle$ is orthogonal to both $|m_1 - 1\rangle \otimes |m_2 + 1\rangle$ and $|m_1 + 1\rangle \otimes |m_2 - 1\rangle$. Hence, we deduce that

$$\langle m_1, m_2 | H | m_1, m_2 \rangle = -\langle m_1, m_2 | S_1^3 S_2^3 | m_1, m_2 \rangle = -m_1 m_2$$

We claim that the state

$$|\Omega\rangle := |-J_1\rangle \otimes |-J_2\rangle$$

is the ground state of H with energy $-J_1 J_2$. Indeed, since $S_j^- |-J_j\rangle = 0$ for $j = 1, 2$, we see that

$$\frac{1}{2}(S_1^+ S_2^- + S_1^- S_2^+)|\Omega\rangle = 0.$$

Thus

$$H|\Omega\rangle = -S_1^3 \otimes S_2^3 |J_1\rangle \otimes |J_2\rangle = -S_1^3 |J_1\rangle \otimes S_2^3 |J_2\rangle = -J_1 J_2 |\Omega\rangle.$$

Next, for $|\psi\rangle = |m_1\rangle \otimes |m_2\rangle$, the previous results indicate that

$$\langle \psi | H | \psi \rangle = -m_1 m_2 \geq -J_1 J_2.$$

The proof is complete by the variational principle.

2 Heisenberg Model on a Graph

From now on, we fix a non-trivial finite simple graph $G = (V, E)$ with $V = (1, 2, \ldots, L)$. Consider a quantum system made up of a spin-S particle on each vertex with nearest-neighbour interaction whose Hamiltonian is given by

$$H = \sum_{\{x,y\}\in E} S^2 - \vec{S}_x \cdot \vec{S}_y. \tag{2.1}$$

The sum is taken over all edges $\{x, y\} \in E$ of the graph G. We shall write $x \sim y$ to denote $\{x, y\} \in E$.

Clearly, H is positive semi-definite.

2.1 The SU_2 symmetry

For $x, y \in V$ and $j = 1, 2, 3$, we have

$$\begin{aligned}&[\vec{S}_x \cdot \vec{S}_y, S_x^j + S_y^j]\\ =&[S_x^1 S_y^1 + S_x^2 S_y^2 + S_x^3 S_y^3, S_x^j + S_y^j]\\ =&0.\end{aligned}$$

It follows that

$$[H, S_{tot}^j] = 0, \qquad [H, \left(\vec{S}_{tot}\right)^2] = 0. \tag{2.2}$$

Indeed, since the Hamiltonian is rotation-invariant, we expect it to commute the with the infinitesimal generators S_{tot}^j of rotations along the three axis.

The relation (2.2) indicates that H acts as a scalar on each of the irreducible components $\mathbb{C}^{2(SL-n)+1}$ in the decomposition (1.3). In particular, all the ground states of H lie in the unique $\mathbb{C}^{2SL+1}$ component in (1.3) and thus the ground state is $(2SL+1)$-fold degerate.

Remark. In general, for fixed n, the eigenvalues of H may differ among the isomorphic copies of irreducible components $\mathbb{C}^{2(SL-n)+1}$ in (1.3). This can be seen for example in Section 4.2.

3 The formalism of second quantisation

3.1 Preliminaries

Let $\mathcal{H}$ be a separable Hilbert space. We use the following notation for tensor products.

$$\mathcal{H}^n = \underbrace{\mathcal{H} \otimes \cdots \otimes \mathcal{H}}_{n\text{-times}}. \tag{3.1}$$

On $\mathcal{H}^n$, we can define the symmetriser and antisymmetriser as a linear operator as follows. Let $\nu = \pm 1$. On the pure tensors $u_1 \otimes \cdots \otimes u_n \in \mathcal{H}^n$, put

$$S_\nu(u_1 \otimes \cdots \otimes u_n) := \frac{1}{N!} \sum_{\sigma\in\mathcal{S}_n} \nu^\sigma u_{\sigma(1)} \otimes \cdots \otimes u_{\sigma(n)},$$

where $\nu^\sigma := 1$ if $\nu = +1$ or the signature of σ is 1 and $\nu^\sigma := -1$ if $\nu = -1$ and the signature of σ is -1. Extend S_ν by linearity and density onto all of $\mathcal{H}^n$. We shall denote $S_\nu(u_1 \otimes \cdots \otimes u_n)$ by $(u_1 \otimes \cdots \otimes u_n)_\nu$. The operators S_ν satisfy the following properties.

$$S_\nu \circ S_\nu = S_\nu = S_\nu^\dagger, \quad S_{+1}S_{-1} = 0. \tag{3.2}$$

Let $(\mathcal{H}^n)_\nu$ be the image $S_\nu(\mathcal{H}^n)$. Since S_ν is a continuous projection map, the subspace $(\mathcal{H}^n)_\nu$ is closed. The inner product between two (anti)-symmetrised elements $(u_1 \otimes \cdots \otimes u_n)_\nu$ and $(v_1 \otimes \cdots \otimes v_n)_\nu$ are given as follows.

$$\begin{aligned}
&\langle (u_1 \otimes \cdots \otimes u_n)_\nu, (v_1 \otimes \cdots \otimes v_n)_\nu \rangle \\
=&\langle S_\nu(u_1 \otimes \cdots \otimes u_n), S_\nu(v_1 \otimes \cdots \otimes v_n) \rangle \\
=&\big\langle u_1 \otimes \cdots \otimes u_n, S_\nu^\dagger S_\nu(v_1 \otimes \cdots \otimes v_n) \big\rangle \\
=&\langle u_1 \otimes \cdots \otimes u_n, S_\nu S_\nu(v_1 \otimes \cdots \otimes v_n) \rangle \\
=&\langle u_1 \otimes \cdots \otimes u_n, S_\nu(v_1 \otimes \cdots \otimes v_n) \rangle \\
=&\frac{1}{N!} \sum_{\sigma \in \mathcal{S}_n} \nu^\sigma \big\langle u_1 \otimes \cdots \otimes u_n, v_{\sigma(1)} \otimes \cdots \otimes v_{\sigma(n)} \big) \big\rangle \\
=&\frac{1}{N!} \sum_{\sigma \in \mathcal{S}_n} \nu^\sigma \prod_{i=1}^n \big\langle u_i, v_{\sigma(i)} \big\rangle \\
\Big(=&\frac{1}{N!} \det(\langle u_i, v_j \rangle_{i,j}) \qquad \text{if } \nu = -1 \Big).
\end{aligned} \tag{3.3}$$

A similar calculation shows that

$$(\mathcal{H}^n)_{+1} \perp (\mathcal{H}^n)_{-1} \quad \text{as orthogonal subspaces in } \mathcal{H}^n.$$

Note that

$$(\mathcal{H}^n)_{+1} \oplus (\mathcal{H}^n)_{-1} \subsetneq \mathcal{H}^n$$

in general. For finite dimensional $\mathcal{H}$, we have $\dim(\mathcal{H}^n)_{+1} = \binom{n-1+\dim(\mathcal{H})}{n}$, which is the number of ways to distribute n identical objects into $\dim(\mathcal{H})$ distinct bins, with no restrictiong on the number of objects in each bin, whereas $\dim(\mathcal{H}^n)_{-1} = \binom{\dim(\mathcal{H})}{n}$ is the number of ways to distribute n identical objects into $\dim(\mathcal{H})$ distinct bins under the constraint that each bin contains at most one object.

3.2 Fock space

Given a separable Hilbert space $\mathcal{H}$, we define the *Fock space* $\mathcal{F}_\nu(\mathcal{H}), \nu = \pm 1$ as the following Hilbert space.

$$\mathcal{F}_\nu(\mathcal{H}) = \mathcal{H}^0 \oplus \mathcal{H}^1 \oplus \mathcal{H}_\nu^2 \oplus \mathcal{H}_\nu^3 \oplus \cdots \oplus \mathcal{H}_\nu^n \oplus \cdots .$$

A complex number of norm one in $\mathcal{H}^0$ is defined as the *vacuum state*, denoted $|\Omega\rangle$.

3.3 Creation and annihilation operators

For each $\psi \in \mathcal{H}$, define the *annihilation operator*, or simply the *annihilator*, of ψ as the linear operator $a(\psi)$ on $\mathcal{F}_\nu(\mathcal{H})$ satisfying

$$a(\psi)(\phi_1 \otimes \phi_2 \otimes \cdots \otimes \phi_n)_\nu = \frac{1}{\sqrt{n}} \sum_{i=1}^{n} \nu^{i-1} \langle \psi, \phi_i \rangle (\phi_1 \otimes \cdots \otimes \widehat{\phi_i} \otimes \cdots \otimes \phi_n)_\nu \quad (3.4)$$

for all $n \geq 1$ and all elements $(\phi_1 \otimes \phi_2 \otimes \cdots \otimes \phi_n)_\nu \in \mathcal{H}_\nu^n$ and

$$a(\psi) = 0 \qquad \text{on } \mathcal{H}^0 \subset \mathcal{F}_\nu(\mathcal{H}).$$

We also define the *creation operator*, or simply the *creator*, of ψ as the Hermitian conjugate $a^\dagger(\psi)$ of $a(\psi)$. One can check directly that $a^\dagger(\psi)$ satisfies

$$a^\dagger(\psi)(\phi_1 \otimes \phi_2 \otimes \cdots \otimes \phi_n)_\nu = \sqrt{n+1}(\psi \otimes \phi_1 \otimes \phi_2 \otimes \cdots \otimes \phi_n)_\nu. \quad (3.5)$$

The creation and annihilation operators satisfy the following commutation relations. For arbitrary $\psi, \phi \in \mathcal{H}$ and for $\nu = +1$, we have

$$[a(\psi), a^\dagger(\phi)] = \langle \psi, \phi \rangle \quad \text{and} \quad [a^\dagger(\psi), a^\dagger(\psi)] = [a(\psi), a(\psi)] = 0. \quad (3.6)$$

For $\nu = -1$, we have

$$\{a(\psi), a^\dagger(\phi)\} = \langle \psi, \phi \rangle \quad \text{and} \quad \{a^\dagger(\psi), a^\dagger(\psi)\} = \{a(\psi), a(\psi)\} = 0. \quad (3.7)$$

Lastly, we define the *number operator* of ψ by

$$n(\psi) := a^\dagger(\phi)a(\phi). \quad (3.8)$$

3.4 Occupation numbers

For a fixed Hilbert basis $\{\psi_1, \psi_2, \ldots\}$ of $\mathcal{H}$, and nonnegative integers n_i and N satisfying $\sum_i n_i = N$, define

$$|n_1, n_2, \ldots, n_r, \ldots\rangle := \begin{cases} \frac{\sqrt{N!}}{\sqrt{n_1! n_2! \cdots n_r! \cdots}} (\psi_{i_1} \otimes \psi_{i_2} \otimes \cdots \otimes \psi_{i_N})_{+1} & \text{if } \nu = +1 \\ \sqrt{N!}(\psi_{i_1} \otimes \psi_{i_2} \otimes \cdots \otimes \psi_{i_N})_{-1} & \text{if } \nu = -1 \end{cases} \quad (3.9)$$

where $\#\{j \mid i_j = r\} = n_r$. A direct computation using (3.3) shows that the vectors $\{|n_1, n_2, \ldots, n_i, \ldots\rangle \mid n_i \geq 0\}$ form a Hilbert basis of $\mathcal{F}_\nu(\mathcal{H})$.[1] The state vectors expressed over this basis is usually referred to as the *occupation number representation*. The integers $n_1, n_2, \ldots, n_r, \ldots$ are called the *occupation numbers*. They indicate that there are n_r particles in the state ψ_r.

With the fixed Hilbert basis as above, put $a_i^\dagger = a^\dagger(\psi_i)$ and $a_i = a(\psi_i)$. The commutation relations in (3.6) and (3.7) becomes

$$\begin{aligned} [a_i, a_j^\dagger] = \delta_{i,j} \quad \text{and} \quad [a_i^\dagger, a_i^\dagger] = [a_i, a_i] = 0, \quad \nu = +1; \\ \{a_i, a_j^\dagger\} = \delta_{i,j} \quad \text{and} \quad \{a_i^\dagger, a_i^\dagger\} = \{a_i, a_i\} = 0, \quad \nu = -1. \end{aligned} \quad (3.10)$$

[1] For any $r \geq 1$, we can permute, up to a sign change, the $\psi_{i_1}, \psi_{i_2}, \psi_{i_3}, \ldots$ in such a way that all the ψ_r's occupy the first n_r slots. Then it is easy to see that when two states have different values of n_r's the inner product between them is zero.

With respect to the Hilbert basis $\{\psi_1, \psi_2, \ldots\}$ given above, a general wave function of N particles can be written as a linear combinations of the vacuum state excited by N creation operators of the form $a_i^\dagger = a^\dagger(\psi_i)$:

$$|\Psi\rangle = \frac{1}{\sqrt{N!}} \sum_{x_1, x_2, \ldots, x_N} \Psi(x_1, \ldots, x_N) a_{x_1}^\dagger \cdots a_{x_N}^\dagger |\Omega\rangle \tag{3.11}$$

where Ψ is a $\mathbb{C}$ valued function on the set $\{1, 2, \ldots, r, \ldots\}^N$. By (3.5), we have

$$a_{x_1}^\dagger \cdots a_{x_N}^\dagger |\Omega\rangle = \sqrt{N!}\big(\psi_{x_1} \otimes \psi_{x_2} \otimes \cdots \otimes \psi_{x_N}\big)_\nu.$$

It follows from (3.9) that (3.11) can be equivalently written as

$$\begin{aligned}
|\psi\rangle &= \sum_{x_1, x_2, \ldots, x_N \in I} \Psi(x_1, \ldots, x_N)\big(\psi_{x_1} \otimes \psi_{x_2} \otimes \cdots \otimes \psi_{x_N}\big)_\nu \\
&= \sum_{x_1, x_2, \ldots, x_N \in I} \Psi(x_1, \ldots, x_N) \frac{\sqrt{n_1! n_2! \cdots n_r! \cdots}}{\sqrt{N!}} |n_1, n_2, \ldots, n_r, \cdots\rangle \\
&\qquad\qquad \text{where } n_r = |\{i \mid x_i = r\}| \\
&= \sum_{n_1 + \cdots + n_r + \cdots = N} \frac{\sqrt{n_1! n_2! \cdots n_r! \cdots}}{\sqrt{N!}} \sum_{|\{x_i = r\}| = n_r} \psi(x_1, \ldots, x_N) |n_1, n_2, \ldots, n_r, \cdots\rangle .
\end{aligned} \tag{3.12}$$

3.5 One-body operators

A particular type of linear operators on the Fock space $\mathcal{F}_\nu(\mathcal{H})$ is the so-called one-body operators. They are defined as follows. Suppose A is a linear operator on $\mathcal{H}$. For each $n \geq 1$ and $1 \leq i \leq n$, let

$$A_n = \sum_{i=1}^{n} \underbrace{\mathrm{id} \otimes \cdots \otimes \mathrm{id}}_{i-1 \text{ times}} \otimes A \otimes \underbrace{\mathrm{id} \otimes \cdots \otimes \mathrm{id}}_{n-i \text{ times}} : \mathcal{H}^{\otimes n} \to \mathcal{H}^{\otimes n}.$$

For $(u_1 \otimes \cdots \otimes u_n)_\nu$, we have

$$\begin{aligned}
A_n(u_1 \otimes \cdots \otimes u_n)_\nu &= \frac{1}{N!} \sum_j \sum_{\sigma \in \mathcal{S}_n} \nu^\sigma u_{\sigma(1)} \otimes \cdots \otimes A u_{\sigma(j)} \otimes \cdots \otimes u_{\sigma(n)} \\
&= \frac{1}{N!} \sum_j \sum_{\sigma \in \mathcal{S}_n} \nu^\sigma u_{\sigma(1)} \otimes \cdots \otimes A u_j \otimes \cdots \otimes u_{\sigma(n)} \\
&= \sum_j (u_1 \otimes \cdots \otimes A u_j \otimes \cdots \otimes u_n)_\nu.
\end{aligned}$$

Thus, A_n preserves the subspaces $\mathcal{H}_\nu^n$ for $\nu = \pm 1$. With the convention $A_0 = \mathrm{id} : \mathbb{C} \to \mathbb{C}$, we can define

$$\bigoplus_{n=0}^{\infty} A_n : \quad \mathcal{F}_\nu(\mathcal{H}) \to \mathcal{F}_\nu(\mathcal{H}).$$

For convenience, the above operator will still be denoted by A. The operators on $\mathcal{F}_\nu(\mathcal{H})$ arising in this manner will be called *one-body operators*.

Example 3.1. The number operator $n(\psi) = a^\dagger(\psi)a_x(\psi)$ associated with ψ is a one-body operator whereas the composed number operator $n(\psi)n(\phi)$ is not a one-body operator, regardless of whether $\psi = \phi$ or not. In fact, the one-body operator on $\mathcal{F}_\nu(\mathcal{H})$ arising from restriction of $n(\psi)n(\phi)$ on $\mathcal{H}^1$ does not agree with $n(\psi)n(\phi)$.

We can represent a one-body operator A with the aid of creation and annihilation operators defined earlier in (3.4) and (3.5). In fact, for any Hilbert basis ϕ_i of $\mathcal{H}$, a direct calculation yields

$$A = \sum_i a^\dagger(A\phi_i)a(\phi_i)$$

as operators on $\mathcal{F}_\nu(\mathcal{H})$. By expressing $A\phi_i$ as $\sum_j \langle \phi_j, A\phi_i\rangle \phi_j$ and using the linearity of $a^\dagger(\cdot)$, we can further infer that

$$A = \sum_{i,j} A_{j,i} a^\dagger(\phi_j)a(\phi_i) \tag{3.13}$$

where $A_{j,i} := \langle \phi_j, A\phi_i\rangle$. If we choose ϕ_i as a orthonormal set of eigenvectors of A with $A\phi_i = \lambda_i\phi_i$, then

$$A = \sum_i \lambda_i a^\dagger(\phi_i)a(\phi_i) = \sum_i \lambda_i n(\phi_i). \tag{3.14}$$

3.6 Thermodynamic quantities

For an isolated quantum system in thermal equilibrium with a heat bath, the *partition function* of the system is defined to be

$$\mathcal{Z} = \operatorname{tr}(e^{-\beta H}) \tag{3.15}$$

where H is the Hermitian operator on a Hilbert space representing the Hamiltonian of the system and β is a quantity proportional to the inverse of temperature. The *free energy* of the system is defined to be

$$F = -\frac{1}{\beta}\ln \operatorname{tr}(e^{-\beta H}). \tag{3.16}$$

Let $\Gamma = \frac{e^{-\beta H}}{\operatorname{tr}(e^{-\beta H})}$. Then the average value of the obervable A on the system will be

$$\operatorname{tr}(A\Gamma).$$

We shall use Fock spaces to describe systems of variable number of bosons and fermions. In this formalism, we can calculate the above thermodynamic quantities quite explicitly.

Let $\{|\psi_i\rangle\}_{i=1,2,3,\ldots}$ be orthonormal set of the energy eigenstates of H in the space $\mathcal{H}$ of single particles with $H|\psi_i\rangle = \epsilon_i|\psi_i\rangle$ with $\epsilon_i \in \mathbb{R}$. [2] To calculate the partition function, we take the trace of $e^{-\beta H}$ over the whole of the Fock space $\mathcal{F} = \mathcal{F}_\nu(\mathcal{H})$. The energy eigenstates of H in $\mathcal{F}$ are given in occupation number representations as

[2] We may assume all ϵ_i are non-negative, for, if not, we can replace H by $H + \lambda I$ where $\lambda < 0$ is the ground state energy. The partition function will include an additional factor of $e^{-\beta\lambda}$.

$|n_1, n_2, \ldots\rangle$ such that $H\,|n_1, n_2, \ldots\rangle = \sum_i n_i \epsilon_i\,|n_1, n_2, \ldots\rangle$. It follows that, for $\nu = +1$, we have

$$\begin{aligned}\mathrm{tr}(e^{-\beta H}) &= \sum_{n_1, n_2, \ldots \geq 0} e^{-\beta(n_1\epsilon_1 + n_2\epsilon_2 + \cdots)} \\ &= \prod_i \sum_{n_i \geq 0} e^{-\beta n_i \epsilon_i} \\ &= \prod_i \frac{1}{1 - e^{-\beta\epsilon_i}}\end{aligned} \tag{3.17}$$

and, in the case where $\nu = -1$, we have

$$\begin{aligned}\mathrm{tr}(e^{-\beta H}) &= \sum_{0 \leq n_1, n_2, \ldots \leq 1} e^{-\beta(n_1\epsilon_1 + n_2\epsilon_2 + \cdots)} \\ &= \prod_i (1 + e^{-\beta\epsilon_i}).\end{aligned} \tag{3.18}$$

The free energies for the two cases of ν follow directly from the above results.

$$F = \begin{cases} \frac{1}{\beta}\sum_i \ln(1 - e^{-\beta\epsilon_i}) & \nu = +1 \\ -\frac{1}{\beta}\sum_i \ln(1 + e^{-\beta\epsilon_i}) & \nu = -1. \end{cases} \tag{3.19}$$

With the identity $\frac{e^x}{(1-e^{-x})^2} = \sum_n n e^{-nx}$ for positive x, the average number of particles $\langle n_i \rangle$ in the eigenstate $|\psi_i\rangle$ can be readily computed as follows. For $\nu = +1$, we have

$$\begin{aligned}\mathrm{tr}_{\mathcal{F}}(a_i^\dagger a_i \Gamma) &= \frac{1}{\mathcal{Z}} \sum_{n_1, n_2, \ldots \geq 0} e^{-\beta(n_1\epsilon_1 + n_2\epsilon_2 + \cdots)}\,\langle n_1, n_2, \ldots|\, a_i^\dagger a_i\,|n_1, n_2, \ldots\rangle \\ &= \frac{1}{\mathcal{Z}} \sum_{n_1, n_2, \ldots \geq 0} n_i e^{-\beta(n_1\epsilon_1 + n_2\epsilon_2 + \cdots)} \\ &= \frac{1}{\mathcal{Z}} \frac{e^{-\beta\epsilon_i}}{(1 - e^{-\beta\epsilon_i})^2} \prod_{j \neq i} \frac{1}{(1 - e^{-\beta\epsilon_j})} \\ &= \frac{e^{-\beta\epsilon_i}}{1 - e^{-\beta\epsilon_i}} \\ &= \frac{1}{e^{\beta\epsilon_i} - 1}.\end{aligned} \tag{3.20}$$

For $\nu = -1$, we have

$$\begin{aligned}\mathrm{tr}_{\mathcal{F}}(a_i^\dagger a_i \Gamma) &= \frac{1}{\mathcal{Z}} \sum_{0 \leq n_1, n_2, \ldots \leq 1} e^{-\beta(n_1\epsilon_1 + n_2\epsilon_2 + \cdots)}\,\langle n_1, n_2, \ldots|\, a_i^\dagger a_i\,|n_1, n_2, \ldots\rangle \\ &= \frac{1}{\mathcal{Z}} \sum_{0 \leq n_1, n_2, \ldots \leq 1} n_i e^{-\beta(n_1\epsilon_1 + n_2\epsilon_2 + \cdots)} \\ &= \frac{1}{\mathcal{Z}} e^{-\beta\epsilon_i} \prod_{j \neq i} (1 + e^{-\beta\epsilon_j}) \\ &= \frac{e^{-\beta\epsilon_i}}{1 + e^{-\beta\epsilon_i}} \\ &= \frac{1}{e^{\beta\epsilon_i} + 1}.\end{aligned} \tag{3.21}$$

Lastly, we can compute in general the average value of any one-body observable, or any one-body linear operator A, by making use of (3.13).

$$\begin{aligned}
\mathrm{tr}_{\mathcal{F}}(A\Gamma) &= \frac{1}{\mathcal{Z}} \sum_{n_1,n_2,\ldots\geq 0} e^{-\beta(n_1\epsilon_1+n_2\epsilon_2+\cdots)} \langle n_1, n_2, \ldots | A | n_1, n_2, \ldots \rangle \\
&= \frac{1}{\mathcal{Z}} \sum_{n_1,n_2,\ldots\geq 0} e^{-\beta(n_1\epsilon_1+n_2\epsilon_2+\cdots)} \sum_{i,j} A_{i,j} \langle n_1, n_2, \ldots | \, a_i^\dagger a_j \, | n_1, n_2, \ldots \rangle \\
&= \frac{1}{\mathcal{Z}} \sum_{n_1,n_2,\ldots\geq 0} e^{-\beta(n_1\epsilon_1+n_2\epsilon_2+\cdots)} \sum_{i,j} A_{i,j}\delta_{i,j} n_i \\
&= \sum_i A_{i,i} \frac{1}{\mathcal{Z}} \sum_{n_1,n_2,\ldots\geq 0} n_i e^{-\beta(n_1\epsilon_1+n_2\epsilon_2+\cdots)} \\
&= \sum_i \frac{A_{i,i}}{e^{\beta\epsilon_i} \pm 1}.
\end{aligned} \tag{3.22}$$

In particular, the average energy is

$$\langle H \rangle_\Gamma = \mathrm{tr}_{\mathcal{F}}(H\Gamma) = \sum_i \frac{\epsilon_i}{e^{\beta\epsilon_i} \pm 1}. \tag{3.23}$$

Remark. The equation (3.22) is applicable only for one-body operator as defined in Section 3.5. It does not work, for example, in the case of the average value $\langle n_x n_y \rangle$, because $n_x n_y = a_x^\dagger a_x a_y^\dagger a_y$ does not admit an expression of the form (3.13).

3.7 An example

We illustrate the earlier notions about Fock spaces using the following example of a system of interacting particles on the graph $G = (V, E)$. Consider the finite dimensional Hilbert space $\mathcal{H} = \mathbb{C}^V$. The Fock space $\mathcal{F}_\nu(\mathcal{H})$ associated with $\mathcal{H}$ describes the states with a variable number of particles on G. An orthonormal basis of $\mathcal{H}$ can be given by $\{|x\rangle \mid x \in V\}$ where $|x\rangle$ is a state with one particle located at the vertex x and no particle in other places. We shall use a_x and $a_x^\dagger$ to denote the creation and annihilation operators of $|x\rangle$ as defined earlier in (3.4) and (3.5).

If $\nu = +1$ (bosons), the Fock space $\mathcal{F}_{+1}(\mathcal{H})$ has a natural isomorphism with the space

$$\bigotimes_{i=1}^{L} \ell^2(\mathbb{N})$$

The space $\ell^2(\mathbb{N})$ has the natural basis $e_0, e_1, e_2, \ldots$ where e_i is the vector $(0, 0, \ldots, 1, \ldots)$ having 1 in the $(i+1)$-th component and zero everywhere else. In occupation number representation, the isomorphism identifies the vector $|n_1, n_2, \ldots, n_L\rangle \in \mathcal{F}$ with the vector $(e_{n_1} \otimes e_{n_2} \otimes \ldots \otimes e_{n_L}) \in \bigotimes_{i=1}^{L} \ell^2(\mathbb{N})$. Similarly, if $\nu = -1$ (fermions), then the Fock space $\mathcal{F}_{-1}(\mathcal{H})$ is isomorphic with

$$\bigotimes_{i=1}^{L} \mathbb{C}^2$$

in an obvious way.

Let

$$\begin{aligned} K &= \sum_{x\sim y} (a_x^\dagger - a_y^\dagger)(a_x - a_y) \\ &= \sum_{x\sim y} \big(- a_x^\dagger a_y - a_y^\dagger a_x + n_x + n_y \big) \end{aligned} \tag{3.24}$$

be a Hermitian operator defined on the Fock space. By commutation relations (3.10), we have the following for both $\nu = \pm 1$,

$$\begin{aligned} a_x^\dagger a_y \big(a_{x_1}^\dagger \cdots a_{x_N}^\dagger \big) &= \sum_j \delta_{x_j,y} \nu^{j-1} a_x^\dagger a_{x_1}^\dagger \cdots \widehat{a_{x_j}^\dagger} \cdots a_{x_N}^\dagger \\ &= \sum_j \delta_{x_j,y} a_{x_1}^\dagger \cdots a_x^\dagger \cdots a_{x_N}^\dagger \end{aligned}$$

Summing the above equation over all pairs $x \sim y$ and over all $y \in V$, we deduce

$$\begin{aligned} &\sum_{x\sim y} \big(a_y^\dagger a_y - a_x^\dagger a_y \big) a_{x_1}^\dagger \cdots a_{x_N}^\dagger \, |\Omega\rangle \\ =& \frac{1}{2} \sum_j \sum_y \delta_{x_j,y} \sum_{x\sim y} \big(a_{x_1}^\dagger \cdots a_{x_j}^\dagger \cdots a_{x_N}^\dagger - a_{x_1}^\dagger \cdots a_x^\dagger \cdots a_{x_N}^\dagger \big) \, |\Omega\rangle \\ =& \frac{1}{2} \sum_j \sum_{x\sim x_j} \big(a_{x_1}^\dagger \cdots a_{x_j}^\dagger \cdots a_{x_N}^\dagger - a_{x_1}^\dagger \cdots a_x^\dagger \cdots a_{x_N}^\dagger \big) \, |\Omega\rangle \end{aligned}$$

It follows that, with $|\psi\rangle$ defined as in (3.11),

$$\begin{aligned} K\,|\psi\rangle &= \sum_{x\sim y} \big(a_y^\dagger a_y - a_x^\dagger a_y \big) \, |\psi\rangle + \sum_{x\sim y} \big(a_x^\dagger a_x - a_y^\dagger a_x \big) \, |\psi\rangle = 2 \sum_{x\sim y} \big(a_y^\dagger a_y - a_x^\dagger a_y \big) \, |\psi\rangle \\ =& \sum_j \sum_{x\sim x_j} \psi(x_1, \ldots, x_j, \ldots, x_N) \big(a_{x_1}^\dagger \cdots a_{x_j}^\dagger \cdots a_{x_N}^\dagger - a_{x_1}^\dagger \cdots a_x^\dagger \cdots a_{x_N}^\dagger \big) \, |\Omega\rangle \\ =& \sum_{x_1,\ldots,x_N \in V} \left(\Big(\sum_j \deg_G(x_j) \Big) \psi(x_1, \ldots, x_N) - \sum_j \sum_{x\sim x_j} \psi(x_1, \ldots, x, \ldots, x_N) \right) a_{x_1}^\dagger \cdots a_{x_N}^\dagger \, |\Omega\rangle \\ =& \sum_{x_1,\ldots,x_N \in V} (-\Delta\psi)\,(x_1, \ldots, x_N) a_{x_1}^\dagger \cdots a_{x_N}^\dagger \, |\Omega\rangle \,, \end{aligned} \tag{3.25}$$

where $-\Delta$ is the Laplacian operator on the product graph $G \times G \times \cdots \times G$ where the edges are of the following form.

$$\{(x_1, \ldots, x, \ldots, x_N), (x_1, \ldots, y, \ldots, x_N)\}, \quad x \sim y \text{ in } G.$$

Let

$$\{\phi_k \mid k = 1, 2, \ldots, L\} \tag{3.26}$$

be an orthonormal set of Laplacian eigenfunctions on G with eigenvalues $0 \le \epsilon_1 \le \epsilon_2 \le \cdots \le \epsilon_L$. Then the eigenfunctions of $-\Delta$ on G^N are given simply by the product

$$\phi_{k_1}(x_1)\phi_{k_2}(x_2) \cdots \phi_{k_N}(x_N) \quad \text{with} \quad k_i = 1, 2, \ldots, L. \tag{3.27}$$

The corresponding eigenvalue is $\epsilon_{k_1} + \cdots + \epsilon_{k_L}$. It is easy to verify these facts since $-\Delta$ acts on a general ψ by the sum $\sum_{j=1}^{N} -\Delta_j \psi$ where $-\Delta_j$ is the Laplacian operator on the variable x_j only. In particular, we obtain the enegy eigenfunctions of a one-particle system (case $N = 1$) as the following state vectors

$$|k\rangle := \sum_k \phi_k(x) \, |x\rangle \, . \tag{3.28}$$

For $N \geq 2$, it is clear that $-\Delta$ preserves both the subspace of symmetric functions and the subspace of anti-symmetric functions on G^N. We can thus diagonalise $-\Delta$ in these two invariant subspaces, where the eigenfunctions in the respective subspaces can be found by symmetrising or anti-symmetrising the functions in (3.27) accordingly. The resulting wavefunctions are nothing but the (anti-)symmetrised states

$$(|k_1\rangle \otimes |k_2\rangle \otimes \cdots \otimes |k_N\rangle)_\nu$$

For $k = 1, 2, 3, \ldots, L$, define the operator

$$\begin{aligned} b_k^\dagger &:= \sum_{x \in V} \phi_k(x) a_x^\dagger . \\ b_k &:= \sum_{x \in V} \overline{\phi_k(x)} a_x . \end{aligned} \tag{3.29}$$

They are essentially the creators and annihilators of energy eigenstates (3.28). Since the states (3.28) are orthonormal, we immediately have the following commutation relations.

$$\begin{aligned} [b_k, b_m^\dagger] = \delta_{k,m}, \quad [b_k^\dagger, b_m^\dagger] = 0, \quad [b_k, b_m] = 0 \quad \text{if } \nu = +1 \\ \{b_k, b_m^\dagger\} = \delta_{k,m}, \quad \{b_k^\dagger, b_m^\dagger\} = 0, \quad \{b_k, b_m\} = 0 \quad \text{if } \nu = -1. \end{aligned} \tag{3.30}$$

It follows from our earlier analysis that for $k_i = 1, 2, \ldots, L$, if

$$b_{k_1}^\dagger b_{k_2}^\dagger \cdots b_{k_N}^\dagger \, |\Omega\rangle \neq 0,$$

then it is an eigenfunction of K with eigenvalue $\epsilon_{k_1} + \cdots + \epsilon_{k_N}$. We may likewise use the occupation number representations as in (3.9):

$$|n_1, \ldots, n_L\rangle := \frac{\sqrt{n_1! \cdots n_L!}}{\sqrt{N!}} \sum_{\sigma \in \mathcal{S}_N} b_{k_{\sigma(1)}}^\dagger b_{k_{\sigma(2)}}^\dagger \cdots b_{k_{\sigma(N)}}^\dagger \, |\Omega\rangle \tag{3.31}$$

where $n_r = \#\{j \mid k_j = r\}$. By construction, we have

$$\begin{aligned} K \, |n_1, \ldots, n_L\rangle &= (n_1\epsilon_1 + n_2\epsilon_2 + \cdots + n_L\epsilon_L) \, |n_1, \ldots, n_L\rangle \, . \\ \left(b_k^\dagger b_k\right) |n_1, \ldots, n_L\rangle &= n_k \, |n_1, \ldots, n_L\rangle \, . \end{aligned} \tag{3.32}$$

The Hamiltonian (3.24) can be rewritten as

$$K = \sum_k \epsilon_k b_k^\dagger b_k \tag{3.33}$$

which describes a set of L uncoupled systems. For $\nu = +1$, the Hamiltonian K describes a set of L uncoupled simple harmonic oscillator. For $\nu = -1$, we have a set of L uncoupled two-state systems since $n_r \in \{0, 1\}$ for all r.

Suppose the system is in the Gibbs state

$$\Gamma = \frac{e^{-\beta K}}{\operatorname{tr} e^{-\beta K}}$$

for some $\beta > 0$. We shall calculate some thermodynamic quantities of this state. By (3.22), the average number of particles $\langle n_x \rangle$ at site x is given by

$$\sum_p \frac{\langle p| \, a_x^\dagger a_x \, |p\rangle}{e^{\beta\epsilon(p)} \pm 1} = \sum_p \frac{|\phi_p(x)|^2}{e^{\beta\epsilon(p)} \pm 1}.$$

The average energy is as in (3.23).

$$\langle K \rangle = \sum_p \frac{\epsilon(p)}{e^{\beta\epsilon(p)} \pm 1}.$$

As a further example, we compute $\left\langle K a_x^\dagger a_x^\dagger a_x a_x a_x \right\rangle$. Note that $K a_x^\dagger a_x^\dagger a_x a_x a_x$ is not a one-body operator. By unitarity of the matrix $(\phi_p(x))_{p,x}$, we have $a_x^\dagger = \sum_p \overline{\phi_p}(x) a_p^\dagger$. Thus, we can express $a_x^\dagger a_x$ in terms the energy eigenstates $|p\rangle$ as

$$a_x^\dagger a_x = \sum_{q,r} \overline{\phi_q}(x) \phi_r(x) a_q^\dagger a_r.$$

Then, Wick's rule implies

$$\begin{aligned}
\left\langle K a_x^\dagger a_x^\dagger a_x a_x a_x \right\rangle &= 2 \langle n_x \rangle^2 \langle K \rangle + 2 \langle n_x \rangle^2 \sum_{p,q,r} \epsilon(p) \overline{\phi_q}(x) \phi_r(x) \left\langle a_p^\dagger a_r \right\rangle \left\langle a_p a_q^\dagger \right\rangle \\
&= 2 \langle n_x \rangle^2 \langle K \rangle + 2 \langle n_x \rangle \sum_{p,q,r} \epsilon(p) \overline{\phi_q}(x) \phi_r(x) \delta_{p,r} \left\langle a_p^\dagger a_r \right\rangle \left\langle a_p^\dagger a_q \mp \delta_{p,q} \right\rangle \\
&= 2 \langle n_x \rangle^2 \langle K \rangle + 2 \langle n_x \rangle \sum_p \epsilon(p) |\phi_p(x)|^2 \frac{1}{e^{\beta\epsilon(p)} \pm 1} \Big(\frac{1}{e^{\beta\epsilon(p)} \pm 1} \mp 1 \Big).
\end{aligned} \tag{3.34}$$

In the case $\nu = +1$,

$$\begin{aligned}
\frac{1}{e^{\beta\epsilon(p)} - 1} \Big(\frac{1}{e^{\beta\epsilon(p)} - 1} + 1 \Big) &= \frac{e^{\beta\epsilon(p)}}{(e^{\beta\epsilon(p)} - 1)^2} \\
&= \frac{1}{(e^{\beta\epsilon(p)/2} - e^{-\beta\epsilon(p)/2})^2} \\
&= \frac{1}{2 \sinh^2(\beta\epsilon(p)/2)}.
\end{aligned}$$

In the case $\nu = -1$,

$$\begin{aligned}
\frac{1}{e^{\beta\epsilon(p)} + 1} \Big(\frac{1}{e^{\beta\epsilon(p)} + 1} - 1 \Big) &= \frac{-e^{\beta\epsilon(p)}}{(e^{\beta\epsilon(p)} + 1)^2} \\
&= \frac{-1}{(e^{\beta\epsilon(p)/2} + e^{-\beta\epsilon(p)/2})^2} \\
&= \frac{-1}{2 \cosh^2(\beta\epsilon(p)/2)}.
\end{aligned}$$

Inserting this back to (3.34), we deduce, for $\nu = +1$,

$$\begin{aligned}\left\langle K a_x^\dagger a_x^\dagger a_x a_x \right\rangle &= 2\left\langle n_x \right\rangle^2 \left\langle K \right\rangle + 2\left\langle n_x \right\rangle \sum_p \epsilon(p)|\phi_p(x)|^2 \frac{1}{2\sinh^2(\beta\epsilon(p)/2)}. \\ &= \Big(\sum_p \frac{|\phi_p(x)|^2}{e^{\beta\epsilon(p)}-1}\Big)^2 \sum_p \frac{2\epsilon(p)}{e^{\beta\epsilon(p)}-1} + \sum_p \frac{|\phi_p(x)|^2}{e^{\beta\epsilon(p)}-1} \sum_p \frac{\epsilon(p)|\phi_p(x)|^2}{\sinh^2(\beta\epsilon(p)/2)},\end{aligned} \tag{3.35}$$

and, for $\nu = -1$,

$$\left\langle K a_x^\dagger a_x^\dagger a_x a_x \right\rangle = \Big(\sum_p \frac{|\phi_p(x)|^2}{e^{\beta\epsilon(p)}+1}\Big)^2 \sum_p \frac{2\epsilon(p)}{e^{\beta\epsilon(p)}+1} - \sum_p \frac{|\phi_p(x)|^2}{e^{\beta\epsilon(p)}+1} \sum_p \frac{\epsilon(p)|\phi_p(x)|^2}{\cosh^2(\beta\epsilon(p)/2)}. \tag{3.36}$$

4 Holstein-Primakoff Transformation

The *Holstein-Primakoff Transformation* establishes an isomorphism between the system of spins described by the Heisenberg model (2.1) and a system of several bosons hopping on $G = (V, E)$. Hence the tools developed in Section 3 can be used to study the Heisenberg model.

we consider the Hilbert basis $\{\psi_x \mid x \in V\}$ of the space $\mathcal{H}$ associated with a particle on the graph $G = (V, E)$, i.e. the state ψ_x describes a particle at the position $x \in V$. Define $a_x^\dagger = a^\dagger(\psi_x)$, $a_x = a(\psi_x)$ and $n_x = a_x^\dagger a_x$. Also define $N = \sum_{x\in V} n_x$ to be the total particle number operator. For each $x \in V$, we define the following operators on the Fock space $\bigotimes_{x\in V} \ell^2(\mathbb{N})$.

$$S_x^+ = \sqrt{2S} a_x^\dagger \left[1 - \frac{a_x^\dagger a_x}{2S}\right]_+^{1/2}, \quad S_x^- = \sqrt{2S}\left[1 - \frac{a_x^\dagger a_x}{2S}\right]_+^{1/2} a_x, \quad S_x^3 = a_x^\dagger a_x - S. \tag{4.1}$$

With the aid of (4.1), we can rewrite (2.1) into the following form.

$$\begin{aligned}H = S\sum_{x\sim y}\Bigg(&-a_x^\dagger\sqrt{1-\frac{n_x}{2S}}\sqrt{1-\frac{n_y}{2S}}a_y - a_y^\dagger\sqrt{1-\frac{n_y}{2S}}\sqrt{1-\frac{n_x}{2S}}a_x \\ &+ n_x + n_y - \frac{1}{S}n_x n_y\Bigg)\end{aligned} \tag{4.2}$$

Alternatively, the Hamiltonian (2.1) can be written as

$$H = S\sum_{x\sim y}\left(a_y^\dagger\sqrt{1-\frac{n_x}{2S}} - a_x^\dagger\sqrt{1-\frac{n_y}{2S}}\right)\left(a_y\sqrt{1-\frac{n_x}{2S}} - a_x\sqrt{1-\frac{n_y}{2S}}\right). \tag{4.3}$$

4.1 Two-particle densities

Let us consider a wavefunction $\Psi(x_1, \ldots, x_n)$ representing n particles in the sense of (3.11). By choice, $N|\Psi\rangle = n|\Psi\rangle$. For $x, y \in V$, define

$$\begin{aligned}\rho_\Psi(x,y) &:= \langle\Psi| a_x^\dagger a_y^\dagger a_y a_x |\Psi\rangle \\ &= \begin{cases}\langle\Psi| n_x n_y |\Psi\rangle & \text{if } x \neq y \\ \langle\Psi| n_x(n_x-1) |\Psi\rangle & \text{if } x = y.\end{cases}\end{aligned} \tag{4.4}$$

Explicitly, since the action of n_x on $\Psi(x_1,\dots,x_n)$ can be written as

$$(n_x\Psi)(x_1,\dots,x_n)=\Big(\sum_{i=1}^n \delta_{x,x_i}\Big)\Psi(x_1,\dots,x_n),$$

we have

$$\begin{aligned}\rho_\Psi(x,x)&=\sum_{x_1,\dots,x_n\in V}\underbrace{\Big(\sum_{i=1}^n\delta_{x,x_i}\Big)\left[\Big(\sum_{i=1}^n\delta_{x,x_i}\Big)-1\right]}_{\geq 2 \text{ if } x_i=x_j=x \text{ for some } i\neq j}|\Psi(x_1,\dots,x_n)|^2\\&\geq 2\sum\left\{|\Psi(x_1,\dots,x_n)|^2\;\middle|\; x_i=x_j=x \text{ for some } i\neq j\right\}\geq 0.\end{aligned}$$

Similarly, for $x\neq y$,

$$\begin{aligned}\rho_\Psi(x,y)&=\sum_{x_1,\dots,x_n\in V}\underbrace{\Big(\sum_{i=1}^n\delta_{x,x_i}\Big)\Big(\sum_{i=1}^n\delta_{y,x_i}\Big)}_{\geq 1 \text{ if } x_i=x \text{ and } x_j=y \text{ for some } i,j}|\Psi(x_1,\dots,x_n)|^2\\&\geq\sum\left\{|\Psi(x_1,\dots,x_n)|^2\;\middle|\; x_i=x \text{ and } x_j=y \text{ for some } i,j\right\}\geq 0.\end{aligned}$$

Moreoever, since

$$\begin{aligned}\sum_{x,y\in V}a_x^\dagger a_y^\dagger a_y a_x&=\sum_x\sum_{y\neq x}n_xn_y+\sum_x(n_xn_x-n_x)=\sum_x n_x\Big(n_x+\sum_{y\neq x}n_y\Big)-\sum_x n_x\\&=\sum_x n_x\sum_y n_y-\sum_x n_x=N(N-1)\end{aligned}$$

we have

$$\sum_{x,y\in V}\rho_\Psi(x,y)=n(n-1). \tag{4.5}$$

For $x,y,z\in V$, define the positive semi-definite operator

$$h^y_{x,z}=\left(a_x^\dagger\sqrt{1-\frac{n_z}{2S}}-a_z^\dagger\sqrt{1-\frac{n_x}{2S}}\right)n_y\left(a_x\sqrt{1-\frac{n_z}{2S}}-a_z\sqrt{1-\frac{n_x}{2S}}\right). \tag{4.6}$$

We can deduce from the commutation relations (3.6) that

$$a_x^\dagger N=(N-1)a_x^\dagger \quad\text{and}\quad Na_x=a_x(N-1),$$

which implies that

$$\begin{aligned}\sum_{x\sim z}\sum_y h^y_{x,z}&=\sum_{x\sim z}\left(a_x^\dagger\sqrt{1-\frac{n_z}{2S}}-a_z^\dagger\sqrt{1-\frac{n_x}{2S}}\right)N\left(a_x\sqrt{1-\frac{n_z}{2S}}-a_z\sqrt{1-\frac{n_x}{2S}}\right)\\&=\sum_{x\sim z}\left(a_x^\dagger\sqrt{1-\frac{n_z}{2S}}-a_z^\dagger\sqrt{1-\frac{n_x}{2S}}\right)\left(a_x\sqrt{1-\frac{n_z}{2S}}-a_z\sqrt{1-\frac{n_x}{2S}}\right)(N-1)\\&=\frac{1}{S}H(N-1)=\frac{1}{S}(N-1)H.\end{aligned} \tag{4.7}$$

Lemma 4.1. *For $x \neq z$, the following inequality holds for all y.*

$$\begin{aligned}&\left|\rho_\Psi(z,y)\left(1-\frac{\delta_{x,y}}{2S}\right)-\rho_\Psi(x,y)\left(1-\frac{\delta_{z,y}}{2S}\right)\right|^2\\ \leq& 2\left\langle\Psi\right| h^y_{x,z}\left|\Psi\right\rangle\left[\rho_\Psi(z,y)\left(1-\frac{\delta_{x,y}}{2S}\right)+\rho_\Psi(x,y)\left(1-\frac{\delta_{z,y}}{2S}\right)\right]\end{aligned}$$

Proof. Using the commutation relation $[n_y, a_x] = -a_x\delta_{x,y}$, we can write

$$\begin{aligned}a_x^\dagger\sqrt{1-\frac{n_z}{2S}}n_y a_x\sqrt{1-\frac{n_z}{2S}} &= \left(1-\frac{n_z}{2S}\right)n_x(n_y-\delta_{x,y})\\ &= n_x(n_y-\delta_{x,y})-\frac{n_xn_yn_z}{2S}+\frac{n_xn_z}{2S}\delta_{x,y}.\end{aligned}$$

Thus

$$\begin{aligned}&a_x^\dagger\sqrt{1-\frac{n_z}{2S}}n_y a_x\sqrt{1-\frac{n_z}{2S}}-a_z^\dagger\sqrt{1-\frac{n_x}{2S}}n_y a_z\sqrt{1-\frac{n_x}{2S}}\\ =&n_x(n_y-\delta_{x,y})-n_z(n_y-\delta_{z,y})+\frac{n_xn_z}{2S}(\delta_{x,y}-\delta_{z,y})\\ =&\begin{cases}n_xn_y-n_zn_y & \text{if } y\neq x \text{ and } y\neq z\\ n_xn_y-n_z(n_y-1)+\frac{n_xn_y}{2S} & \text{if } y=z\\ n_x(n_y-1)-(n_zn_y+\frac{n_zn_y}{2S}) & \text{if } y=x.\end{cases}\end{aligned}$$

Thus, with

$$u := a_y a_x\sqrt{1-\frac{n_z}{2S}}\left|\Psi\right\rangle \quad \text{and} \quad v := a_y a_z\sqrt{1-\frac{n_x}{2S}}\left|\Psi\right\rangle,$$

we have

$$\rho_\Psi(x,y)\left(1-\frac{\delta_{z,y}}{2S}\right)-\rho_\Psi(z,y)\left(1-\frac{\delta_{x,y}}{2S}\right)=\langle u,u\rangle-\langle v,v\rangle=\Re\left\langle u-v,u+v\right\rangle.$$

By Cauchy-Schwartz inequality and the parallelogram inequality,

$$\|\Re\left\langle u-v,u+v\right\rangle\|^2\leq\|u-v\|^2\|u+v\|^2\leq\|u-v\|^2(2\|u\|^2+2\|v\|^2).$$

Since $\|v\|^2$ and $\|u\|^2$ are bounded by $\rho_\Psi(x,y)(1-\frac{\delta_{z,y}}{2S})$ and $\rho_\Psi(z,y)(1-\frac{\delta_{x,y}}{2S})$ respectively, and $\|u-v\|^2=\left\langle\Psi|h^y_{x,z}\Psi\right\rangle$ by definition of $h^y_{x,z}$, we have finally

$$\|\Re\left\langle u-v,u+v\right\rangle\|^2\leq 2\left\langle\Psi|h^y_{x,z}\Psi\right\rangle(\rho_\Psi(x,y)(1-\frac{\delta_{z,y}}{2S})+\rho_\Psi(z,y)(1-\frac{\delta_{x,y}}{2S})) \quad (4.8)$$

as desired. □

As a corollary of Lemma 4.1, we can bound certain sums of two particle densities. We shall derive an inequality in a general form as follows.

Fix an arbitrary map

$$y\mapsto y'$$

which sends each vertex y in G to a *different* vertex $y'\neq y$ in G. Let $G'(y,y')=G'(y)=G'$ be the largest connected component of the graph obtained by removing y and y' from

G. Suppose that y' is joint with G' by an edge in G. Let x_* be the vertex of G' which minimises $G' \ni z \mapsto \rho_\Psi(y,z)$ and choose a shortest path $(x_* = x_0, x_1, x_2, \ldots, x_m = y')$ going from x_* to y'. By the choice of x_*, we have

$$\rho_\Psi(y,x_*) \leq \frac{1}{|G'|}\sum_{z\in G'}\rho_\Psi(y,z) \leq \frac{1}{|G'|}\sum_{w,w'\in V}\rho_\Psi(w,w') \leq \frac{n(n-1)}{|G'|}.$$

On the other hand, the succesive differences $\rho_\Psi(y,x_i) - \rho_\Psi(y,x_{i+1})$ can be bounded from above by Lemma 4.1. since $x_i \neq y$ for all i and $x_i \neq x_j$ for all $i \neq j$, we have

$$\begin{aligned}
&\sum_{y\in V}\sum_i |\rho_\Psi(y,x_i) - \rho_\Psi(y,x_{i+1})| \\
\leq&\sqrt{2}\sum_{y\in V}\sum_i \sqrt{\langle\Psi| h^y_{x_i,x_{i+1}} |\Psi\rangle}\sqrt{\rho_\Psi(x_{i+1},y)+\rho_\Psi(x_i,y)} \\
\leq&\sqrt{2}\sum_{y\in V}\sum_{x\sim z} \sqrt{\langle\Psi| h^y_{x,z} |\Psi\rangle}\sqrt{\rho_\Psi(x,y)+\rho_\Psi(z,y)} \\
\leq&\sqrt{2}\sqrt{\sum_{y\in V}\sum_{x\sim z}\langle\Psi| h^y_{x,z} |\Psi\rangle}\sqrt{\sum_{y\in V}\sum_{x\sim z}(\rho_\Psi(x,y)+\rho_\Psi(z,y))} \\
=&\sqrt{2}\sqrt{\frac{n-1}{S}}\langle\Psi| H |\Psi\rangle^{\frac{1}{2}}\sqrt{\sum_{y\in V}\sum_{x\sim z}(\rho_\Psi(x,y)+\rho_\Psi(z,y))} \\
\leq&\sqrt{2}\sqrt{\frac{n-1}{S}}\langle\Psi| H |\Psi\rangle^{\frac{1}{2}}\sqrt{2\Delta(G)n(n-1)} \\
\leq&2\sqrt{\Delta(G)}(n-1)\sqrt{\frac{n}{S}}\langle\Psi| H |\Psi\rangle^{\frac{1}{2}}
\end{aligned}$$

In the second last line, we denoted the maximal degree of G by $\Delta(G)$ and used (4.5). Since $\rho_\Psi(y,y') = \rho_\Psi(y',y)$, the same calculation applies in the case where y is joint with G' via an edge instead of y'. Therefore, we have

$$\sum_{y\in V}\rho_\Psi(y,y') \leq \frac{n(n-1)}{\min_y |G'(y,y')|} + 2\sqrt{\Delta(G)}(n-1)\sqrt{\frac{n}{S}}\langle\Psi| H |\Psi\rangle^{\frac{1}{2}}. \tag{4.9}$$

In particular, the sum over pairs of neighbours $y \sim y'$ is bounded from above by

$$\sum_{y\sim y'}\rho_\Psi(y,y') \leq \Delta(G)\frac{n(n-1)}{\min_{y\sim y'}|G'(y,y')|} + 2\Delta(G)^{\frac{3}{2}}(n-1)\sqrt{\frac{n}{S}}\langle\Psi| H |\Psi\rangle^{\frac{1}{2}}. \tag{4.10}$$

We can bound $\rho_\Psi(y,y)$ as follows. In the case $S = \frac{1}{2}$, we have $\rho_\Psi(y,y) = 0$. Suppose $S \geq 1$. For each y, choose a neighbour of y and denote it by y'. We have

$$\sum_{y\in V}\rho_\Psi(y,y) \leq \sum_{y\in V}\left(1-\frac{1}{2S}\right)\rho(y,y') + \sum_{y\in V}\left|\left(1-\frac{1}{2S}\right)\rho_\Psi(y,y') - \rho_\Psi(y,y)\right|. \tag{4.11}$$

The first term in (4.11) can be bounded from above by (4.9). By Lemma 4.1, the second term is bounded from above by

$$\begin{aligned}
&\sum_{y\in V}\sqrt{2}\sqrt{\langle\Psi|\, h^y_{y,y'}\,|\Psi\rangle\left|\left(1-\frac{1}{2S}\right)\rho_\Psi(y,y')+\rho_\Psi(y,y)\right|}\\
\leq&\sum_{y\in V}\sqrt{2}\sqrt{\langle\Psi|\, h^y_{y,y'}\,|\Psi\rangle\,|\rho_\Psi(y,y')+\rho_\Psi(y,y)|}\\
\leq&\sqrt{2}\sqrt{\sum_{y\in V}\langle\Psi|\, h^y_{y,y'}\,|\Psi\rangle}\sqrt{\sum_{y\in V}|\rho_\Psi(y,y')+\rho_\Psi(y,y)|}\\
\leq&\sqrt{2}\sqrt{\frac{n-1}{S}}\,\langle\Psi|\, H\,|\Psi\rangle^{\frac{1}{2}}\,\sqrt{2n(n-1)}\\
\leq&2(n-1)\sqrt{\frac{n}{S}}\,\langle\Psi|\, H\,|\Psi\rangle^{\frac{1}{2}}\,.
\end{aligned}$$

Combining the upper bounds for the two terms in (4.11), we deduce

$$\sum_{y\in V}\rho_\Psi(y,y)\leq\frac{n(n-1)}{\min_y|G'(y,y')|}+2\big(\sqrt{\Delta(G)}+1\big)(n-1)\sqrt{\frac{n}{S}}\,\langle\Psi|\, H\,|\Psi\rangle^{\frac{1}{2}}\,. \quad (4.12)$$

Remark. For the ladder graph of length ℓ and $(x,\theta)' := (x+1,-\theta)$, we have $|G'(y,y')|\geq \ell-1$ and $\Delta(G)=3$. It follows from (4.9) that

$$\sum_{y\in V}\rho_\Psi(y,y')\leq\frac{n(n-1)}{\ell-1}+2\sqrt{3}(n-1)\sqrt{\frac{n}{S}}\,\langle\Psi|\, H\,|\Psi\rangle^{\frac{1}{2}}\,.$$

and

$$\sum_{y\in V}\rho_\Psi(y,y)\leq\frac{n(n-1)}{\ell-1}+2\big(\sqrt{3}+1\big)(n-1)\sqrt{\frac{n}{S}}\,\langle\Psi|\, H\,|\Psi\rangle^{\frac{1}{2}}\,.$$

4.2 Spin waves

Let $\Psi\in\ell^2(V^N)$ represent a wave function of n particles in the sense of (3.11). We have assumed without loss of generality that Ψ is a symmetric function, i.e.

$$\Psi(x_1,\ldots,x_N)=\Psi(x_{\sigma(1)},\ldots,x_{\sigma(N)})\quad\text{for all permutations }\sigma\text{ of }\{1,2,\ldots,N\}.$$

The map $\ell^2_{sym}(V^N) \ni \Psi(x_1, \dots, x_N) \mapsto |\Psi\rangle$ is an isometry. Indeed,

$$\begin{aligned}
\langle \Psi | \Psi \rangle &= \left\| \sum_{n_1+\cdots+n_L=N} \frac{\sqrt{n_1! \cdots n_L!}}{\sqrt{N!}} \sum_{|\{x_i=j\}|=n_j} \Psi(x_1, \dots, x_N) \, |n_1, \dots, n_L\rangle \right\|^2 \\
&= \sum_{n_1+\cdots+n_L=N} \frac{n_1! \cdots n_L!}{N!} \left\| \sum_{|\{x_i=j\}|=n_j} \Psi(x_1, \dots, x_N) \right\|^2 \\
&= \sum_{n_1+\cdots+n_L=N} \frac{n_1! \cdots n_L!}{N!} \Big(\frac{N!}{n_1! \cdots n_L!} \Big)^2 \|\Psi(1, \dots, 2, \dots, 3, \dots)\|^2 \\
&= \sum_{n_1+\cdots+n_L=N} \frac{N!}{n_1! \cdots n_L!} \|\Psi(1, \dots, 2, \dots, 3, \dots)\|^2 \\
&= \sum_{1 \le x_1, \dots, x_N \le L} \|\Psi(x_1, \dots, x_N)\|^2 \\
&= \|\Psi\|^2_{\ell^2_{sym}(V^N)}
\end{aligned}$$

4.2.1 First excitation states

Let us consider the case $n = 1$. The general wave function is given by

$$|\Psi\rangle = \sum_{x \in V} \Psi(x) a_x^\dagger \, |\Omega\rangle \, . \tag{4.13}$$

The action of the Hamiltonian (4.2) on $|\Psi\rangle$ coincides with the action of K as defined in (3.24) up to a multiple of S. More precisely, we have

$$H \, |\Psi\rangle = SK \, |\Psi\rangle \, .$$

By (3.25), we see that

$$H \, |\Psi\rangle = S \sum_{x \in V} (-\Delta\psi)(x) a_x^\dagger \, |\Omega\rangle \, .$$

Therefore, for (4.13) to be an energy eigenstate, we need Ψ to be an eigenfunction of the graph Laplacian $-\Delta$ on G, for example a constant function $\Psi \equiv 1$. Since $-\Delta$ is a positive symmetric operator on $\mathbb{C}^L$, it can be diagonalised with non-negative eigenvalues

$$\lambda_1 = 0 \le \lambda_2 \le \cdots \le \lambda_L .$$

For each $-\Delta\Psi_k = \lambda_k \Psi_k$, the wave function $|k\rangle := \sum_x \Psi_k(x) a_x^\dagger \, |\Omega\rangle$ is an energy eigenstate of H with energy $S\lambda_k$. In particular, the state $|k = 0\rangle$ has the ground energy 0 and lies in the irreducible component $\mathbb{C}^{2SL+1}$ in the decomposition (1.3) whereas the states $|k = 1\rangle \, , |k = 2\rangle \, , \dots, |k = L\rangle$ lie in each of the other $L-1$ irreducible components $\mathbb{C}^{2(SL-1)+1}$. In principle, we can obtain the rest of the energy eigenstates in $\mathbb{C}^{2SL+1}$ and $\mathbb{C}^{2(SL-1)+1}$ by applying the raising operator S^+_{tot} onto $|\Psi_k\rangle \, , k = 1, 2, \dots, L$ repeatedly.

Essentially, the sum of eigenspaces of the total number operator $\sum_x n_x$ corresponding to eigenvalues 0 and 1 is isomorphic to the space $\mathbb{C}^L$. The action of the Hamiltonian (2.1) then coincides with the operator $-S\Delta_G$ on the space $\mathbb{C}^L$.

Example 4.2. Consider a linear graph G representing a chain of $\ell+2$ spin-S particles as follows.

$$\overset{\bullet}{0} - \overset{\bullet}{1} - \overset{\bullet}{2} - \overset{\bullet}{3} - \cdots - \overset{\bullet}{\ell} - \overset{\bullet}{\ell+1}. \tag{4.14}$$

We have $-\Delta_G \Psi = 0$ for all Ψ in the two-dimensional subspace of affine functions on the lattice $(0, 1, 2, \ldots, \ell+1)$. There are ℓ other eigenfunctions of $-\Delta_G$.

Suppose the Dirichlet boundary condition is imposed, i.e. $\Psi(0) = \Psi(\ell+1) = 0$. Equivalently, we restrict to the joint eigenspace $\mathcal{H}^D$ of S_0^3 and $S_{\ell+1}^3$ corresponding to the eigenvalue $-S$. For each state $|\Psi\rangle \in \mathcal{H}^D$,

$$\langle \Psi | H | \Psi \rangle = \langle \Psi | H^D | \Psi \rangle$$

where

$$H^D = 2S^2 + S(S_1^3 + S_\ell^3) + \sum_{x=1}^{\ell-1} S^2 - \vec{S}_x \cdot \vec{S}_{x+1}. \tag{4.15}$$

This can be easily verified over the basis $\{|-S, m_1, m_2, \ldots, m_\ell, -S\rangle\}_{|m_j| \le S}$ of the subspace $\mathcal{H}^D$. Note that the Hamiltonian H, as defined in (2.1), does not preserve the subspace $\mathcal{H}^D$.

The eigenfunctions of H^D are precisely the eigenfunctions of the graph Laplacian on the linear graph with Dirichlet boundary condition. They are parametrised by $k \in \{1, 2, \ldots, \ell\}$ with

$$\Psi_k(x) = \sin\Big(\frac{\pi k x}{\ell+1}\Big), \quad x = 0, 1, 2, \ldots, \ell+1. \tag{4.16}$$

One can easily verify that

$$-\Delta \Psi_k(x) = 2\Big(1 - \cos\Big(\frac{\pi k}{\ell+1}\Big)\Big)\Psi_k(x) \quad \text{for} \quad x = 1, 2, \ldots, \ell.$$

4.3 Higher excitation states

The action of H on $|\Psi\rangle$ for particle number greater than 1 is more complicated. The spin-wave apprximation consists of formally replacing the factor $\sqrt{1 - \frac{n_x}{2S}}$ in the expression (4.3) or (4.2) by finitely many terms in the Taylor series $1 - \frac{1}{2}\frac{n_x}{2S} + \cdots$. If only the constant term $\sqrt{1 - \frac{n_x}{2S}} \approx 1$ is kept, then we have essentially the free boson Hamiltonian as defined in (3.24).

5 One-dimensional systems

We consider the ferromagnetic quantum Heisenberg spin chain modeled by the linear graph $G = (V, E)$ with $V = (1, 2, 3, \ldots, L)$ and $\{x, y\} \in E$ if and only if $|x - y| = 1$. The Hamiltonian H_L of the system has been defined in (2.1). The *specific free energy* of the system is defined as

$$f_L(\beta, S) = -\frac{1}{\beta L} \ln \operatorname{tr} e^{-\beta H_L}. \tag{5.1}$$

We shall examine the *thermodynamic limit* of $f_L(\beta, S)$

$$f(\beta, S) = \lim_{L\to\infty} f_L(\beta, S) \tag{5.2}$$

in the low temperature limit $\beta \to \infty$. We will begin by proving the existence of the limit in (5.2) in the next section.

5.1 Existence of thermodynamic limits

The well-known Fekete's lemma states that if a_n is a subadditive sequence, i.e.

$$a_{n+m} \leq a_n + a_m,$$

then

$$\lim_{n\to\infty} \frac{a_n}{n} = \inf_{n\to\infty} \frac{a_n}{n} \in [-\infty, \infty).$$

We can use this lemma to establish the existence of the limit in (5.2) by showing the subadditivity of $\ln \operatorname{tr}(e^{-\beta H_L})$ in L. Indeed, for $L_1 + L_2 = L$, the original Hilbert space $\mathcal{H}$ can be written as

$$\mathcal{H}_1 \otimes \mathcal{H}_2.$$

where $\mathcal{H}_i$ is the Hilbert space $\bigotimes_{x=1}^{L_i} \mathbb{C}^{2S+1}$. The Hamiltonian H_L can be written as

$$K_1 + K_2 + (S^2 - \vec{S}_l \cdot \vec{S}_{l+1})$$

where K_1 acts on $\mathcal{H}_1 \otimes \mathcal{H}_2$ as $H_{L_1} \otimes \mathrm{id}$ and K_2 acts on $\mathcal{H}_1 \otimes \mathcal{H}_2$ as $\mathrm{id} \otimes H_{L_2}$. Let ϵ_i and ϵ'_j be the eigenvalues of H_{L_1} and H_{L_2} respectively. Then

$$\begin{aligned}
\operatorname{tr}(e^{-\beta(K_1+K_2)}) &= \sum_{i,j} e^{-\beta(\epsilon_i+\epsilon'_j)} \\
&= \Big(\sum_i e^{-\beta\epsilon_i}\Big)\Big(\sum_j e^{-\beta\epsilon'_j}\Big) \\
&= \operatorname{tr}(e^{-\beta H_{L_1}}) \operatorname{tr}(e^{-\beta H_{L_2}}).
\end{aligned}$$

It follows from $K_1 + K_2 \leq H_L$ and the above equality that the subadditivity of $\ln \operatorname{tr}(e^{-\beta H_L})$ holds:

$$\ln \operatorname{tr} e^{-\beta H_{L_1}} + \ln \operatorname{tr} e^{-\beta H_{L_2}} \geq \ln \operatorname{tr}(e^{-\beta H_L}).$$

This, together with Fekete's lemma, proves the existence of the limit in (5.2). Moreover, Fekete's lemma also implies that

$$f(\beta, S) \geq f_\ell(\beta, S) \tag{5.3}$$

for all finite $\ell \geq 1$.

5.2 Localisation

5.2.1 Gibbs variational principle

The *Gibbs variational principle* states that, for any Hermitian operator H on a finite dimensional Hilbert space $\mathcal{H}$, the following inequality holds

$$-\frac{1}{\beta}\ln \mathrm{tr}\big(e^{-\beta H}\big) = \inf\left\{ \mathrm{tr}(H\Gamma) + \frac{1}{\beta}\,\mathrm{tr}(\Gamma\ln\Gamma) \;\middle|\; 0 \le \Gamma \le 1 \right\}. \tag{5.4}$$

In fact, the minimum of (5.4) is attained at

$$\Gamma = \frac{e^{-\beta H}}{\mathrm{tr}_{\mathcal{H}}\, e^{-\beta H}}. \tag{5.5}$$

It can be verified that the left hand side of (5.4) is equal to the free energy associated with the choice (5.5).

To prove (5.4), we first state the *Gibbs inequality*. Let $P = (p_i)_{i\in X}$ and $Q = (q_i)_{i\in X}$ be two probability distributions on a finite set X. The Gibbs inequality states that

$$\sum_i p_i \ln p_i \ge \sum_i p_i \ln q_i,$$

which follows easily from the concavity of $x \mapsto \ln x$. By Gibbs' inequality, we deduce that the so-called *Kullback-Leibler divergence* between P and Q is always non-negative:

$$D_{\mathrm{KL}}(P\|Q) \equiv \sum_{i=1}^{n} p_i \log\frac{p_i}{q_i} \ge 0.$$

Coming back to the proof of (5.4), we consider an arbitrary density matrix

$$\Gamma = \sum_i p_i \left|\psi_i\right\rangle \left\langle\psi_i\right|$$

where $\{|\psi_i\rangle\}_i$ is a basis of $\mathcal{H}$ (not necessarily orthonormal) and $0 \le p_i \le 1$ for all i such that $\sum_i p_i = 1$. Let $\{|\phi_j\rangle\}_j$ be an orthonormal basis consisting of eigenvectors of H and

$$H\left|\phi_j\right\rangle = E_j\left|\phi_j\right\rangle, \quad E_j \in \mathbb{R}.$$

Let

$$\left|\psi_i\right\rangle = \sum_j \alpha_{i,j}\left|\phi_j\right\rangle, \quad \alpha_{i,j} \in \mathbb{C}.$$

Note that $\sum_j |\alpha_{i,j}|^2 = 1$ for all i. By a direct computation,

$$\begin{aligned}
&\mathsf{tr}(\Gamma H) + \mathsf{tr}(\Gamma \ln \Gamma) \\
=&\sum_j \langle\psi_j| \sum_i p_i |\psi_i\rangle \langle\psi_i|H|\psi_j\rangle + \sum_i p_i \ln p_i \\
=&\sum_i p_i \langle\psi_i|H|\psi_i\rangle + \sum_i p_i \ln p_i \\
=&\sum_{i,j} p_i |\alpha_{i,j}|^2 \langle\phi_j|H|\phi_j\rangle + \sum_i p_i \ln p_i \\
=&\sum_i p_i \sum_j |\alpha_{i,j}|^2 E_j + \sum_i p_i \ln p_i \\
=&\sum_i p_i \Big[\ln \Big(e^{\sum_j |\alpha_{i,j}|^2 E_j} \mathsf{tr}\big(e^{-H}\big) \Big) - \ln \mathsf{tr}\big(e^{-H}\big) \Big] + \sum_i p_i \ln p_i \\
=&-\ln \mathsf{tr}\big(e^{-H}\big) + \sum_i p_i \ln \Big(e^{\sum_j |\alpha_{i,j}|^2 E_j} \mathsf{tr}\big(e^{-H}\big) \Big) + \sum_i p_i \ln p_i \\
=&-\ln \mathsf{tr}\big(e^{-H}\big) + \sum_i p_i \left[\sum_i \ln p_i - \ln \left(\frac{e^{-\sum_j |\alpha_{i,j}|^2 E_j}}{\mathsf{tr}\big(e^{-H}\big)} \right) \right].
\end{aligned}$$

It suffices to show that the second term is non-negative for all probability distribution $(p_i)_i$ and all choices of basis $\{|\psi_i\rangle\}_i$ (which boils down to choices of $\alpha_{i,j}$). We proceed with the convexity of $x \mapsto e^x$ to deduce

$$e^{-\sum_j |\alpha_{i,j}|^2 E_j} \leq \sum_j |\alpha_{i,j}|^2 e^{-E_j} \quad \text{for all } i.$$

Thus

$$\sum_i p_i \left[\sum_i \ln p_i - \ln \left(\frac{e^{-\sum_j |\alpha_{i,j}|^2 E_j}}{\mathsf{tr}\big(e^{-H}\big)} \right) \right] \geq \sum_i p_i \left[\sum_i \ln p_i - \ln \left(\frac{\sum_j |\alpha_{i,j}|^2 e^{-E_j}}{\mathsf{tr}\big(e^{-H}\big)} \right) \right].$$

Since

$$\frac{\sum_j |\alpha_{i,j}|^2 e^{-E_j}}{\mathsf{tr}\big(e^{-H}\big)} > 0 \quad \text{for all } i$$

and

$$\begin{aligned}
\sum_i \frac{\sum_j |\alpha_{i,j}|^2 e^{-E_j}}{\mathsf{tr}\big(e^{-H}\big)} &= \sum_i \frac{\sum_j |\alpha_{i,j}|^2 \langle\phi_j| e^{-H} |\phi_j\rangle}{\mathsf{tr}\big(e^{-H}\big)} \\
&= \sum_i \frac{\langle\psi_i| e^{-H} |\psi_i\rangle}{\mathsf{tr}\big(e^{-H}\big)} \\
&= \frac{\mathsf{tr}\big(e^{-H}\big)}{\mathsf{tr}\big(e^{-H}\big)} \\
&= 1,
\end{aligned}$$

we deduce from Gibbs' inequality with $q_i = \frac{\sum_j |\alpha_{i,j}|^2 e^{-E_j}}{\mathsf{tr}\big(e^{-H}\big)}$ that

$$\sum_i p_i \left[\sum_i \ln p_i - \ln \left(\frac{\sum_j |\alpha_{i,j}|^2 e^{-E_j}}{\mathsf{tr}\big(e^{-H}\big)} \right) \right] \geq 0.$$

This completes the proof.

5.2.2 Upper bound by finite intervals

We can use Gibbs variational principle to give an upper bound on $f(\beta, S)$ using the specific free energy of a modified Hamiltonian H_ℓ^D on a finite system of ℓ sites. Consider a spin chain of length $\ell+2$ whose sites are indexed by $0, 1, 2, \ldots, \ell, \ell+1$. In the subspace of $\mathcal{H}$ consisting of the states $|\psi\rangle$ such that the spins of the first and the last particles point maximally downwards, i.e.

$$S_0^3 |\psi\rangle = -S \quad \text{and} \quad S_{\ell+1}^3 |\psi\rangle = -S,$$

the action of H_ℓ coincides with the following Hamiltonian.

$$H_\ell^D = \sum H_\ell + 2S^2 + S(S_1^3 + S_\ell^3). \tag{5.6}$$

Generally, for arbitrary states $|\psi\rangle$, we have

$$\langle \psi | H_L^D | \psi \rangle \geq \langle \psi | H_L | \psi \rangle ,$$

which follows from the fact that $2S^2 + S(S_1^3 + S_\ell^3)$ is a positive operator. For convenience, we also define

$$f_\ell^D(\beta, S) := -\frac{1}{\beta \ell} \ln \operatorname{tr} e^{-\beta H_\ell^D}. \tag{5.7}$$

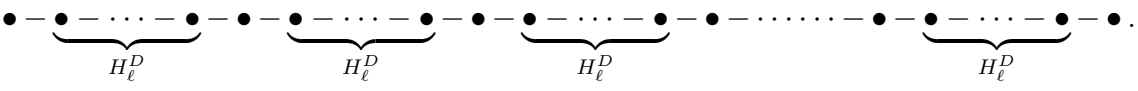
With a total spin chain length

$$L = k(\ell + 1) + 1,$$

we can decompose the original Hilbert space $\mathcal{H}$ into

$$\mathbb{C}^{2S+1} \otimes \Big(\bigotimes_{x=1}^{\ell} \mathbb{C}^{2S+1} \Big) \otimes \mathbb{C}^{2S+1} \otimes \Big(\bigotimes_{x=1}^{\ell} \mathbb{C}^{2S+1} \Big) \otimes \mathbb{C}^{2S+1} \otimes \cdots \otimes \mathbb{C}^{2S+1} \otimes \Big(\bigotimes_{x=1}^{\ell} \mathbb{C}^{2S+1} \Big). \tag{5.8}$$

This corresponds to subdividing the spin chain into k regular intervals of length ℓ and adjacent intervals are separated by 1 site. This subdivision can be schematised as follows.



Let

$$\Gamma_\ell = \frac{e^{-\beta H_\ell^D}}{\operatorname{tr} e^{-\beta H_\ell^D}}$$

be the density matrix on $\Big(\bigotimes_{x=1}^{\ell} \mathbb{C}^{2S+1} \Big)$ which minimises the free energy associated with H_ℓ^D as in (5.4). Consider the state

$$\Gamma = |-S\rangle \langle -S| \otimes \Gamma_\ell \otimes |-S\rangle \langle -S| \otimes \Gamma_\ell \otimes \cdots \otimes |-S\rangle \langle -S| \otimes \Gamma_\ell \otimes |-S\rangle \langle -S| . \tag{5.9}$$

By properties of Γ, we have

$$\operatorname{tr}(H_L\Gamma) = \sum_{i=1}^{k} \operatorname{tr}(H_\ell^D \Gamma_\ell) = k \operatorname{tr}(H_\ell^D \Gamma_\ell)$$

and

$$\operatorname{tr}(\Gamma \ln \Gamma) = \sum_{i=1}^{k} \operatorname{tr}(\Gamma_\ell \ln \Gamma_\ell) = k \operatorname{tr}(\Gamma_\ell \ln \Gamma_\ell)$$

It follows (5.4) and the choice of Γ_ℓ that

$$\begin{aligned} Lf_L(\beta, S) &\le \operatorname{tr}(H_L\Gamma) + \operatorname{tr}(\Gamma \ln \Gamma) \\ &\le k(\operatorname{tr}(H_\ell^D \Gamma_\ell) + \operatorname{tr}(\Gamma_\ell \ln \Gamma_\ell)) \\ &\le k\ell f_\ell^D(\beta, S) \end{aligned}$$

which implies

$$f_L(\beta, S) \le (1 + \ell^{-1})^{-1} f_\ell^D(\beta, S).$$

By letting $k \to \infty$, we have $L \to \infty$ and thus

$$f(\beta, S) \le (1 + \ell^{-1})^{-1} f_\ell^D(\beta, S). \tag{5.10}$$

for arbitrarily large ℓ.

From (5.3) and (5.10), we have an estimate of $f(\beta, S)$ by the specific free energy of finite systems as follows.

$$f_\ell(\beta, S) \le f(\beta, S) \le f_\ell^D(\beta, S) \qquad \text{for arbitrarily large } \ell. \tag{5.11}$$