CHAPTER 2

Fermionic and bosonic systems

In condensed matter physics, more precise models deal with itinerant particles on lattices, which may carry spins. We review the setting in this chapter. Excellent introductory textbooks include Martin and Rothen [2004], ... We restrict to lattice systems, which are simpler and relevant for our purpose, but it is worth noting that all notions can be extended to the continuum setting, see Bratteli and Robinson [1987] for a thorough description. We then introduce two important models, namely the Hubbard model of electrons, and the Bose-Hubbard model of lattice bosons. We explain how spin systems can be derived from itinerant particle systems, and we also explain the Bose-Einstein condensation.

2.1. 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

$$\langle\varphi|\psi\rangle = \sum_{x\in\Lambda} \overline{\varphi(x)}\,\psi(x), \qquad \varphi,\psi \in \ell^2(\Lambda). \tag{2.1}$$

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

$$\mathcal{H}_{\Lambda,n} = \otimes_{i=1}^n \ell^2(\Lambda) \cong \ell^2(\Lambda^n). \tag{2.2}$$

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

$$\Big\{ \bigotimes_{i=1}^n e_{x_i} \Big\}_{x_1,\dots,x_n\in\Lambda}, \tag{2.3}$$

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

$$e_{x_1,\dots,x_n}(y_1,\dots,y_n) = \prod_{i=1}^n \delta_{x_i,y_i}. \tag{2.4}$$

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

$$\begin{aligned} \big(P_+\varphi\big)(x_1,\dots,x_n) &= \frac{1}{n!}\sum_{\sigma\in\mathfrak{S}_n} \varphi(x_{\sigma(1)},\dots,x_{\sigma(n)}), \qquad \varphi\in\ell^2(\Lambda^n) \\ P_+\bigotimes_{i=1}^n \varphi_i &= \frac{1}{n!}\sum_{\sigma\in\mathfrak{S}_n}\bigotimes_{i=1}^n \varphi_{\sigma(i)}, \qquad \varphi_i\in\ell^2(\Lambda) \text{ for } i=1,\dots,n. \end{aligned} \tag{2.5}$$

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

$$\begin{aligned} \big(P_-\varphi\big)(x_1,\dots,x_n) &= \frac{1}{n!}\sum_{\sigma\in\mathfrak{S}_n} (-1)^\sigma \varphi(x_{\sigma(1)},\dots,x_{\sigma(n)}), \qquad \varphi\in\ell^2(\Lambda^n) \\ P_-\bigotimes_{i=1}^n \varphi_i &= \frac{1}{n!}\sum_{\sigma\in\mathfrak{S}_n}(-1)^\sigma\bigotimes_{i=1}^n \varphi_{\sigma(i)}, \qquad \varphi_i\in\ell^2(\Lambda) \text{ for } i=1,\dots,n, \end{aligned} \tag{2.6}$$

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 orthogonal projection operators in the sense that

$$P_\pm^2 = P_\pm, \qquad P_\pm^* = P_\pm. \tag{2.7}$$

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

$$\mathcal{H}_{\Lambda,n}^{(\pm)} \cong P_\pm \ell^2(\Lambda^n) \cong P_\pm \bigotimes_{i=1}^n \ell^2(\Lambda). \tag{2.8}$$

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

$$\begin{aligned} \mathcal{H}_{\Lambda,n}^{(+)} &= \Big\{\varphi\in\mathbb{C}^\Lambda : \varphi(x_{\sigma(1)},\dots,x_{\sigma(n)}) = \varphi(x_1,\dots,x_n)\ \forall\sigma\in\mathfrak{S}_n\Big\}; \\ \mathcal{H}_{\Lambda,n}^{(-)} &= \Big\{\varphi\in\mathbb{C}^\Lambda : \varphi(x_{\sigma(1)},\dots,x_{\sigma(n)}) = (-1)^\sigma\varphi(x_1,\dots,x_n)\ \forall\sigma\in\mathfrak{S}_n\Big\}. \end{aligned} \tag{2.9}$$

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

$$\begin{aligned} \mathcal{N}_{\Lambda,n}^{(+)} &= \big\{(n_x)_{x\in\Lambda} : n_x\in\mathbb{N}_0 \text{ and } \sum_{x\in\Lambda} n_x = n\big\}; \\ \mathcal{N}_{\Lambda,n}^{(-)} &= \big\{(n_x)_{x\in\Lambda} : n_x\in\{0,1\} \text{ and } \sum_{x\in\Lambda} n_x = n\big\}. \end{aligned} \tag{2.10}$$

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

$$\mathcal{H}_{\Lambda,n}^{(\pm)} \cong \ell^2(\mathcal{N}_{\Lambda,n}^{(\pm)}). \tag{2.11}$$

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

$$\begin{aligned} |\boldsymbol{n}\rangle &= \Big(\frac{n!}{\prod_x n_x!}\Big)^{1/2} P_+ e_{x_1,\dots,x_n} \qquad \text{in } \mathcal{H}^{(+)}_{\Lambda,n}; \\ |\boldsymbol{n}\rangle &= (n!)^{1/2} P_+ e_{x_1,\dots,x_n} \qquad \text{in } \mathcal{H}^{(-)}_{\Lambda,n}. \end{aligned} \tag{2.12}$$

The vectors $e_{x_1,\dots,x_n}$ above are the basis vectors defined in (2.4); 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 $x_1 \prec \dots \prec x_n$ 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 2.3. 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

$$\begin{aligned} \dim \mathcal{H}^{(+)}_{\Lambda,n} &= |\mathcal{N}^{(+)}_{\Lambda,n}| = \binom{n + |\Lambda| - 1}{|\Lambda| - 1}, \\ \dim \mathcal{H}^{(-)}_{\Lambda,n} &= |\mathcal{N}^{(-)}_{\Lambda,n}| = \binom{|\Lambda|}{n} \qquad \text{if } n \leq |\Lambda|; \end{aligned} \tag{2.13}$$

this is verified in Exercise 2.4.

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

$$\mathcal{F}^{(+)}_\Lambda = \bigoplus_{n=0}^{\infty} \mathcal{H}^{(+)}_{\Lambda,n}, \qquad \mathcal{F}^{(-)}_\Lambda = \bigoplus_{n=0}^{|\Lambda|} \mathcal{H}^{(-)}_{\Lambda,n}. \tag{2.14}$$

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

$$\langle \varphi, \psi \rangle = \sum_{n \geq 0} \langle \varphi_n, \psi_n \rangle_{\mathcal{H}^{(+)}_{\Lambda,n}}. \tag{2.15}$$

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

$$\mathcal{F}^{(+)}_\Lambda \cong \ell^2(\mathcal{N}^{(+)}_\Lambda) \tag{2.16}$$

where

$$\mathcal{N}^{(+)}_\Lambda = \bigcup_{n \geq 0} \mathcal{N}^{(+)}_{\Lambda,n} = \mathbb{N}^\Lambda. \tag{2.17}$$

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

$$\langle \varphi, \psi \rangle = \sum_{n=0}^{|\Lambda|} \langle \varphi_n, \psi_n \rangle_{\mathcal{H}^{(-)}_{\Lambda,n}}. \tag{2.18}$$

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

$$\mathcal{F}_\Lambda^{(-)} \cong \ell^2(\mathcal{N}_\Lambda^{(-)}) \tag{2.19}$$

where

$$\mathcal{N}_\Lambda^{(-)} = \bigcup_{n\geq 0} \mathcal{N}_{\Lambda,n}^{(+)} = \{0,1\}^\Lambda. \tag{2.20}$$

2.2. Creation and annihilation operators

These operators are most useful in defining the models and in basic calculations. We define them as operators in the spaces of bosonic or fermionic particles, but physicists (and operator algebraists) usually specify their commutation relations, which indeed fixes the whole setting. Following the tradition in physics, we denote a_x, a_x^* the annihilation and creation operators of bosons, and c_x, c_x^* those of fermions.

$$\begin{aligned}
\text{Bosons:}\qquad & a_x : \mathcal{H}_{\Lambda,n}^{(+)} \to \mathcal{H}_{\Lambda,n-1}^{(+)} \\
& \quad a_x|\boldsymbol{n}\rangle = \begin{cases} \sqrt{n_x}\,|\boldsymbol{n}-\delta_x\rangle & \text{if } n_x \geq 1, \\ 0 & \text{if } n_x = 0. \end{cases} \\
& a_x^* : \mathcal{H}_{\Lambda,n}^{(+)} \to \mathcal{H}_{\Lambda,n+1}^{(+)} \\
& \quad a_x^*|\boldsymbol{n}\rangle = \sqrt{n_x+1}\,|\boldsymbol{n}+\delta_x\rangle.
\end{aligned} \tag{2.21}$$

The above operators are bounded since they are defined between finite-dimensional Hilbert spaces. Their extensions to $\mathcal{F}_\Lambda^{(+)}$ are unbounded and, in case we do work in this space (which is not altogether necessary), we need to specify the domains. This is actually straightforward, we take the largest subspace where the image is a bounded vector. Namely,

$$\begin{aligned}
\mathrm{Dom}(a_x) &= \Big\{ \varphi = (\varphi_0, \varphi_1, \dots) \in \mathcal{F}_\Lambda^{(+)} : \sum_{n\geq 1} \big\| a_x \varphi_n \big\|^2_{\mathcal{H}_{\Lambda,n-1}^{(+)}} < \infty \Big\}, \\
\mathrm{Dom}(a_x^*) &= \Big\{ \varphi = (\varphi_0, \varphi_1, \dots) \in \mathcal{F}_\Lambda^{(+)} : \sum_{n\geq 0} \big\| a_x^* \varphi_n \big\|^2_{\mathcal{H}_{\Lambda,n+1}^{(+)}} < \infty \Big\}.
\end{aligned} \tag{2.22}$$

These operators are clearly closed. In Exercise 2.5 you can check that a_x^* is the adjoint of a_x (and conversely), and that these bosonic operators satisfy the commutation relations

$$[a_x, a_y] = 0; \qquad [a_x^*, a_y^*] = 0; \qquad [a_x, a_y^*] = \delta_{x,y}\mathbb{1}. \tag{2.23}$$

One can also check that

$$a_x^* a_x |\boldsymbol{n}\rangle = n_x\,|\boldsymbol{n}\rangle. \tag{2.24}$$

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

$$
\begin{aligned}
\text{Fermions:} \qquad & c_x : \mathcal{H}^{(-)}_{\Lambda,n} \to \mathcal{H}^{(-)}_{\Lambda,n-1} \\
& c_x|\boldsymbol{n}\rangle = \begin{cases} (-1)^{\sum_{y\prec x} n_y} \, |\boldsymbol{n} - \delta_x\rangle & \text{if } n_x = 1, \\ 0 & \text{if } n_x = 0. \end{cases} \\
& c^*_x : \mathcal{H}^{(-)}_{\Lambda,n} \to \mathcal{H}^{(-)}_{\Lambda,n+1} \\
& c^*_x|\boldsymbol{n}\rangle = \begin{cases} (-1)^{\sum_{y\prec x} n_y} \, |\boldsymbol{n} + \delta_x\rangle & \text{if } n_x = 0, \\ 0 & \text{if } n_x = 1. \end{cases}
\end{aligned}
\tag{2.25}
$$

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

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

$$
\{c_x, c_y\} = 0; \qquad \{c^*_x, c^*_y\} = 0; \qquad \{c_x, c^*_y\} = \delta_{x,y} \mathbb{1}. \tag{2.26}
$$

Here also we have that

$$
c^*_x c_x |\boldsymbol{n}\rangle = n_x \, |\boldsymbol{n}\rangle. \tag{2.27}
$$

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 $\mathcal{H}_{\Lambda,n}$:

$$
\boldsymbol{B} = \sum_{i=1}^n B_i, \tag{2.28}
$$

where

$$
B_i = \mathbb{1} \otimes \cdots \otimes \underbrace{B}_{i\text{th particle}} \otimes \cdots \otimes \mathbb{1}. \tag{2.29}
$$

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 2.1. *[One-body operator in the Fock space]*
If $B = (b_{x,y})_{x,y\in\Lambda}$ is an operator on $\ell^2(\Lambda)$, the operator (2.28) in $\mathcal{H}^{(+)}_{\Lambda,n}$ or $\mathcal{H}^{(-)}_{\Lambda,n}$ is equal to

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

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

$$
\langle \boldsymbol{m} | b_{x,y} a^*_x a_y | \boldsymbol{n}\rangle = \sqrt{m_x n_y} \; \delta_{\boldsymbol{m}-\delta_x, \boldsymbol{n}-\delta_y}. \tag{2.30}
$$

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

$$\begin{aligned}\langle \boldsymbol{m}|\boldsymbol{B}|\boldsymbol{n}\rangle &= \frac{n!}{\sqrt{\prod_z m_z! n_z!}} \langle e_{x_1,\dots,x_n}|P_+^2 \boldsymbol{B}|e_{y_1,\dots,y_n}\rangle \\ &= \frac{n!}{\sqrt{\prod_z m_z! n_z!}} \sum_{i=1}^n \langle e_{x_1,\dots,x_n}|P_+^2 B_i|e_{y_1,\dots,y_n}\rangle.\end{aligned} \tag{2.31}$$

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

$$B_i|e_{y_1,\dots,y_n}\rangle = \delta_{y_i,y}|e_{y_1,\dots,x,\dots,y_n}\rangle \tag{2.32}$$

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

$$\begin{aligned}\langle \boldsymbol{m}|\boldsymbol{B}|\boldsymbol{n}\rangle &= \Big(\frac{n!}{\prod_z n_z!}\Big)^{1/2} \sum_{i=1}^n \delta_{y_i,y} \langle \boldsymbol{m}|P_+|e_{y_1,\dots,x,\dots,y_n}\rangle \\ &= \Big(\frac{n!}{\prod_z n_z!}\Big)^{1/2} n_y \Big(\frac{n!}{\prod_z (n_z - \delta_y + \delta_x)!}\Big)^{-1/2} \langle \boldsymbol{m}|\boldsymbol{n} - \delta_y + \delta_x\rangle \\ &= n_y \big(\tfrac{n_x+1}{n_y}\big)^{1/2} \, \delta_{\boldsymbol{m}-\delta_x, \boldsymbol{n}-\delta_y}.\end{aligned} \tag{2.33}$$

This agrees with (2.30). □

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

$$H_\Lambda = -\sum_{i=1}^n \Delta_i + \sum_{1 \le i < j \le n} V_{i,j}, \tag{2.34}$$

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

$$(\Delta\varphi)(x) = \sum_{y \in \Lambda} t_{x,y} \varphi(y). \tag{2.35}$$

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

$$V_{i,j} \varphi(x_1, \dots, x_n) = W(x_i - x_j) \varphi(x_1, \dots, x_n). \tag{2.36}$$

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

$$H_\Lambda = -\sum_{x,y \in \Lambda} t_{x,y} a_x^* a_y + \tfrac12 W(0) \sum_{x \in \Lambda} a_x^* a_x (a_x^* a_x - 1) + \tfrac12 \sum_{\substack{x,y \in \Lambda \\ x \neq y}} W(x-y) a_x^* a_x a_y^* a_y. \tag{2.37}$$

As an operator in $\mathcal{F}_\Lambda^{(+)}$ it is unbounded. It is well defined on $\ell^2_{\mathrm{f}}(\mathcal{N}_\Lambda^{(+)})$; 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

$$a_x \equiv S_x^{(-)}, \qquad a_x^* \equiv S_x^{(+)}, \qquad a_x^* a_x \equiv S_x^{(3)} + \tfrac{1}{2}. \tag{2.38}$$

2.3. The Bose-Hubbard model

A simple interacting model is obtained by choosing the potential function to be on-site only, that is, $W(0) = U$ and $W(x) = 0$ for $x \neq 0$, with U a positive constant. This is known as the Bose-Hubbard model.

Bose-Hubbard hamiltonian:

$$H_\Lambda = -t \sum_{xy \in \mathcal{E}(\Lambda)} \big(a_x^* a_y + a_y^* a_x\big) + \tfrac{1}{2} U \sum_{x \in \Lambda} n_x(n_x - 1) - \mu \sum_{x \in \Lambda} n_x. \tag{2.39}$$

The first term gives the kinetic energy of the lattice bosons. Interactions are on-site only. Notice that $\frac{1}{2}n(n-1)$ is the number of pairs among n particles; in this model, any pair contributes energy U. The last term involves the chemical potential μ. Despite its simplicity, the model is difficult to study. One can check that in the limit $U \to \infty$, we get hard-core bosons, and the hamiltonian is equivalent to the quantum XY spin model.

The phase diagram is depicted in Fig. 2.1. For small t the system is in "Mott insulating phases", which are phases whose insulating properties are due to interactions (this contrasts to free fermions in solids, where the insulating properties are due to gaps in the band structure of the spectrum of the hamiltonian). For large t, or equivalently, small U, the system is expected to display Bose-Einstein condensation.

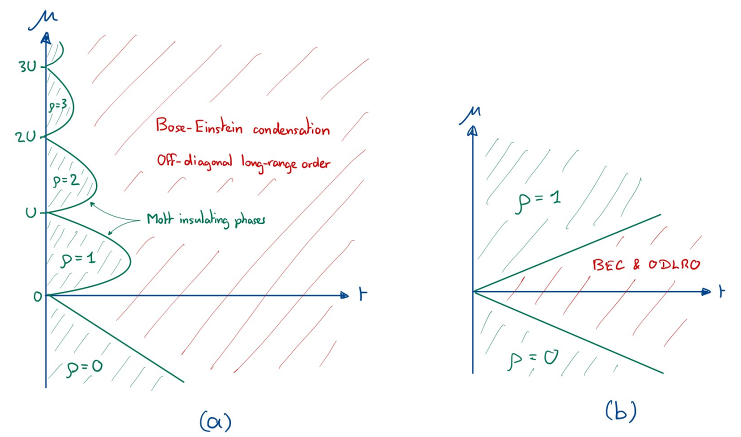

FIGURE 2.1. (a) Ground state phase diagram of the **Bose-Hubbard model** for dimensions $d \geq 2$. (b) The same, in the limit $U \to \infty$; this is the hard-core Bose gas.

2.4. Bose–Einstein condensation

We now consider the *ideal Bose gas* on the lattice, where particles do not interact. The situation is non-trivial nonetheless because of the Bose statistics. Einstein understood in 1925 that a phase transition takes place. His description was for particles in the continuum, but the situation on the lattice is essentially identical.

The hamiltonian is then

$$H_\Lambda = -t \sum_{xy \in \mathcal{E}(\Lambda)} \bigl(a_x^* a_y + a_y^* a_x\bigr) - 2d \sum_{x \in \Lambda} n_x. \tag{2.40}$$

The $2d$ term is mathematically not important, it means that the lowest eigenvalue of H_Λ is essentially 0 and that $\mu = 0$ is the value where the pressure ceases to be finite (see below).

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

$$\begin{aligned} f_{\Lambda,n}(\beta) &= -\frac{1}{\beta|\Lambda|} \log \operatorname{Tr}_{\mathcal{H}^{(+)}_{\Lambda,n}} \mathrm{e}^{-\beta H_\Lambda}. \\ f(\beta,\rho) &= \lim_{\Lambda \Uparrow \mathbb{Z}^d} f_{\Lambda,\lfloor \rho|\Lambda| \rfloor}(\beta). \end{aligned} \tag{2.41}$$

Here, the parameter ρ is the **density**. Existence of the limit can be proved in a similar fashion as for spin systems (see a later chapter). The **pressure** by

$$\begin{aligned} p_\Lambda(\beta,\mu) &= \frac{1}{|\Lambda|} \log \sum_{n \geq 0} \mathrm{e}^{\beta\mu n} \operatorname{Tr}_{\mathcal{H}^{(+)}_{\Lambda,n}} \mathrm{e}^{-\beta H_\Lambda}. \\ p(\beta,\mu) &= \lim_{\Lambda \Uparrow \mathbb{Z}^d} p_\Lambda(\beta,\mu). \end{aligned} \tag{2.42}$$

One can check that $p_\Lambda(\beta,\mu)$ is finite for $\mu < 0$, infinite for $\mu > 0$, and is increasing and convex in μ.

Proposition 2.2. *The functions $f(\beta,\rho)$ and $p(\beta,\mu)$ are related by Legendre transforms:*

$$\begin{aligned} f(\beta,\rho) &= \sup_{\mu<0} \bigl(\rho\mu - \tfrac{1}{\beta} p(\beta,\mu)\bigr), \\ p(\beta,\mu) &= \sup_{\rho \geq 0} \bigl(\beta\rho\mu - \beta f(\beta,\rho)\bigr). \end{aligned}$$

Proof. The pressure is equal to

$$p_\Lambda(\beta,\mu) = \frac{1}{|\Lambda|} \log \sum_{\rho \in \frac{1}{|\Lambda|}\mathbb{N}_0} \mathrm{e}^{|\Lambda|(\beta\rho\mu - \beta f_\Lambda(\beta,\rho))}. \tag{2.43}$$

Keeping only the largest term in the sum, we get

$$p_\Lambda(\beta,\mu) \geq \sup_\rho (\beta\rho\mu - \beta f_{\Lambda,\rho|\Lambda|}(\beta)). \tag{2.44}$$

Recall that, if (a_{ij}) is double sequence, we have $\liminf_i (\sup_j a_{ij}) \geq \sup_j (\liminf_i a_{ij})$. This allows to take the limit $\Lambda \Uparrow \mathbb{Z}^d$.

For the upper bound, let $\varepsilon > 0$. From (2.43) we have

$$\begin{aligned} p_\Lambda(\beta, \mu - \varepsilon) &= \frac{1}{|\Lambda|} \log \sum_{\rho \in \frac{1}{|\Lambda|}\mathbb{N}_0} \mathrm{e}^{|\Lambda|(\beta\rho\mu - \beta f_{\Lambda,\rho|\Lambda|}(\beta))} \, \mathrm{e}^{-|\Lambda|\beta\rho\varepsilon} \\ &\leq \sup_\rho (\beta\rho\mu - \beta f_{\Lambda,\rho|\Lambda|}(\beta)) + \tfrac{1}{|\Lambda|} \log \tfrac{1}{1-\mathrm{e}^{-\beta\varepsilon}} \\ &\leq p_\Lambda(\beta,\mu) + \tfrac{1}{|\Lambda|} \log \tfrac{1}{1-\mathrm{e}^{-\beta\varepsilon}}. \end{aligned} \tag{2.45}$$

The remaining difficulty is to take the limit $\Lambda \Uparrow \mathbb{Z}^d$ and interchange it with $\sup_\rho$. One possibility is to establish that $f_{\Lambda,\rho|\Lambda|}(\beta)$ converges to $f(\beta,\rho)$ uniformly in ρ, which allows to replace $f_{\Lambda,\rho|\Lambda|}(\beta)$ with $f(\beta,\rho) + \epsilon$. We do not give details here. Since the inequalities hold for arbitrarily small ε, ϵ, we get that the pressure is indeed the Legendre transform of the free energy. Both functions being convex, the converse Legendre transform is also clear. □

The pressure can be calculated exactly. The result is depicted in Fig. 2.2, also with its Legendre transform. We see that in dimensions 3 and higher, the free energy is not analytic at a point $\rho_c = \rho_c(\beta)$.

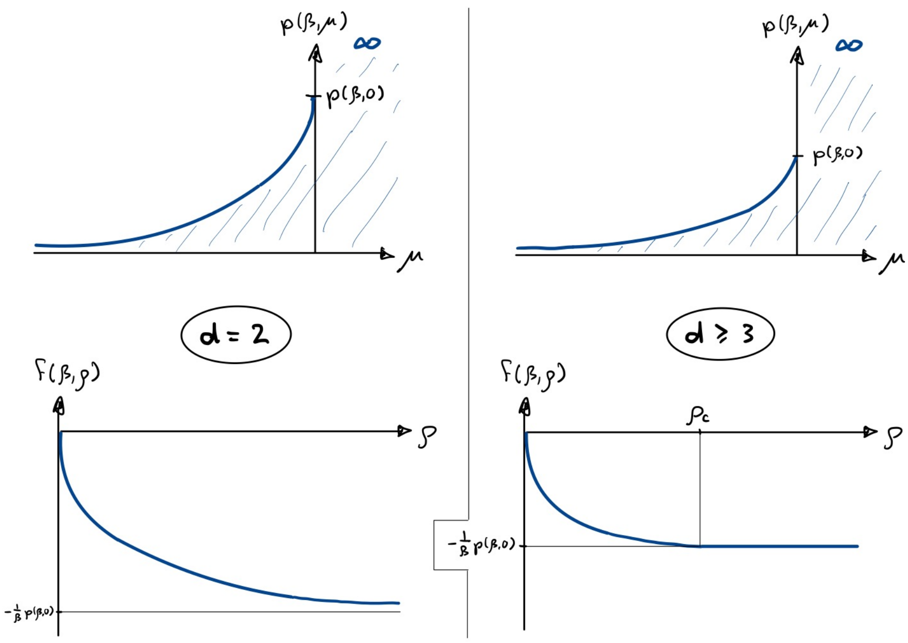

FIGURE 2.2. Pressure and free energy of the ideal Bose gas, in dimensions two and three (or higher).

THEOREM 2.3 (Pressure of the ideal Bose gas). *For $\mu < 0$, the pressure is*

$$p(\beta,\mu) = -\frac{1}{(2\pi)^d}\int_{[-\pi,\pi]^d}\log\Big(1-\mathrm{e}^{-\beta(\varepsilon(k)-\mu)}\Big)\mathrm{d}k,$$

where

$$\varepsilon(k) = 2\sum_{i=1}^d (1-\cos k_i).$$

Note that $\varepsilon(k) \sim \|k\|^2$ for small k. For $\mu > 0$ the pressure is infinite.

The density of the system is

$$\rho(\beta,\mu) = \frac{1}{\beta}\frac{\partial}{\partial\mu}p(\beta,\mu) = \frac{1}{(2\pi)^d}\int_{[-\pi,\pi]^d}\frac{1}{\mathrm{e}^{\beta(\varepsilon(k)-\mu)}-1}\mathrm{d}k. \tag{2.46}$$

The critical density is equal to the limit $\mu \uparrow 0$ of $\rho(\beta,\mu)$:

$$\rho_{\mathrm{c}}(\beta) = \frac{1}{(2\pi)^d}\int_{[-\pi,\pi]^d}\frac{1}{\mathrm{e}^{\beta\varepsilon(k)}-1}\mathrm{d}k. \tag{2.47}$$

The critical density is finite for $d \geq 3$, but infinite for $d = 1,2$. In the continuum the expression for the critical density is the same, except that $\varepsilon(k)$ is replaced by $\|k\|^2$ and the integral is over all $\mathbb{R}^d$. One can then expand the fraction as a geometric series, integrate the gaussians, and one gets the well-known formula of Einstein.

PROOF OF THEOREM 2.3. We work in a box with periodic boundary conditions (the infinite limit does not depend on the choice of boundary conditions, so we can choose the most convenient). That is, $\Lambda_\ell^{\mathrm{per}} = \{1,\dots,\ell\}^d_{\mathrm{per}}$, and we define the dual Fourier space to be $\Lambda_\ell^* = \frac{\pi}{\ell}\{-\frac{\ell}{2}+1,\dots,\frac{\ell}{2}\}^d \subset [-\pi,\pi]^d$. We have $|\Lambda_\ell^*| = |\Lambda_\ell^{|rmper}| = \ell^d$. We introduce the creation and annihilation operators of the Fourier modes, namely

$$\hat{a}_k = \frac{1}{\ell^{d/2}}\sum_{x\in\Lambda_\ell^{\mathrm{per}}}\mathrm{e}^{-\mathrm{i}kx}\,a_x, \qquad k \in \Lambda_\ell^*. \tag{2.48}$$

Then we have

$$a_x = \frac{1}{\ell^{d/2}}\sum_{k\in\Lambda_\ell^*}\mathrm{e}^{\mathrm{i}kx}\,\hat{a}_k \tag{2.49}$$

and

$$\sum_{x,y\in\mathcal{E}_{\Lambda_\ell^{|rmper}}} a_x^* a_y - 2d\sum_{x\in\Lambda_\ell^{\mathrm{per}}} a_x^* a_x = \sum_{k\in\Lambda_\ell^*}\varepsilon(k)\hat{a}_k^*\hat{a}_k. \tag{2.50}$$

One can check that the eigenvalues of $\hat{a}_k^*\hat{a}_k$ are $0,1,2,\dots$. Using occupation numbers (n_k) with respect to $k \in \Lambda_\ell^*$ we have

$$p_{\Lambda_\ell^{\mathrm{per}}}(\beta,\mu) = \frac{1}{\ell^d}\log\sum_{(n_k)}\mathrm{e}^{-\beta\sum_k(\varepsilon(k)-\mu)n_k} = \frac{1}{\ell^d}\sum_{k\in\Lambda_\ell^*}\log\frac{1}{1-\mathrm{e}^{-\beta(\varepsilon(k)-\mu)}}. \tag{2.51}$$

As $\ell \to \infty$ the sum over k converges to a Riemann integral and we get the expression of the theorem. For $\mu > 0$ we clearly get ∞. $\square$

Let us clarify the notion of symmetry breaking that is associate with Bose-Einstein condensation. 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:

$$H_\Lambda = \mathrm{e}^{\mathrm{i}\theta N_\Lambda} H_\Lambda \mathrm{e}^{-\mathrm{i}\theta N_\Lambda}, \qquad \theta \in [0, 2\pi). \tag{2.52}$$

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 grand-canonical ensemble). The question is whether it remains positive in the infinite volume limit, and as $\|x - y\| \to \infty$. This can be established in the ideal gas.

THEOREM 2.4.

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

where the critical density $\rho_{\mathrm{c}}(\beta)$ is defined in Eq. (2.47).

PROOF. We invoke the Fourier transform of the creation and annihilation operators as in the proof of Theorem 2.3. We have

$$\frac{1}{\ell^d} \sum_{x\in\Lambda_\ell^{\mathrm{per}}} \langle a_0^* a_x \rangle_{\Lambda_\ell^{\mathrm{per}},\beta,n} = \frac{1}{\ell^{2d}} \sum_{x,y\in\Lambda_\ell^{\mathrm{per}}} \langle a_x^* a_y \rangle_{\Lambda_\ell^{\mathrm{per}},\beta,n} = \frac{1}{\ell^d} \langle \hat a_0^* \hat a_0 \rangle_{\Lambda_\ell^{\mathrm{per}},\beta,n}. \tag{2.53}$$

The average can be written as an expectation with occupation numbers $(n_k)_{k\in\Lambda_\ell^*}$ satisfying $\sum_k n_k = n$. Namely,

$$\frac{1}{\ell^d} \sum_{x\in\Lambda_\ell^{\mathrm{per}}} \langle a_0^* a_x \rangle_{\Lambda_\ell^{\mathrm{per}},\beta,n} = \frac{1}{\ell^d} \langle \hat a_0^* \hat a_0 \rangle_{\Lambda_\ell^{\mathrm{per}},\beta,n} = \frac{1}{Z_{\Lambda_\ell^{\mathrm{per}},\beta,\rho}} \sum_{(n_k)_{k\in\Lambda_\ell^*}: \sum_k n_k = n} \frac{n_0}{\ell^k} \mathrm{e}^{-\beta\sum_k \varepsilon(k) n_k}. \tag{2.54}$$

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

$$\begin{aligned}
\frac{1}{\ell^d} \sum_{x\in\Lambda_\ell^{\mathrm{per}}} \langle a_0^* a_x \rangle_{\Lambda_\ell^{\mathrm{per}},\beta,n} &= \frac{1}{\ell^d} \mathbb{E}[n_0] = \frac{n}{\ell^d} - \frac{1}{\ell^d} \sum_{k\neq 0} \mathbb{E}[n_k] \\
&= \frac{n}{\ell^d} - \frac{1}{\ell^d} \sum_{k\neq 0} \sum_{i\geq 1} \mathbb{P}[n_k \geq i] \\
&= \frac{n}{\ell^d} - \frac{1}{\ell^d} \sum_{k\neq 0} \frac{1}{Z_{\Lambda_\ell^{\mathrm{per}},\beta,n}} \sum_{i\geq 1} \sum_{(n_{k'}): \sum_{k'} n_{k'} = n, n_k \geq i} \mathrm{e}^{-\beta\sum_{k'} \varepsilon(k') n_{k'}} \\
&= \frac{n}{\ell^d} - \frac{1}{\ell^d} \sum_{k\neq 0} \sum_{i\geq 1} \mathrm{e}^{-\beta\varepsilon(k) i} \frac{Z_{\Lambda_\ell^{\mathrm{per}},\beta,n-i}}{Z_{\Lambda_\ell^{\mathrm{per}},\beta,n}} \\
&\geq \frac{n}{\ell^d} - \frac{1}{\ell^d} \sum_{k\neq 0} \frac{1}{\mathrm{e}^{\beta\varepsilon(k)} - 1}.
\end{aligned} \tag{2.55}$$

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 $\rho - \rho_c(\beta)$.

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.

Let us prove the converse inequality. For any $\eta \geq 0$, we have that

$$\lim_{\ell\to\infty} \frac{1}{\beta\ell^d} \log \mathbb{P}[n_0 \geq \ell^d \eta] = \lim_{\ell\to\infty} \frac{1}{\beta\ell^d} \log \frac{Z_{\Lambda_\ell^{\rm per},\beta,n-\ell^d\eta}}{Z_{\Lambda_\ell^{\rm per},\beta,n}} = f(\beta,\rho) - f(\beta,\rho-\eta). \tag{2.56}$$

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

$$\mathbb{P}[n_0 \geq \ell^d \eta] \leq \mathrm{e}^{-\ell^d \delta} \tag{2.57}$$

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

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.

2.5. The Hubbard model

The Hubbard model is a lattice model that involves itinerant electrons, which are fermions carrying $S = \frac{1}{2}$ spins. It is the most important model in condensed matter physics. It is a gross simplification of the description of a large system of electrons that interact among themselves and with fixed nuclei. It is nonetheless a difficult model to study, and people expect it to have very rich phase diagrams. At low temperatures, and depending on the lattice and on the particle density, the system may exhibit spontaneous magnetisation, antiferromagnetic long-range order, or superconductivity. We recommend the recent book of Tasaki [**30**] for an excellent introduction to the Hubbard model. Here we give a minimal introduction to the setting and we show a connection to the Heisenberg antiferromagnet using a suitable perturbative expansion.

Let $\Lambda \Subset \mathbb{Z}^d$. A configuration of electrons carrying spins is denoted $\eta = (\eta_{x,\sigma})$ where $\eta_{x,\sigma} \in \{0,1\}$ with $x \in \Lambda$ and $\sigma \in \{\uparrow,\downarrow\}$. Let E_Λ denote the set of configurations:

$$E_\Lambda = \{0,1\}^{\Lambda\times\{\uparrow,\downarrow\}} \simeq \{0,\uparrow,\downarrow,2\}^\Lambda. \tag{2.58}$$

We have $|E_\Lambda| = 4^{|\Lambda|}$. The Hilbert space is $\mathcal{H}_\Lambda = \ell^2(E_\Lambda)$ whose dimension is $4^{|\Lambda|}$.

We need to choose an order on $\Lambda \times \{\uparrow,\downarrow\}$. It is convenient to consider the spiral order in $\mathbb{Z}^d$ (it is illustrated in Fig. 2.3), which has the advantage that the number of preceding sites is always finite. We also decide that $\downarrow<\uparrow$. Then

$$(x,\sigma) < (y,\sigma') \quad\Longleftrightarrow\quad x < y \text{ or } \big(x = y \text{ and } \sigma < \sigma'\big). \tag{2.59}$$

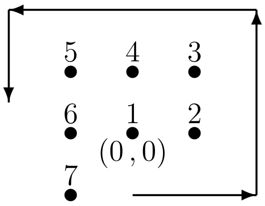

FIGURE 2.3. The spiral order in $\mathbb{Z}^2$ (figure taken from [**6**]).

This allows to define the creation and annihilation operators as follows. Given $\eta \in E_\Lambda$ and $x \in \Lambda$, $\sigma \in \{\uparrow, \downarrow\}$,

$$
\begin{aligned}
c^*_{x,\sigma}|\eta\rangle &= (-1)^{\sum_{(y,\sigma')<(x,\sigma)} \eta_{y,\sigma'}} \begin{cases} |\eta + \delta_{x,\sigma}\rangle & \text{if } \eta_{x,\sigma} = 0, \\ 0 & \text{otherwise.} \end{cases} \\
c_{x,\sigma}|\eta\rangle &= (-1)^{\sum_{(y,\sigma')<(x,\sigma)} \eta_{y,\sigma'}} \begin{cases} |\eta - \delta_{x,\sigma}\rangle & \text{if } \eta_{x,\sigma} = 1, \\ 0 & \text{otherwise.} \end{cases}
\end{aligned} \tag{2.60}
$$

The prefactor looks cumbersome but one rarely invokes it in calculations. One should rather keep in mind that $c^*_{x,\sigma}$ and $c_{x,\sigma}$ are adjoint of each other, and that we have the following anticommutation relations, for any $x, y \in \Lambda$ and $\sigma, \sigma' \in \{\uparrow, \downarrow\}$:

$$
\begin{aligned}
\{c^*_{x,\sigma}, c^*_{y,\sigma'}\} &= \{c_{x,\sigma}, c_{y,\sigma'}\} = 0, \\
\{c^*_{x,\sigma}, c_{y,\sigma'}\} &= \delta_{x,y}\delta_{\sigma,\sigma'}\mathbb{1}.
\end{aligned} \tag{2.61}
$$

We also introduce the number operators $n_{x,\sigma} = c^*_{x,\sigma} c_{x,\sigma}$ that satisfy

$$
n_{x,\sigma}|\eta\rangle = \eta_{x,\sigma}|\eta\rangle. \tag{2.62}
$$

Let $n_x = n_{x,\uparrow} + n_{x,\downarrow}$. Further, all basis vectors can be expressed using a product a creation operators that act on the “vacuum state” $|0\rangle$, which is the vector that corresponds to the empty configuration $\eta \equiv 0$. Namely,

$$
|\eta\rangle = c^*_{x_1,\sigma_1} c^*_{x_2,\sigma_2} \dots c^*_{x_N,\sigma_N} |0\rangle. \tag{2.63}
$$

Here $(x_1, \sigma_1) < \dots < (x_N, \sigma_N)$ are such that $\eta_{x_i,\sigma_i} = 1$ and the order is according to (2.59). N is the number of particles in the state $|\eta\rangle$, it is equal to $\sum_{x,\sigma} \eta_{x,\sigma}$. The relations (2.61)–(2.63) are verified in Exercise 2.9.

The Hubbard model depends on three real parameters. t is in front of the kinetic energy of the electrons and is related to their mass; U is the strength of the onsite interactions (whose physical origin is the Coulomb interactions between electrons); μ is the chemical potential that allows to vary the density.

Hubbard hamiltonian:

$$
H_\Lambda = -t \sum_{xy \in \mathcal{E}(\Lambda)} \sum_{\sigma=\downarrow,\uparrow} \bigl(c^*_{x,\sigma} c_{y,\sigma} + c^*_{y,\sigma} c_{x,\sigma} \bigr) + U \sum_{x \in \Lambda} n_{x,\uparrow} n_{x,\downarrow} - \mu \sum_{x \in \Lambda} (n_{x,\uparrow} + n_{x,\downarrow}). \tag{2.64}
$$

Partition functions and Gibbs states are defined exactly as for spin systems. The terms in the Hubbard model are made of *even* numbers of creation and annihilation operators, and they therefore commute when their supports are disjoint. The construction of the evolution operator, Proposition 3.17, remains valid, and KMS states are well defined. The other characterisations of infinite volume Gibbs states also hold.

2.6. Spin operators and symmetries

Using creation and annihilation operators, we define

$$S_x^{(+)} = c^*_{x,\uparrow} c_{x,\downarrow}, \qquad S_x^{(-)} = c^*_{x,\downarrow} c_{x,\uparrow}, \qquad S_x^{(3)} = \tfrac12 (n_{x,\uparrow} - n_{x,\downarrow}). \tag{2.65}$$

We further set $S_x^{(1)} = \frac12 (S_x^{(+)} + S_x^{(-)})$ and $S_x^{(2)} = \frac{1}{2\mathrm{i}} (S_x^{(+)} - S_x^{(-)})$. Then we have (Exercise 2.10)

$$\begin{aligned}
&[S_x^{(1)}, S_y^{(2)}] = \mathrm{i}\delta_{x,y} S_x^{(3)}, \quad [S_x^{(2)}, S_y^{(3)}] = \mathrm{i}\delta_{x,y} S_x^{(1)}, \quad [S_x^{(3)}, S_y^{(1)}] = \mathrm{i}\delta_{x,y} S_x^{(2)}, \\
&(S_x^{(1)})^2 + (S_x^{(2)})^2 + (S_x^{(3)})^2 = \tfrac34 \mathbb{1}.
\end{aligned} \tag{2.66}$$

Let us list some symmetries of the Hubbard hamiltonian.

PROPOSITION 2.5.

(a) SU(2) symmetry: $[H_\Lambda, \sum_{x\in\Lambda} S_x^{(i)}] = 0$ *for* $i = 1, 2, 3$.

(b) Gauge invariance: $[H_\Lambda, \sum_{x\in\Lambda} n_x] = 0$.

The proof is in Exercise 2.11. This allow to construct the unitary operators $U_\Lambda^{(\vec a)} = \mathrm{e}^{\mathrm{i} \sum_{x\in\Lambda} \vec a \cdot \vec S_x}$, $\vec a \in \mathbb{R}^3$, and $U_\Lambda^{(\theta)} = \mathrm{e}^{\mathrm{i}\theta \sum_{x\in\Lambda} n_x}$ that allow to establish that finite-volume Gibbs states satisfy

$$\langle S_x^{(i)} \rangle_{\Lambda,\beta} = 0, \qquad \langle c^*_{x,\uparrow} c^*_{y,\downarrow} \rangle_{\Lambda,\beta} = 0. \tag{2.67}$$

But one cannot rule out the existence of infinite-volume Gibbs states where the above expectations differ from 0; the first is a state displaying magnetic properties, the second is a superconductive state with Cooper pairs.

Next we consider particle-hole transformations. This is not a symmetry of the model, but it allows to relate hamiltonians with different parameters. Let $U^{\mathrm{ph}}_{x,\sigma} = \mathrm{i}(c^*_{x,\sigma} + c_{x,\sigma})$. We then have

$$(U^{\mathrm{ph}}_{x,\sigma})^{-1} c_{x,\sigma} U^{\mathrm{ph}}_{x,\sigma} = c^*_{x,\sigma}, \qquad (U^{\mathrm{ph}}_{x,\sigma})^{-1} c^*_{x,\sigma} U^{\mathrm{ph}}_{x,\sigma} = c_{x,\sigma}. \tag{2.68}$$

Let $U^{\mathrm{ph}}_\Lambda = \prod_{x\in\Lambda} U^{\mathrm{ph}}_{x,\uparrow} U^{\mathrm{ph}}_{x,\downarrow}$. Then we have

$$(U^{\mathrm{ph}}_\Lambda)^{-1} H_\Lambda^{t,U,\mu} U^{\mathrm{ph}}_\Lambda = H_\Lambda^{-t,U,U-\mu} + (U-\mu)|\Lambda|. \tag{2.69}$$

This is checked in Exercise 2.13. This shows that the sign of t does not matter.

2.7. Relation to the antiferromagnetic Heisenberg model

We now explain a perturbation expansion that applies to half-filling (density 1) and U large. The particular feature of the expansion is to deal with interactions rather than operators; it was first developed and used in [**6**].

We consider the hamiltonian $H_\Lambda = H_\Lambda^{(0)} + tT_\Lambda$ where

$$\begin{aligned} H_\Lambda^{(0)} &= U \sum_{x\in\Lambda} (n_{x,\uparrow} - \tfrac12)(n_{x,\downarrow} - \tfrac12), \\ T_\Lambda &= \sum_{xy\in\mathcal{E}(\Lambda)} \sum_{\sigma=\uparrow,\downarrow} \bigl(c^*_{x,\sigma} c_{y,\sigma} + c^*_{y,\sigma} c_{x,\sigma} \bigr). \end{aligned} \tag{2.70}$$

This the Hubbard model at half-filling, where a particle-hole symmetry guarantees that $\langle n_x \rangle_{\Lambda,\beta} = 1$ for any bipartite lattice Λ and any β (see Exercise 2.14).

In order to introduce the expansion, recall the definition of the adjoint operation and of its inverse: For A, B hermitian matrices, we let

$$\begin{aligned} \mathrm{ad}_A B &= [A, B], \\ \mathrm{ad}_A^{-1} B &= \sum_{\substack{a,a'\in\mathrm{Spec}(A) \\ a\neq a'}} P_a \frac{B}{a-a'} P_{a'}. \end{aligned} \tag{2.71}$$

Here P_a is the projector onto the eigensubspace of A with eigenvalue a. One can check (Exercise 2.15) that ad_A and ad_A^{-1} are inverse operations, in the sense that

$$\mathrm{ad}_A \mathrm{ad}_A^{-1} B = \mathrm{ad}_A^{-1} \mathrm{ad}_A B = B^{\mathrm{od}}, \tag{2.72}$$

where $B^{\mathrm{od}} = \sum_{a\neq a'} P_a B P_{a'}$ is the off-diagonal part of B in the basis of eigenvectors of A.

Let S_Λ such that $S_\Lambda^* = -S_\Lambda$ and let $U_\Lambda = \mathrm{e}^{tS_\Lambda}$. By the Lie-Schwinger expansion (Lemma 3.16) we have

$$U_\Lambda H_\Lambda U_\Lambda^{-1} = H_\Lambda^{(0)} + tT_\Lambda + t\,\mathrm{ad}_{S_\Lambda} H_\Lambda^{(0)} + t^2 \mathrm{ad}_{S_\Lambda} T_\Lambda + \tfrac12 t^2 \mathrm{ad}^2_{S_\Lambda} H_\Lambda^{(0)} + O(t^3). \tag{2.73}$$

We require that $T_\Lambda = -\mathrm{ad}_{S_\Lambda} H_\Lambda^{(0)} = \mathrm{ad}_{H_\Lambda^{(0)}} S_\Lambda$, so we choose

$$S_\Lambda = \mathrm{ad}^{-1}_{H_\Lambda^{(0)}} T_\Lambda = \sum_{xy\in\mathcal{E}(\Lambda)} \mathrm{ad}^{-1}_{H_\Lambda^{(0)}} T_{xy} \equiv \sum_{xy\in\mathcal{E}(\Lambda)} S_{xy}. \tag{2.74}$$

We also have $\mathrm{ad}^2_{S_\Lambda} H_\Lambda^{(0)} = -\mathrm{ad}_{S_\Lambda} T_\Lambda$. We obtain the expansion

$$U_\Lambda H_\Lambda U_\Lambda^{-1} = H_\Lambda^{(0)} + \tfrac12 t^2 \mathrm{ad}_{S_\Lambda} T_\Lambda + O(t^3). \tag{2.75}$$

We can check that

$$\begin{aligned} \langle 0,2 | S_{xy} | \uparrow,\downarrow \rangle = \langle 2,0 | S_{xy} | \uparrow,\downarrow \rangle = -\frac{1}{U} = -\langle \uparrow,\downarrow | S_{xy} | 0,2 \rangle = -\langle \uparrow,\downarrow | S_{xy} | 2,0 \rangle, \\ \langle 0,2 | S_{xy} | \downarrow,\uparrow \rangle = \langle 2,0 | S_{xy} | \downarrow,\uparrow \rangle = +\frac{1}{U} = -\langle \downarrow,\uparrow | S_{xy} | 0,2 \rangle = -\langle \downarrow,\uparrow | S_{xy} | 2,0 \rangle. \end{aligned} \tag{2.76}$$

We now restrict on the subspace with exactly one particle per site. Let $P_\Lambda^{(1)}$ be the corresponding projector, namely

$$P_\Lambda^{(1)} = \otimes_{x\in\Lambda}\big(|\uparrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow|\big). \tag{2.77}$$

Notice that $P_\Lambda^{(1)} H_\Lambda P_\Lambda^{(1)} = -\frac14 U|\Lambda| P_\Lambda^{(1)}$; in order to obtain a nontrivial perturbation result, we need to expand before we apply the projector! One can check that $P_\Lambda^{(1)}(\mathrm{ad}_{S_\Lambda} T_\Lambda) P_\Lambda^{(1)}$ is a sum of nearest-neighbour terms only. We have

$$\begin{aligned} \langle\uparrow,\downarrow|S_{xy}T_{xy}|\uparrow,\downarrow\rangle &= \langle\downarrow,\uparrow|S_{xy}T_{xy}|\downarrow,\uparrow\rangle = -\frac{2}{U}, \\ \langle\uparrow,\downarrow|S_{xy}T_{xy}|\downarrow,\uparrow\rangle &= \langle\downarrow,\uparrow|S_{xy}T_{xy}|\uparrow,\downarrow\rangle = +\frac{2}{U}. \end{aligned} \tag{2.78}$$

The matrix elements involving $|\uparrow,\uparrow\rangle$ and $|\downarrow,\downarrow\rangle$ are zero. One gets (Exercise 2.16)

$$P_{xy}^{(1)}[S_{xy}, T_{xy}] P_\Lambda^{(1)} = \frac{8}{U} P_\Lambda^{(1)}\big(\vec S_x\cdot\vec S_y - \tfrac14\big) P_\Lambda^{(1)}. \tag{2.79}$$

We have obtained:

THEOREM 2.6.

$$P_\Lambda^{(1)} U_\Lambda H_\Lambda U_\Lambda^{-1} P_\Lambda^{(1)} = \frac{4t^2}{U}\sum_{xy\in\Lambda} P_\Lambda^{(1)}\,\vec S_x\cdot\vec S_y\,P_\Lambda^{(1)} - \tfrac14 U|\Lambda| P_\Lambda^{(1)} + O(t^3).$$

The $O(t^3)$ term is a sum of local interactions with exponential decay. The first term is indeed the antiferromagnetic Heisenberg model. This expansion suggests the existence of a phase with antiferromagnetic long-range order. But the Hubbard hamiltonian is not reflection positive and such a phase has not been mathematically proved.

EXERCISE 2.1. *Verify that the operators $P_\pm$ defined in (2.5)–(2.6) are indeed projectors.*

EXERCISE 2.2. *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 2.3. *Let $(n_x) \in \mathcal{N}_{\Lambda,n}^{(\pm)}$ and $(x_1,\dots,x_n)$ such that $\#\{i=1,\dots,n : x_i = x\} = n_x$ for all $x\in\Lambda$. Verify that*

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

EXERCISE 2.4. *Verify Eq. (2.13) about the dimensions of the symmetric and antisymmetric spaces.*

EXERCISE 2.5. *Verify that that a_x and a_x^* are adjoint of one another. In the bosonic case, this involves their domains.*

EXERCISE 2.6. *Verify the commutation relations (2.23) and (2.26).*

EXERCISE 2.7. *Give the proof of Lemma 2.1 in the fermionic case.*

EXERCISE 2.8. *In this exercise we outline a variant of the proof of Theorem 2.4, starting from the probabilistic representation in (2.54) and (2.55).*

(1) *Show that we can write*

$$\frac{1}{\ell^d}\sum_{k\neq 0}\mathbb{E}[n_k] = \mathbb{E}[X_\ell \mid X_\ell \le \rho] \tag{2.80}$$

where

$$X_\ell = \frac{1}{\ell^d}\sum_{k\in\Lambda_\ell^*\setminus\{0\}} N_k \tag{2.81}$$

and the N_k are independent geometric random variables:

$$\mathbb{P}(N_k = r) = (\,\mathrm{e}^{-\beta\varepsilon(k)}\,)^r(1-\mathrm{e}^{-\beta\varepsilon(k)}\,), \qquad r \ge 0. \tag{2.82}$$

The goal is thus to show that

$$\lim_{\ell\to\infty}\mathbb{E}[X_\ell \mid X_\ell \le \rho] = \begin{cases}\rho & \text{if } \rho \le \rho_{\mathrm{c}},\\ \rho_{\mathrm{c}} & \text{if } \rho \ge \rho_{\mathrm{c}}.\end{cases} \tag{2.83}$$

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

(3) *Show that*

$$\mathbb{E}[(X_\ell-\rho_{\mathrm{c}})^2] \to 0, \qquad \text{as } \ell\to\infty. \tag{2.84}$$

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

$$\lim_{\ell\to\infty}\mathbb{E}[X_\ell \mid X_\ell \le \rho] = \rho_{\mathrm{c}} \tag{2.85}$$

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

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

(a) *Show that*

$$\Lambda(t) := \lim_{\ell\to\infty}\frac{1}{\ell^d}\log\mathbb{E}[\,\mathrm{e}^{t\ell^d X_\ell}\,] \tag{2.86}$$

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

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

$$\lim_{\ell\to\infty} -\frac{1}{\ell^d}\log\mathbb{P}(X_\ell \le x) = \Lambda^*(x) := \sup_{t\in\mathbb{R}}\,(xt-\Lambda(t)) \tag{2.87}$$

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

$$\mathbb{E}[X_\ell \mid X_\ell \le \rho] \ge (\rho-\delta)\Big(1-\frac{\mathbb{P}(X_\ell \le \rho-\delta)}{\mathbb{P}(X_\ell \le \rho-\delta/2)}\Big). \tag{2.88}$$

(d) *Deduce the result.*

EXERCISE 2.9.

(a) *From the definition (2.60) of the creation and annihilation operators, check that the relations (2.61) and (2.62) hold true.*

(b) *Check that the vectors $|\eta\rangle$ defined in (2.63) form an orthonormal basis of $\mathcal{H}_\Lambda$.*

(c) Consider a vector of the form (2.63) where $(x_i, \sigma_i) = (x_j, \sigma_j)$ *for some* $i \neq j$ *(such a vector does not correspond to a configurattion). Check that such a vector is 0.*

EXERCISE 2.10. *Check the spin relations in (2.66).*

EXERCISE 2.11. *Prove Proposition 2.5. For this, you may find it convenient to prove*

(a) $[H_\Lambda, \sum_{x\in\Lambda} S_x^{(\pm)}] = 0$, $[H_\Lambda, \sum_{x\in\Lambda} S_x^{(3)}] = 0$.

(b) $\mathrm{e}^{\mathrm{i}\theta n_x}\, c_{x,\sigma}^* \,\mathrm{e}^{-\mathrm{i}\theta n_x} = \mathrm{e}^{\mathrm{i}\theta}\, c_{x,\sigma}^*$ *and* $\mathrm{e}^{\mathrm{i}\theta n_x}\, c_{x,\sigma} \,\mathrm{e}^{-\mathrm{i}\theta n_x} = \mathrm{e}^{-\mathrm{i}\theta}\, c_{x,\sigma}^*$.

EXERCISE 2.12. *Use the symmetries of the Hubbard model to prove the relations (2.67).*

EXERCISE 2.13. *Check that the particle-hole symmetry operator* $U_{x,\sigma}^{\mathrm{ph}}$ *is unitary and check the relations (2.68) and (2.69).*

EXERCISE 2.14. *Show that* $\langle n_x \rangle_{\Lambda,\beta} = 1$ *where the hamiltonian is that of the half-filled Hubbard model defined in (2.70). The lattice is assumed here to be bipartite, that is,* $\Lambda = \Lambda_A \cup \Lambda_B$ *and* $\mathcal{E}(\Lambda)$ *only involve edges with one endpoint in* Λ_A *and the other in* Λ_B.

EXERCISE 2.15. *Prove the relations (2.72).*

EXERCISE 2.16. *Check Eqs (2.78) and (2.79). You may use* $\vec{S}_x \cdot \vec{S}_y = \frac{1}{2}(S_x^{(+)} S_y^{(-)} + S_x^{(-)} S_y^{(+)}) + S_x^{(3)} S_y^{(3)}$.