Chapter 11
The Origin of Ferromagnetism

In the present chapter we focus on ferromagnetism (or, more precisely, saturated ferromagnetism) in the ground states of the Hubbard model. Recalling that both the non-interacting models and the non-hopping models exhibit paramagnetism, we see that ferromagnetism can be generated only through nontrivial "competition" between wave-like nature and particle-like nature of electrons. After discussing basic properties of saturated ferromagnetism in the Hubbard model in Sect. 11.1, we present some rigorous results which establish that the ground states of certain versions of the Hubbard models exhibit ferromagnetism. They include Nagaoka's ferromagnetism for systems with infinitely large U (Sect. 11.2), flat-band ferromagnetism by Mielke and by Tasaki (Sect. 11.3), and ferromagnetism in nearly-flat-band Hubbard model due to Tasaki (Sect. 11.4). The final result is of particular importance since it deals with a situation where ferromagnetism is intrinsically a non-perturbative phenomenon, and above mentioned competition plays an essential role. We end the chapter by briefly discussing the fascinating but extremely difficult problem of metallic ferromagnetism in Sect. 11.5.

11.1 Basic Properties of Ferromagnetism

We shall now focus on the emergence of ferromagnetism in several versions of the Hubbard model. As we discussed in Sect. 9.1, to study the origin of ferromagnetism was the main motivation for the introduction of the Hubbard model. Let us remark at this point that ferromagnetism, despite being quite remarkable and interesting phenomenon, is indeed not ubiquitous. We are very much familiar with ferromagnetism in iron, but most metals are paramagnets. The examples of Hubbard models exhibiting ferromagnetism that we treat in Sects. 11.3 and 11.4 describe insulators, but in reality ferromagnetic insulators do exist but are very rare. We might say that ferromagnetism is a phenomenon that is robust enough to be observed in nature, but is found only in relatively small ranges in the "parameter space".

In this preparatory section, we discuss some basic properties of saturated ferromagnetism, to which we simply refer as ferromagnetism throughout the chapter. In Sect. 11.1.1, we give a precise definition of ferromagnetism, and state a basic propo-

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sition which characterizes the nature of ferromagnetic ground states. In Sect. 11.1.2, we present two elementary theorems which show that ferromagnetism is impossible in certain situations. These theorems should make clear that ferromagnetism is indeed a non-perturbative phenomenon in general. In Sect. 11.1.3, we introduce and discuss a simple toy model, which illustrates some essential properties of ferromagnetism in the Hubbard model. Finally in Sect. 11.1.4, we briefly discuss the Stoner criterion, which suggests that ferromagnetism should be sought in models with large (single-electron) density of states and/or large Coulomb interaction.

Let us also make a brief comment on the problem of ferromagnetism at nonzero temperatures. It has been shown rigorously that any Hubbard model with short range hopping in one or two dimensions does not exhibit any magnetic ordering at nonzero temperatures [12, 21]. The mechanism behind this statement is essentially the same as that for quantum spin systems, which we have discussed thoroughly in Sect. 4.4.3. In fact the Proofs of Theorems 4.24 and 4.25 (p. 124) can be applied to the Hubbard model (or a more general lattice electron model) almost as they are.[1] Therefore we must treat models in (at least) three dimensions in order to have ferromagnetism stable at nonzero temperatures. We expect that ferromagnetism in three dimensional versions of some of the models treated in this chapter survives at finite temperatures, but there are no rigorous results in this direction. As we have noted in Sect. 4.4.4, the existence of ferromagnetic order in the quantum ferromagnetic Heisenberg model at low enough temperatures is not yet proved [8]. The corresponding problem in the Hubbard model must be much harder.

11.1.1 Definition and Basic Theorem

We consider the standard Hubbard Hamiltonian

$$\hat{H} = \hat{H}_{\text{hop}} + \hat{H}_{\text{int}}, \tag{11.1.1}$$

with

$$\hat{H}_{\text{hop}} = \sum_{\substack{x,y\in\Lambda \\ \sigma=\uparrow,\downarrow}} t_{x,y}\, \hat{c}^{\dagger}_{x,\sigma}\hat{c}_{y,\sigma}, \quad \hat{H}_{\text{int}} = U\sum_{x\in\Lambda} \hat{n}_{x,\uparrow}\hat{n}_{x,\downarrow}, \tag{11.1.2}$$

which are (9.3.17) and (9.3.29), respectively. We can treat the interaction Hamiltonian (9.3.28) with site dependent interaction U_x in most cases, but shall stick to the above simpler form.

In the present chapter we study the strongest form of ferromagnetism, namely saturated ferromagnetism, which is defined as follows. We write $S_{\max} := N/2$.

[1] One uses the same complex rotation (4.4.26), regarding the spin operator as written in terms of the fermion operators.

Definition 11.1 (*Saturated ferromagnetism*) Consider the Hubbard model with Hamiltonian (11.1.1) with N electrons. We say that the model exhibits ferromagnetism (or, more precisely, saturated ferromagnetism) if any ground state $|\Phi_{\mathrm{GS}}\rangle$ has the maximum possible total spin $S_{\mathrm{tot}} = S_{\max}$, i.e., $(\hat{\boldsymbol{S}}_{\mathrm{tot}})^2|\Phi_{\mathrm{GS}}\rangle = S_{\max}(S_{\max}+1)|\Phi_{\mathrm{GS}}\rangle$.

We should note that saturated ferromagnetism is indeed a very special form of ferromagnetism. In general we expect partial ferromagnetism where S_{tot} of the ground states is macroscopically large but the ratio $S_{\mathrm{tot}}/S_{\max}$ is strictly less than unity.[2] In the present book, we however concentrate only on saturated ferromagnetism, and refer to it simply as ferromagnetism. This is mainly because the study of partial ferromagnetism is so difficult that there are almost no rigorous results to be discussed. Theoretical study of (saturated) ferromagnetism in the Hubbard model is relatively easier because of the property stated in the following Proposition 11.2.

As in Sect. 9.3.2, we denote by $\hat{a}^\dagger_{j,\sigma}$ the creation operator of the single-electron energy eigenstate $\boldsymbol{\psi}^{(j)}$ with energy eigenvalue ε_j, where $j = 1, 2, \ldots, |\Lambda|$. It satisfies the commutation relation $[\hat{H}_{\mathrm{hop}}, \hat{a}^\dagger_{j,\sigma}] = \varepsilon_j \hat{a}^\dagger_{j,\sigma}$, which is (9.3.21). We have seen that the eigenstates of $\hat{H}_{\mathrm{hop}}$ are explicitly written as (9.3.22). Let us define

$$E_{\mathrm{ferro}} := \min_{\substack{\Gamma\subset\{1,\ldots,|\Lambda|\}\\(|\Gamma|=N)}} \sum_{j\in\Gamma} \varepsilon_j, \tag{11.1.3}$$

which is the ground state energy of the system of N spin-less fermions with non-interacting Hamiltonian $\hat{H}_{\mathrm{hop}}$.

Proposition 11.2 *Suppose that a Hubbard model exhibits (saturated) ferromagnetism as in Definition 11.1. Then for any $\Gamma \subset \{1, \ldots, |\Lambda|\}$ such that $|\Gamma| = N$ and $\sum_{j\in\Gamma} \varepsilon_j = E_{\mathrm{ferro}}$, and for any $M = -S_{\max}, S_{\max}+1, \ldots, S_{\max}$, the state*

$$|\Phi^{\Gamma,M}_{\mathrm{GS}}\rangle := (\hat{S}^-_{\mathrm{tot}})^{S_{\max}-M}\Big(\prod_{j\in\Gamma}\hat{a}^\dagger_{j,\uparrow}\Big)|\Phi_{\mathrm{vac}}\rangle, \tag{11.1.4}$$

is a ground state of the Hubbard model. Moreover any ground state is a linear combination of these ground states.

This proposition shows that the ground states of a Hubbard model simplifies considerably when the model exhibits saturated ferromagnetism. To see the essence of the proof, consider a subspace of states that consists only of up-spin electrons. Since the interaction Hamiltonian $\hat{H}_{\mathrm{int}}$ always gives zero when acting on such states, the Hubbard model, when restricted on this subspace, reduces to a non-interacting electron model. The energy eigenstates then take the simple Slater determinant form (9.3.22) with $S_\downarrow = \emptyset$. In particular, the lowest energy state in the subspace is given by (11.1.4) with $M = S_{\max}$.

[2] Lieb's example in Sect. 10.2.3 satisfies this criterion, but it should better be interpreted as ferrimagnetism rather than partial ferromagnetism.

This drastic simplification is a result of the particular form of the Hubbard interaction, where only electrons on the same site interact. We should note however that the appearance of ferromagnetism is a highly nontrivial phenomenon, which must be caused by the interaction effect.

Proof of Proposition 11.2 The proposition relies essentially on the SU(2) invariance of the Hubbard model. As in Appendix A.3, we denote by $\mathscr{H}_{J,M}$ the space of states with $(\hat{\boldsymbol{S}}_{\rm tot})^2|\Phi\rangle = J(J+1)|\Phi\rangle$ and $\hat{S}^{(3)}_{\rm tot}|\Phi\rangle = M|\Phi\rangle$. (Here we set $\hat{J} = \hat{\boldsymbol{S}}_{\rm tot}$.)

We first note that there is a ground state in[3] $\mathscr{H}_{S_{\max},S_{\max}}$, i.e., the space of states consisting of N up-spin electrons. Then we see from the above discussion that $|\Phi^{\Gamma,S_{\max}}_{\rm GS}\rangle$, which is the lowest energy state within $\mathscr{H}_{S_{\max},S_{\max}}$, must be a ground state of the Hubbard model. Note that Lemma A.14 (p. 471) implies that $|\Phi^{\Gamma,M}_{\rm GS}\rangle$ is nonzero for $M = -S_{\max}, S_{\max}+1, \dots, S_{\max}$. Since $[\hat{S}^-_{\rm tot}, \hat{H}] = 0$, we see that $|\Phi^{\Gamma,M}_{\rm GS}\rangle$ is a ground state for any M.

To see that any ground state is a linear combination of the states (11.1.4), take an arbitrary ground state $|\Phi_{\rm GS}\rangle$, and decompose it as $|\Phi_{\rm GS}\rangle = \sum_{M=-N/2}^{N/2} |\Phi^M_{\rm GS}\rangle$, where $|\Phi^M_{\rm GS}\rangle \in \mathscr{H}_{S_{\max},M}$. Note that each $|\Phi^M_{\rm GS}\rangle$, if nonzero, is a ground state. For each nonzero $|\Phi^M_{\rm GS}\rangle$, let $|\Phi^{M,\uparrow}_{\rm GS}\rangle = (\hat{S}^+_{\rm tot})^{S_{\max}-M}|\Phi^M_{\rm GS}\rangle$, which is nonzero by Lemma A.14. Since $|\Phi^{M,\uparrow}_{\rm GS}\rangle$ is a ground state and belongs to $\mathscr{H}_{S_{\max},S_{\max}}$, it is written as a linear combination of the states (11.1.4) with $M = S_{\max}$. Since $|\Phi^M_{\rm GS}\rangle = ({\rm const.})(\hat{S}^-_{\rm tot})^{S_{\max}-M}|\Phi^{M,\uparrow}_{\rm GS}\rangle$, we see that $|\Phi^M_{\rm GS}\rangle$ is also a linear combination of states (11.1.4). ∎

Suppose that the single-electron energy eigenstates (which are ordered so that $\varepsilon_j \le \varepsilon_{j+1}$) satisfy $\varepsilon_N < \varepsilon_{N+1}$. Then the choice of Γ in the ground state (11.1.4) is unique, and we must set $\Gamma = \{1, 2, \dots, N\}$. In such a case the ground states are exactly $2S_{\max}+1 = N+1$ fold degenerate.

11.1.2 Instability of Ferromagnetism

To see that ferromagnetism is indded a delicate phenomenon, we discuss some results which show that the Hubbard model with certain conditions does not exhibit ferromagnetism.

We have seen in Sect. 9.3.2 that the non-interacting model, whose Hamiltonian is $\hat{H}_{\rm hop}$, in general exhibits Pauli paramagnetism as in (9.3.24). See, in particular, Fig. 9.3. In the same section, we have also seen that the non-hopping model, whose Hamiltonian is $\hat{H}_{\rm int}$, exhibits a simple paramagnetism. Neither $\hat{H}_{\rm hop}$ nor $\hat{H}_{\rm int}$ favors ferromagnetism.

We next consider the situation in which the Coulomb interaction U is nonzero but small. One can easily prove the following theorem which states that there cannot be (saturated) ferromagnetism when U is small, unless the single-electron energy

[3] ***Proof*** Since $\hat{H}$ and $\hat{S}^{(3)}_{\rm tot}$ are simultaneously diagonalizable, there is a ground state in $\mathscr{H}_{S_{\max},M_0}$ for some M_0. Then Theorem A.16 (p. 473) implies that there is a ground state in $\mathscr{H}_{S_{\max},M}$ for each M.

eigenvalues ε_j are highly degenerate. We again denote by $\hat{a}^\dagger_{j,\sigma}$ the creation operator of the single-electron energy eigenstate with eigenvalue ε_j, where $j = 1, 2, \ldots, |\Lambda|$. We also assume that the energy eigenvalues are ordered as $\varepsilon_j \le \varepsilon_{j+1}$.

Theorem 11.3 (Impossibility of ferromagnetism for small U) *Suppose* $0 \le U < \varepsilon_N - \varepsilon_1$. *Then the ground state of the Hubbard model does not have* $S_{\rm tot} = S_{\rm max}$, *i.e., the model does not exhibit (saturated) ferromagnetism.*

Note that $\varepsilon_N - \varepsilon_1$, which is known as the fermi energy, is usually independent of the system size when the filling factor $N/(2|\Lambda|)$ is fixed.

Proof One of the lowest energy states with $S_{\rm tot} = S_{\rm max}$ is given by

$$|\Phi^{\uparrow}_{\rm GS}\rangle = \Big(\prod_{j=1}^{N} \hat{a}^\dagger_{j,\uparrow}\Big)|\Phi_{\rm vac}\rangle, \tag{11.1.5}$$

whose energy is $E_{\rm ferro} = \sum_{j=1}^{N} \varepsilon_j$. Consider a normalized trial state

$$|\Psi\rangle = \hat{a}^\dagger_{1,\downarrow}\Big(\prod_{j=1}^{N-1} \hat{a}^\dagger_{j,\uparrow}\Big)|\Phi_{\rm vac}\rangle, \tag{11.1.6}$$

which is obtained from (11.1.5) by removing the up-spin electron which has the highest energy and then adding a down-spin electron which has the lowest energy. Noting the $SU(2)$ invariance of $\hat{a}^\dagger_{1,\downarrow}\hat{a}^\dagger_{1,\uparrow}$ as shown in (9.2.70) and (9.2.71), one finds that $|\Psi\rangle$ has $S_{\rm tot} = S_{\rm max} - 1$. We want to evaluate the energy expectation value $\langle\Psi|\hat{H}|\Psi\rangle$. For the kinetic energy, we readily see that $\langle\Psi|\hat{H}_{\rm hop}|\Psi\rangle = \varepsilon_1 + \sum_{j=1}^{N-1} \varepsilon_j$. For $\hat{H}_{\rm int}$, we note that the trivial inequality $\hat{n}_{x,\uparrow} \le 1$ implies $\hat{H}_{\rm int} \le U \sum_{x\in\Lambda} \hat{n}_{x,\downarrow}$ to get $\langle\Psi|\hat{H}_{\rm int}|\Psi\rangle \le \langle\Psi|U \sum_{x\in\Lambda} \hat{n}_{x,\downarrow}|\Psi\rangle = U$. We therefore have

$$\langle\Psi|\hat{H}|\Psi\rangle - E_{\rm ferro} \le \varepsilon_1 - \varepsilon_N + U < 0. \tag{11.1.7}$$

From the variational principle, we see that $E_{\rm ferro}$ is not the ground state energy of $\hat{H}$. ∎

Although the above theorem ensures that the ground state cannot be ferromagnetic, it does not provide any information about the nature of the true ground state of the model. To study the latter explicitly is in general a very difficult problem.

Let us also discuss the situation in which the interaction may be large but the density of electrons is very low. It is expected that the chance of electrons to collide with each other in this case becomes very small. It is likely that the model is close to an ideal gas, and there is no ferromagnetism.

This naive guess is justified for "healthy" models in dimensions three (or higher). The dimensionality of the lattice is taken into account by assuming that there are

positive constants[4] c, n_0, ρ_0, and d, and the single electron energy eigenvalues satisfy

$$\varepsilon_n - \varepsilon_1 \geq c \left(\frac{n - n_0}{|\Lambda|} \right)^{2/d}, \tag{11.1.8}$$

for any n such that $n \geq n_0$ and $n/|\Lambda| \leq \rho_0$. Note that the right-hand side represents the n dependence of energy levels in the standard quantum mechanical system of a single particle in d-dimensions. Then we have the following theorem due to Pieri, Daul, Baeriswyl, Dzierzawa, and Fazekas [46].

Theorem 11.4 (Impossibility of ferromagnetism at low densities) *Take a $\hat{H}_{\text{hop}}$ which has translation invariance and satisfies (11.1.8) with positive c, n_0, ρ_0, and $d > 2$. Then there exists a constant $\rho_1 > 0$, and the corresponding Hubbard model does not exhibit (saturated) ferromagnetism for any $U \geq 0$ if $N/|\Lambda| \leq \rho_1$ holds.*

Outline of Proof The naive trial state (11.1.6) does not work for large U. We follow [52], and consider the Roth state [49]

$$|\tilde{\Psi}\rangle = \hat{P}_0 |\Psi\rangle, \tag{11.1.9}$$

where $|\Psi\rangle$ is defined in (11.1.6), and

$$\hat{P}_0 = \prod_{x \in \Lambda} (1 - \hat{n}_{x,\uparrow} \hat{n}_{x,\downarrow}) \tag{11.1.10}$$

is the orthogonal projection (called the Gutzwiller projection) onto the space with no doubly occupied sites. Because of the projection, the state (11.1.9) minimizes the Coulomb interaction as $\hat{H}_{\text{int}} |\Psi\rangle = 0$. Thus we only need to evaluate the expectation value of $\hat{H}_{\text{hop}}$. After a slightly complicated calculation whose details can be found in Appendix F of [73], we find

$$\frac{\langle \widetilde{\Psi} | H | \widetilde{\Psi} \rangle}{\langle \widetilde{\Psi} | \widetilde{\Psi} \rangle} - E_{\text{ferro}} \leq \varepsilon_1 - \varepsilon_N + c' \rho, \tag{11.1.11}$$

where $\rho = N/|\Lambda|$ is the electron density and $c' > 0$ is a constant. From the assumption (11.1.8), we find that the right-hand side becomes strictly negative for sufficiently small ρ provided that $d > 2$. ∎

That we have a restriction on dimensionality in Theorem 11.4 is not merely technical. In a one-dimensional system, moving electrons must eventually collide with each other for an obvious geometric reason. Thus a one-dimensional model cannot be regarded as close to an ideal gas, no matter how low the electron density is. We do not know whether the inapplicability of the theorem to two-dimensional systems is physically meaningful or not.

[4] The constants n_0 and d represent the degeneracy of the single-electron ground states and the dimension of the system, respectively.

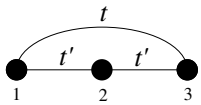

Fig. 11.1 The lattice and the hopping amplitude of the toy model. By considering the system with two electrons on this lattice, we can observe some very important aspects of ferromagnetism in the Hubbard model (© Hal Tasaki 2020. All Rights Reserved)

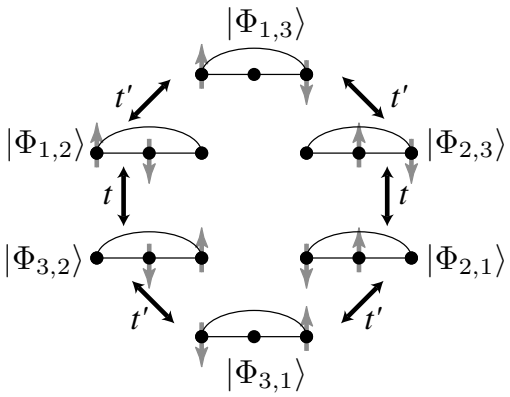

Fig. 11.2 Allowed states and transition amplitude in the toy model with $U = \infty$, which leads to the ring exchange process. The total spin of the ground states can be easily read off from this diagram (© Hal Tasaki 2020. All Rights Reserved)

11.1.3 Toy Model with Two Electrons

As a starting point of our study of ferromagnetism, we consider a very simple toy model with two electrons. Interestingly, some essential features of ferromagnetism found in many-electron systems (that we will discuss in the following sections) are already present in this model.

The smallest possible Hubbard model which is away from half-filling is that with two electrons on a lattice with three sites. Consider the lattice $\Lambda = \{1, 2, 3\}$, and put one electron with $\sigma = \uparrow$ and one with $\sigma = \downarrow$. The hopping matrix is defined by $t_{1,2} = t_{2,3} = t'$, and $t_{1,3} = t$. Note that there are two kinds of hoppings t and t'. Since the sign of t' can be changed by the gauge transformation $\hat{c}_{2,\sigma} \to -\hat{c}_{2,\sigma}$ (see Sect. 9.3.3), we shall fix $t' > 0$. Figure 11.1 shows the lattice and the hopping amplitude. For simplicity, we assume there is only one kind of interaction, and set $U_1 = U_2 = U_3 = U \geq 0$. We have $S_{\max} = 1$ because $N = 2$. Therefore we can say that there appears ferromagnetism if the ground state has $S_{\text{tot}} = 1$, i.e., if it is a spin-triplet.

Let us take the limit $U \uparrow \infty$, in which the effect of the interaction becomes most drastic, and consider only those states with finite energies. This is equiva-

lent to considering only states in which two electrons never occupy a same site.[5] There are six basis states which satisfy the constraint, and they can be written as $|\Phi_{x,y}\rangle = \hat{c}^{\dagger}_{x,\uparrow}\hat{c}^{\dagger}_{y,\downarrow}|\Phi_{\rm vac}\rangle$ where $x, y = 1, 2, 3$, and $x \neq y$. Transition amplitudes between these states are shown in Fig. 11.2. We find that the problem is equivalent to that of a quantum mechanical particle hopping around on a ring consisting of six sites. The basic structure of the ground state can be determined by the standard Perron–Frobenius sign convention.[6] By also taking into account the symmetry between the basis states, the ground state for $t < 0$ is written as

$$|\Phi^{(t<0)}_{\rm GS}\rangle = |\Phi_{1,2}\rangle + |\Phi_{3,2}\rangle - \alpha(t,t')|\Phi_{3,1}\rangle + |\Phi_{2,1}\rangle + |\Phi_{2,3}\rangle - \alpha(t,t')|\Phi_{1,3}\rangle, \tag{11.1.12}$$

and that for $t > 0$ as

$$|\Phi^{(t>0)}_{\rm GS}\rangle = |\Phi_{1,2}\rangle - |\Phi_{3,2}\rangle + \beta(t,t')|\Phi_{3,1}\rangle - |\Phi_{2,1}\rangle + |\Phi_{2,3}\rangle - \beta(t,t')|\Phi_{1,3}\rangle, \tag{11.1.13}$$

where $\alpha(t,t')$ and $\beta(t,t')$ are positive functions of t and t'.

To find the total spin of these states, it suffices to concentrate on two lattice sites, say sites 1 and 2, and note that $|\Phi^{(t<0)}_{\rm GS}\rangle = |\Phi_{1,2}\rangle + |\Phi_{2,1}\rangle + \cdots$, and $|\Phi^{(t>0)}_{\rm GS}\rangle = |\Phi_{1,2}\rangle - |\Phi_{2,1}\rangle + \cdots$. It immediately follows that $|\Phi^{(t<0)}_{\rm GS}\rangle$ has $S_{\rm tot} = 0$, and $|\Phi^{(t>0)}_{\rm GS}\rangle$ has $S_{\rm tot} = 1$. See (9.2.76) and (9.2.77). We see that ferromagnetic coupling is generated when t is positive.

It will be useful to see the mechanism that generates the ferromagnetism in this simple model. Note that the states $|\Phi_{1,2}\rangle$ and $|\Phi_{2,1}\rangle$ can be found in the upper left and and the lower right, respectively, in the diagram of Fig. 11.2. By starting from $|\Phi_{1,2}\rangle$ and following the possible transitions, one reaches the state $|\Phi_{2,1}\rangle$. In other words, electrons hop around in the lattice, and the spins on sites 1 and 2 are "exchanged." When $t > 0$, the quantum mechanical amplitude associated with the exchange process generates the superposition of the two states which precisely yields ferromagnetism. The process leading to ferromagnetic coupling may be called the ring exchange.

Let us briefly look at the cases with finite U. Let $E_{\rm min}(S_{\rm tot})$ be the lowest energy among the states which have total spin $S_{\rm tot}$. In Fig. 11.3, we plotted $E_{\rm min}(0)$ and $E_{\rm min}(1)$ for the toy model with $t = t'/2 > 0$ as functions of $U \geq 0$. As is suggested by the result in the $U \uparrow \infty$ limit, we have ferromagnetism in the sense that $E_{\rm min}(0) > E_{\rm min}(1)$ when U is sufficiently large. A level crossing takes place at finite U, and the system is no longer ferromagnetic for small U. Even in the simplest toy model, ferromagnetism is a nonperturbative phenomenon which takes place only when U is sufficiently large.

The only exception is the case with $t = t' > 0$. See Fig. 11.4. For this parameter value, the ground states are degenerate and have both $S_{\rm tot} = 0$ and 1 when $U = 0$. Ferromagnetic state is the only ground state for any $U > 0$.

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[5] See the Proof of Theorem 11.5 in Sect. 11.2 for the treatment of the $U \uparrow \infty$ limit.

[6] If the transition amplitude between two states is negative (*resp.*, positive), one superposes the two states with the same (*resp.*, opposite) signs.

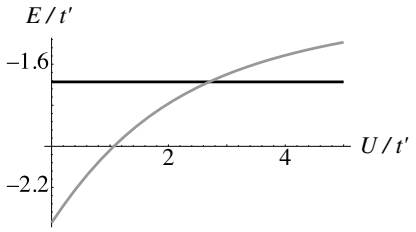

Fig. 11.3 The U dependence of $E_{\min}(0)$ (gray curve) and $E_{\min}(1)$ (black line) in the toy model with $t = t'/2 > 0$. We have ferromagnetism in the sense that $E_{\min}(0) > E_{\min}(1)$ when U is sufficiently large. We find that ferromagnetism is a nonperturbative phenomenon ()

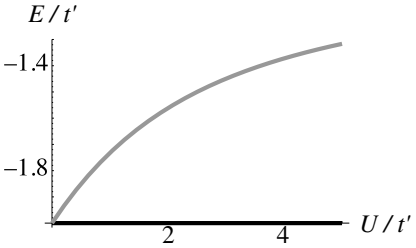

Fig. 11.4 The U dependence of $E_{\min}(0)$ (gray curve) and $E_{\min}(1)$ (black line) in the toy model with $t = t' > 0$. Only for this special parameter, we have ferromagnetism $E_{\min}(0) > E_{\min}(1)$ for any value of $U > 0$. One can regard this case as the simplest example of the flat-band ferromagnetism that we will discuss in Sect. 11.3 ()

Figures 11.3 and 11.4 show that the energy $E_{\min}(1)$ of ferromagnetic states is independent of U. This is because ferromagnetic states do not feel the on-site Coulomb interaction, as we have seen in the Proof of Proposition 11.2.

11.1.4 Stoner Criterion

Before closing the present preparatory section, we briefly discuss a simple condition, known as the Stoner criterion, for ferromagnetism in interacting electron systems. It is based on a very crude mean-field type approximation, and represents a condition for instability of Pauli paramagnetism against ferromagnetic ordering. Although the Stoner criterion should not be regarded as a reliable condition, it gives us a rough idea about the roles played by the interaction U and the density of states D_{F} at the Fermi energy.

Consider the Hubbard model in the space with $N_\uparrow$ up-spin electrons and $N_\downarrow$ down-spin electrons, where $N_\uparrow + N_\downarrow = N$ is fixed. We shall make a bold approximation to the interaction Hamiltonian, and replace $\hat{n}_{x,\uparrow}$ and $\hat{n}_{x,\downarrow}$ by their averages as

$$\hat{H}_{\rm int} = U \sum_{x\in\Lambda} \hat{n}_{x,\uparrow}\hat{n}_{x,\downarrow} \;\to\; U \sum_{x\in\Lambda} \langle \hat{n}_{x,\uparrow}\rangle \langle \hat{n}_{x,\downarrow}\rangle = U\,|\Lambda| \frac{N_\uparrow}{|\Lambda|}\frac{N_\downarrow}{|\Lambda|} = U\frac{N_\uparrow N_\downarrow}{|\Lambda|}. \tag{11.1.14}$$

We again denote by $\hat{a}^\dagger_{j,\sigma}$ the creation operator of the the single-electron energy eigenstate with ε_j, where $j = 1, 2, \ldots, |\Lambda|$ and $\varepsilon_j \le \varepsilon_{j+1}$. Then the state with the lowest kinetic energy with given $N_\uparrow$ and $N_\downarrow$ is

$$|\Phi_{MF}^{N_\uparrow,N_\downarrow}\rangle = \Big(\prod_{j=1}^{N_\uparrow} \hat{a}^\dagger_{j,\uparrow}\Big)\Big(\prod_{j=1}^{N_\downarrow} \hat{a}^\dagger_{j,\downarrow}\Big)|\Phi_{\rm vac}\rangle. \tag{11.1.15}$$

The total energy of this state is thus given by

$$E_{\rm MF}(N_\uparrow, N_\downarrow) = \sum_{j=1}^{N_\uparrow} \varepsilon_j + \sum_{j=1}^{N_\downarrow} \varepsilon_j + U\frac{N_\uparrow N_\downarrow}{|\Lambda|}. \tag{11.1.16}$$

Let us compare the energies of the paramagnetic state $|\Phi_{MF}^{N/2,N/2}\rangle$ and the state $|\Phi_{MF}^{(N/2)+n,(N/2)-n}\rangle$ obtained by flipping n spins from down to up. Note that the latter state has $S_{\rm tot} = n$. From (11.1.16), we find that the energy difference is

$$\begin{aligned}\Delta E &= E_{\rm MF}\Big(\frac{N}{2}+n, \frac{N}{2}-n\Big) - E_{\rm MF}\Big(\frac{N}{2}, \frac{N}{2}\Big)\\ &= \sum_{\ell=1}^{n} (\varepsilon_{(N/2)+\ell} - \varepsilon_{(N/2)-n+\ell}) - U\frac{n^2}{|\Lambda|}\\ &\simeq n^2\Delta\varepsilon - U\frac{n^2}{|\Lambda|}.\end{aligned} \tag{11.1.17}$$

We here approximated $\varepsilon_{(N/2)+\ell} - \varepsilon_{(N/2)-n+\ell} \simeq n\,\Delta\varepsilon$, where $\Delta\varepsilon$ is the average spacing of the single-electron energy eigenvalues near the Fermi energy $\varepsilon_{N/2}$. In a standard system, the energy level spacing behaves as $\Delta\varepsilon \simeq (|\Lambda|\,D_{\rm F})^{-1}$ with a size independent quantity $D_{\rm F}$ known as the (single-electron) density of states (per volume) at the Fermi energy. We thus find

$$\Delta E \simeq \frac{n^2}{|\Lambda|\,D_{\rm F}}(1 - D_{\rm F}\,U). \tag{11.1.18}$$

This estimate implies that the paramagnetic state with $n = 0$ is unstable towards increasing n if

$$D_{\rm F}\,U \gtrsim 1, \tag{11.1.19}$$

which is the Stoner criterion.

As is clear from the derivation, which is not justified in any reasonable limits, the criterion is far from being reliable. There are many examples in which $D_{\rm F}\,U$ is

extremely large but ferromagnetism is not observed. Nevertheless the Stoner criterion provides us with a rough guiding principle that ferromagnetism should be sought in models with large D_{F} and/or large U.

11.2 Nagaoka's Ferromagnetism

In the present section we discuss Nagaoka's ferromagnetism, which historically was the first rigorous example of ferromagnetism in the Hubbard model. In short Nagaoka's theorem [42] states that some Hubbard models exhibit ferromagnetism when the Coulomb repulsion U is infinitely large, and the number of electrons is one less than the number of the lattice sites (i.e., $N = |\Lambda| - 1$). Given the general fact that a half-filled system with $N = |\Lambda|$, where Lieb's theorem apply, never shows ferromagnetism, this is a rather striking result. It demonstrates that strongly interacting electron systems can exhibit very rich and sometimes surprising properties. Note also that the necessity to take $U \uparrow \infty$ is roughly compatible with the Stoner criterion (11.1.19).

When $U = \infty$ and $N = |\Lambda| - 1$, states with finite energies have no doubly occupied sites, and there is exactly one empty site, which we call the "hole." The basic mechanism of Nagaoka's ferromagnetism is that the hole hops around the lattice and generates a suitable linear combination of the basis states, in such a way that the resulting state exhibits ferromagnetism. It is remarkable that the motion of a single hole can turn (expected) antiferromagnetism at exact half-filling into ferromagnetism.[7] See Fig. 11.5. Thouless also discussed a similar mechanism in a different context [75]. Note that the ferromagnetism observed in the toy model studied in Sect. 11.1.3 can be regarded as the simplest version of Nagaoka's ferromagnetism. See, in particular, Fig. 11.2.

Here we give a complete proof of Nagaoka's theorem in its most generalized form due to Tasaki [66]. We believe that the reader will find the general proof [66, 73], which is a refinement of that by Nagaoka [42], straightforward and simple. In Sect. 11.2.1, we state and prove a weak version of Nagaoka's theorem. Then we shall see in Sect. 11.2.2 that this theorem can be easily strengthened to give the full theorem of Nagaoka's if we properly formulate the notion of connectivity of configurations.

Although Nagaoka's ferromagnetism is of considerable interest from theoretical and mathematical points of view, it is now understood that the ferromagnetic state obtained through this mechanism is rather pathological and has little to do with realistic ferromagnetism. There have been many studies which indicate that Nagaoka's ferromagnetism is destroyed when one relaxes the extreme conditions necessary for

[7] In Japanese institutions it often happens that the presence of a single foreign participant in a seminar room makes everybody shift from Japanese to English. I used to mention this phenomenon in the introduction to talks about Nagaoka's ferromagnetism. I remember one seminar at RIMS in Kyoto, where I had a perfect situation for this joke; the topic was about my refinement of Nagaoka's theorem, there was exactly one foreign participant at the seminar, and among many Japanese participants was Yosuke Nagaoka!

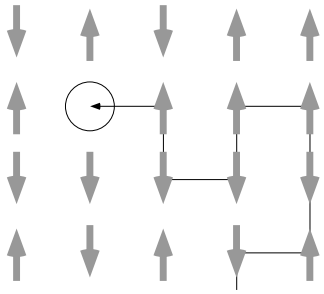

Fig. 11.5 Schematic picture of the origin of Nagaoka's ferromagnetism. When the hole hops around the lattice, the spin configuration changes. For a model with $t_{x,y} \geq 0$, the hole motion produces a precise linear combination of various spin configurations, which leads to a ferromagnetic state ()

the theorem to be valid. We shall briefly summarize some of such results about instability of Nagaoka's ferromagnetism in Sect. 11.2.3.

11.2.1 Weak Version of Nagaoka's Theorem

We consider the standard Hubbard Hamiltonian $\hat{H} = \hat{H}_{\text{hop}} + \hat{H}_{\text{int}}$ with

$$\hat{H}_{\text{hop}} = \sum_{\substack{x,y\in\Lambda \\ \sigma=\uparrow,\downarrow}} t_{x,y}\, \hat{c}^{\dagger}_{x,\sigma}\hat{c}_{y,\sigma}, \quad \hat{H}_{\text{int}} = U \sum_{x\in\Lambda} \hat{n}_{x,\uparrow}\hat{n}_{x,\downarrow}. \tag{11.2.1}$$

Then we have the following.

Theorem 11.5 (Weak version of Nagaoka's theorem) *Assume that the hopping amplitude satisfies $t_{x,y} = t_{y,x} \geq 0$ for any x, $y \in \Lambda$, and consider the Hubbard model with $N = |\Lambda| - 1$ in the limit $U \uparrow \infty$. Then among the ground states there are at least $(2S_{\text{tot}} + 1)$ states with total spin $S_{\text{tot}} = S_{\max}(= N/2)$.*

Note that the theorem does not establish the existence of ferromagnetism since it does not state that the ferromagnetic states are the only ground states. In fact the condition of the theorem is valid even in the trivial non-hopping model with $t_{x,y} = 0$ for all x, $y \in \Lambda$, which exhibits paramagnetism as we have seen in Sect. 9.3.2.

Proof of Theorem 11.5 We shall prove the theorem, following [66, 73]. Let $\mathscr{H}_N^{\text{hc}}$ be the subspace (of the whole Hilbert space $\mathscr{H}_N$ with N electrons) which consists of states without any doubly occupied sites.[8] Here the script "hc" stands for "hardcore".

[8] To be precise, $\mathscr{H}_N^{\text{hc}}$ is spanned by the basis states (9.2.35) with the constraint that $x_j \neq x_k$ when $j \neq k$.

Note that any $|\Phi\rangle \in \mathscr{H}_N^{\rm hc}$ satisfies $\hat{H}_{\rm int}|\Phi\rangle = 0$. We denote by $\hat{P}_{\rm hc}$ the orthogonal projection onto $\mathscr{H}_N^{\rm hc}$.

We are interested in the ground state of the Hubbard Hamiltonian $\hat{H} = \hat{H}_{\rm hop} + \hat{H}_{\rm int}$ in the limit $U \uparrow \infty$. The model in the limit is described by the effective Hamiltonian

$$\hat{H}_{\rm eff} := \hat{P}_{\rm hc}\, \hat{H}\, \hat{P}_{\rm hc}, \tag{11.2.2}$$

which is an operator on the hardcore subspace $\mathscr{H}_N^{\rm hc}$. This fact should be obvious, but is proved in Theorem A.12 (p. 470). In particular the desired ground states of $\hat{H}$ in the $U \uparrow \infty$ limit are ground states of $\hat{H}_{\rm eff}$.

We follow Nagaoka [42], and prepare a basis for the Hilbert space $\mathscr{H}_N^{\rm hc}$, which is most convenient for the present proof. Our basis states are specified by the position $x \in \Lambda$ of the hole and the spin configuration $\boldsymbol{\sigma} = (\sigma_y)_{y\in\Lambda\setminus\{x\}} \in \mathscr{S}_{\Lambda\setminus\{x\}}$ in $\Lambda\setminus\{x\}$, which is the rest of the lattice. (For any subset $\Lambda' \subset \Lambda$, we denote by $\mathscr{S}_{\Lambda'}$ the set of all spin configurations $(\sigma_x)_{x\in\Lambda'}$ with $\sigma_x = \uparrow, \downarrow$.) We define

$$|\Phi_{x,\boldsymbol{\sigma}}\rangle := \hat{c}_{x,\uparrow}\left(\prod_{y\in\Lambda}\hat{c}^\dagger_{y,\sigma'_y}\right)|\Phi_{\rm vac}\rangle = \hat{c}_{x,\downarrow}\left(\prod_{y\in\Lambda}\hat{c}^\dagger_{y,\sigma''_y}\right)|\Phi_{\rm vac}\rangle, \tag{11.2.3}$$

where the product is taken over all the sites in Λ with an arbitrary but fixed order. We gave two equivalent expressions for $|\Phi_{x,\boldsymbol{\sigma}}\rangle$. The spin configurations $(\sigma'_y)_{y\in\Lambda}$ and $(\sigma''_y)_{y\in\Lambda}$ are almost the same as $\boldsymbol{\sigma} = (\sigma_y)_{y\in\Lambda\setminus\{x\}}$, and defined by $\sigma'_y = \sigma''_y = \sigma_y$ for all $y \in \Lambda\setminus\{x\}$. As for the missing site x, we set $\sigma'_x = \uparrow$ and $\sigma''_x = \downarrow$. Thus, in the definition (11.2.3), we are simply supplying an electron at the hole site x, and then annihilating the electron by $\hat{c}_{x,\uparrow}$ or $\hat{c}_{x,\downarrow}$. This may appear as redundant, but, in this way, we get precise fermion signs appropriate for our purpose.

We wish to examine the action of $\hat{H}_{\rm eff} = \hat{P}_{\rm hc}\, \hat{H}_{\rm hop} \hat{P}_{\rm hc}$ on the states (11.2.3). In order to get a nonvanishing contribution, an electron must hop into the hole site x from one of the sites connected to x via nonzero $t_{x,z}$. We therefore examine the action of $\sum_{\sigma=\uparrow,\downarrow}\hat{c}^\dagger_{x,\sigma}\hat{c}_{z,\sigma} = -\sum_{\sigma=\uparrow,\downarrow}\hat{c}_{z,\sigma}\hat{c}^\dagger_{x,\sigma}$ on $|\Phi_{x,\boldsymbol{\sigma}}\rangle$. Using the two equivalent expressions (11.2.3) for $|\Phi_{x,\boldsymbol{\sigma}}\rangle$, we get

$$\begin{aligned}
\sum_{\sigma=\uparrow,\downarrow}\hat{c}^\dagger_{x,\sigma}c_{z,\sigma}|\Phi_{x,\boldsymbol{\sigma}}\rangle &= -\hat{c}_{z,\uparrow}\hat{n}_{x,\uparrow}\Big(\prod_{y\in\Lambda}\hat{c}^\dagger_{y,\sigma'_y}\Big)|\Phi_{\rm vac}\rangle - \hat{c}_{z,\downarrow}\hat{n}_{x,\downarrow}\Big(\prod_{y\in\Lambda}\hat{c}^\dagger_{y,\sigma''_y}\Big)|\Phi_{\rm vac}\rangle \\
&= -\hat{c}_{z,\uparrow}\Big(\prod_{y\in\Lambda}\hat{c}^\dagger_{y,\sigma'_y}\Big)|\Phi_{\rm vac}\rangle - \hat{c}_{z,\downarrow}\Big(\prod_{y\in\Lambda}\hat{c}^\dagger_{y,\sigma''_y}\Big)|\Phi_{\rm vac}\rangle \\
&= -|\Phi_{z,\boldsymbol{\sigma}_{z\to x}}\rangle,
\end{aligned} \tag{11.2.4}$$

where $\boldsymbol{\sigma}_{z\to x} \in \mathscr{S}_{\Lambda\setminus z}$ is the new spin configuration on $\Lambda\setminus z$ obtained from $\boldsymbol{\sigma}$ by moving σ_z to the site x. Note that, in the second and the third expressions in (11.2.4), only one of the two terms survive depending on the value of σ_z. Therefore the matrix elements of the effective Hamiltonian $\hat{H}_{\rm eff}$ are given by

$$\langle \Phi_{y,\boldsymbol{\tau}} | \hat{H}_{\rm eff} | \Phi_{x,\boldsymbol{\sigma}} \rangle = \begin{cases} -t_{x,y} & \text{if } \boldsymbol{\tau} = \boldsymbol{\sigma}_{y\to x} \\ 0 & \text{otherwise.} \end{cases} \tag{11.2.5}$$

Let $|\Phi_{\rm GS}\rangle$ be an arbitrary normalized ground state of $\hat{H}_{\rm eff}$, and expand it using the above basis as

$$|\Phi_{\rm GS}\rangle = \sum_{x\in\Lambda} \sum_{\boldsymbol{\sigma}\in\mathscr{S}_{\Lambda\setminus\{x\}}} \varphi(x,\boldsymbol{\sigma}) |\Phi_{x,\boldsymbol{\sigma}}\rangle. \tag{11.2.6}$$

Since the matrix elements (11.2.5) of $\hat{H}_{\rm eff}$ are real, we can assume that the coefficients $\varphi(x,\boldsymbol{\sigma})$ are real.[9] For each $x \in \Lambda$ we define

$$\xi_x = \Big(\sum_{\boldsymbol{\sigma}\in\mathscr{S}_{\Lambda\setminus\{x\}}} \{\varphi(x,\boldsymbol{\sigma})\}^2 \Big)^{1/2}. \tag{11.2.7}$$

Let the corresponding normalized ferromagnetic state be

$$|\Phi_\uparrow\rangle := \sum_{x\in\Lambda} \xi_x |\Phi_{x,(\uparrow)}\rangle, \tag{11.2.8}$$

where $(\uparrow)$ denotes the spin configuration with all spins up.

By using (11.2.6) and (11.2.5), we find

$$\begin{aligned} \langle \Phi_{\rm GS} | \hat{H}_{\rm eff} | \Phi_{\rm GS} \rangle &= \sum_{x,y\in\Lambda} \sum_{\substack{\boldsymbol{\sigma}\in\mathscr{S}_{\Lambda\setminus\{x\}} \\ \boldsymbol{\tau}\in\mathscr{S}_{\Lambda\setminus\{y\}}}} \varphi(y,\boldsymbol{\tau})\varphi(x,\boldsymbol{\sigma}) \langle \Phi_{y,\boldsymbol{\tau}} | \hat{H}_{\rm eff} | \Phi_{x,\boldsymbol{\sigma}} \rangle \\ &= -\sum_{x,y\in\Lambda} t_{x,y} \sum_{\boldsymbol{\sigma}\in\mathscr{S}_{\Lambda\setminus\{x\}}} \varphi(y,\boldsymbol{\sigma}_{y\to x})\varphi(x,\boldsymbol{\sigma}) \\ &\ge -\sum_{x,y\in\Lambda} t_{x,y} \Big(\sum_{\boldsymbol{\sigma}\in\mathscr{S}_{\Lambda\setminus\{x\}}} \{\varphi(y,\boldsymbol{\sigma}_{y\to x})\}^2 \Big)^{1/2} \Big(\sum_{\boldsymbol{\sigma}\in\mathscr{S}_{\Lambda\setminus\{x\}}} \{\varphi(x,\boldsymbol{\sigma})\}^2 \Big)^{1/2} \\ &= -\sum_{x,y\in\Lambda} t_{x,y}\, \xi_y \xi_x = \langle \Phi_\uparrow | \hat{H}_{\rm eff} | \Phi_\uparrow \rangle, \end{aligned} \tag{11.2.9}$$

where we used the Schwarz inequality (with the assumption $t_{x,y} \ge 0$) to get the third line. This bound shows that $|\Phi_\uparrow\rangle$ is also a ground state. ∎

[9] If this is not the case, we redefine $ia\{\varphi(x,\boldsymbol{\sigma}) - \varphi(x,\boldsymbol{\sigma})^*\}$ as $\varphi(x,\boldsymbol{\sigma})$, where $a \in \mathbb{R}$ is a normalization factor. The corresponding $|\Phi_{\rm GS}\rangle$ is also a ground state.

11.2.2 Nagaoka's Theorem and the Connectivity Condition

We now state a stronger theorem, namely, Nagaoka's theorem in its most general form [42, 66, 73]. Under an additional condition (which are verified in many situations), we prove that the model exhibits ferromagnetism in the sense of Definition 11.1, i.e., ferromagnetic ground states are the only possible ground states. See [20] for an extension of Nagaoka's theorem to the SU(n) version of the Hubbard model, and [41] for a unified extension to the Hubbard model coupled to phonons or photons.

The key is the Perron–Frobenius theorem, Theorem A.18 in p. 475. To apply the theorem to the present problem, we identify the matrix M with the matrix representation (11.2.5) of the effective Hamiltonian in the basis states (11.2.3) with a fixed $S^{(3)}_{\mathrm{tot}} = \sum_{y\in\Lambda\setminus\{x\}} \sigma_y$. Because of (11.2.5) and the assumption $t_{x,y} \geq 0$, the condition (i) (for Theorem A.18) on the non-positivity of off-diagonal matrix elements is satisfied. The condition (ii) on the connectivity, on the other hand, is not always valid. This motivates us to introduce the following connectivity condition.

Definition 11.6 (*Connectivity condition*) A Hubbard model with $U = \infty$ and $N = |\Lambda| - 1$ is said to satisfy the connectivity condition if all the basis states $|\Phi_{x,\boldsymbol{\sigma}}\rangle$ with common $S^{(3)}_{\mathrm{tot}} = \sum_{y\in\Lambda\setminus\{x\}} \sigma_y$ are connected (in the sense of the Perron–Frobenius theorem) with each other through nonvanishing matrix elements of $\hat{H}_{\mathrm{eff}}$.

Note that the connectivity condition is a condition for hopping amplitude $(t_{x,y})_{x,y\in\Lambda}$ (or the graph defined by the hopping amplitude). As we shall see below, the connectivity condition is known to be satisfied in the Hubbard model with nearest neighbor hopping on essentially any standard lattices in two or higher dimensions.

Consider a model which satisfies the connectivity condition. Then we can readily apply the Perron–Frobenius theorem to see that the ground state in each subspace with a fixed $S^{(3)}_{\mathrm{tot}}$ is unique. Then Theorem 11.5 implies that this ground state must be ferromagnetic. We have thus proved the following.

Theorem 11.7 (Nagaoka's theorem) *Consider an arbitrary Hubbard model with $t_{x,y} \geq 0$ for any $x, y \in \Lambda$, $N = |\Lambda| - 1$, and $U = \infty$, and further assume that the model satisfies the connectivity condition. Then the ground states have total spin $S_{\mathrm{tot}} = S_{\max} (= N/2)$, and are non-degenerate apart from the trivial $(2S_{\max} + 1)$-fold degeneracy.*

In contrast to the weak theorem (Theorem 11.5), the above theorem states that all the ground states are ferromagnetic. This improvement is essential if one is interested in the emergence of ferromagnetism.

Since the theorem asserts the non-degeneracy of the ferromagnetic ground states for $U = \infty$, the continuity of energy eigenvalues in U implies that the statement of the theorem is valid also for sufficiently large but finite U. However, we have no meaningful estimates on how large U should be. When U is finite it is expected that antiferromagnetic interaction is generated by the mechanism (which does not involve the hole) discussed in Sect. 10.1. Then it is very likely that U must grow indefinitely as $|\Lambda|$ is increased in order to maintain ferromagnetism.

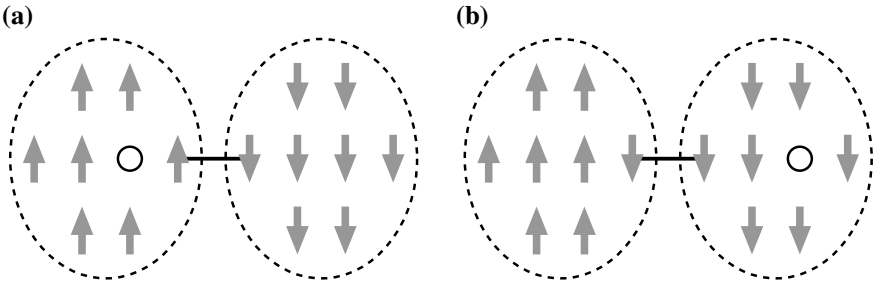

Fig. 11.6 A lattice which is connected but not biconnected. The lattice can be decomposed into two parts (within which one may have any connections) connected by a single bond. Suppose that one starts from a configuration (**a**), where the left part contains only up-spin electrons and a hole, while the right part contains only down-spin electrons. When the hole moves to the right part, one gets a configuration (**b**). If the hole go backs to the left part, one again gets a configuration as in **a**. It is impossible to carry an up-spin electron to the right part. The connectivity condition is violated ()

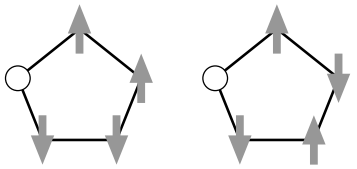

Fig. 11.7 The connectivity condition does not hold on a pentagon. It is interesting to compare the situation with those in a triangle (Fig. 11.8) and a square (Fig. 11.9) ()

Connectivity condition In order to make Theorem 11.7 meaningful, we still need to verify the connectivity condition for some concrete models. Let $\mathscr{B}$ be the set of bonds $\{x, y\} = \{y, x\}$ such that $x \neq y$ and $t_{x,y} \neq 0$. We shall examine the validity of the connectivity condition for the lattice (or the graph) $(\Lambda, \mathscr{B})$.

Let us first discuss a necessary and sufficient condition for the connectivity condition [4]. Obviously the connectivity condition does not always hold. If $(\Lambda, \mathscr{B})$ is a one-dimensional lattice with open boundary conditions, for example, it is easy to see that there is no way of modifying spin configurations by the motion of a hole. Generalizing this observation, one sees that the connectivity condition does not hold if the lattice $(\Lambda, \mathscr{B})$ is not biconnected.[10] See Fig. 11.6. Another counter example is $(\Lambda, \mathscr{B})$ which forms a hexagon. It is obvious that one can never connect the two configurations depicted in Fig. 11.7 by moving the hole.

[10] A lattice (or a graph) is biconnected (or non-separable) if and only if one cannot make it disconnected by removing a single site.

In fact it is known that these two examples essentially represent all cases where the connectivity condition fails. By making use of a graph theoretic result by Wilson [81] on the "15 puzzle" problem,[11] Bobrow, Stubis, and Li recently derived the following necessary and sufficient condition for the connectivity [4].

Theorem 11.8 (Necessary and sufficient condition for the connectivity) *A lattice* $(\Lambda, \mathscr{B})$ *satisfies the connectivity condition if and only if it is biconnected and it is not a simple loop (i.e., periodic chain) with more than four sites.*

We thus see that the connectivity condition is satisfied in essentially any standard lattice in two or higher dimensions. We leave the Proof of Theorem 11.8 to the original papers [4, 81].

Let us next state a simple sufficient condition for the connectivity, which can be proved easily.[12] The sufficient condition is implicit in Nagaoka's original work [42].

We introduce some terminology to state the condition. By a loop of length m, we mean an ordered set $(x_1, \ldots, x_m)$ of sites in Λ such that $\{x_i, x_{i+1}\} \in \mathscr{B}$ for all $i = 1, \ldots, m-1$, and $\{x_m, x_1\} \in \mathscr{B}$. We say that a pair $\{x, y\}$ of lattice sites (which may not be in $\mathscr{B}$) is an exchange bond if (E1) x and y belong to a common loop of length three or four, and (E2) the whole lattice remains connected (through bonds in $\mathscr{B}$) when both the sites x and y are removed.

Lemma 11.9 (A sufficient condition for the connectivity) *If the whole lattice is connected by exchange bonds, then the model satisfies the connectivity condition.*

Note that all bonds in $\mathscr{B}$ are also exchange bonds in triangular, square, simple cubic, fcc, or bcc lattices. These lattices trivially satisfy the above sufficient condition. The hexagonal lattice does not satisfy the sufficient condition, but it does satisfy the connectivity condition because of Theorem 11.8.

Proof of Lemma 11.9 Suppose that we are given an arbitrary configuration of $N = |\Lambda| - 1$ electrons on Λ. Our goal is to show that we can get an arbitrary configuration with the same $S^{(3)}_{\mathrm{tot}}$ by moving the single hole along bonds in $\mathscr{B}$.

Let $\{x, y\}$ be an exchange bond. We show below that we can exchange the spins at sites x and y without changing the configuration outside $\{x, y\}$. Since the whole lattice is connected via exchange bonds, this means we can generate any permutation of spin configurations by successive exchanges on the exchange bonds.[13] This proves the connectivity condition.

We now prove the desired property of exchange bonds. Let $\{x, y\}$ be an exchange bond, and assume that x and y are occupied by electrons with opposite spins. We first bring the hole (by successive hops outside $\{x, y\}$) to a site other than x or y on the loop (of length three or four) that contains both x and y. Next we let the hole move

[11] Those who read Japanese might enjoy a short article by Nagaoka entitled "The 15 Puzzle" [43].

[12] The sufficient condition is, in a sense, physical since it only makes use of basic exchange processes caused by local motions of the hole. But, after all, we should note that Nagaoka's ferromagnetism itself is not quite physical.

[13] For a proof of this property, see "Proof of the property (iii)" in p. 41.

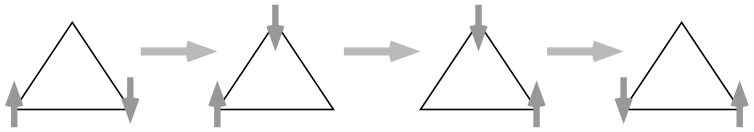

Fig. 11.8 The two spins are exchanged when the hole hops around the loop once. This is the same as Fig. 11.2 for the toy model discussed in Sect. 11.1.3 ()

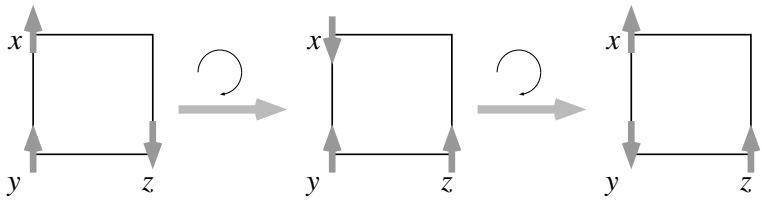

Fig. 11.9 The spins at x and z are exchanged when the hole hops around the loop once. The spins at y and z are exchanged when the hole hops around the loop twice (or once in the opposite orientation) ()

along the loop until the spins at x and y are exchanged. In a loop of length three, this is realized after the hole goes around the loop once, as in Fig. 11.8. In a loop of length four, we have to move the hole along the loop once or twice, depending on the spin configuration, as in Fig. 11.9. Note that the exchange on a length four loop is possible because electronic spins take (only) two values.[14] Finally, we bring the hole back to the original location by following the same path as before backwards. We then recover exactly the same spin configuration, except on sites x and y. ∎

11.2.3 Instability of Nagaoka's Ferromagnetism

There is no doubt that Nagaoka's ferromagnetism is nontrivial and interesting. We have seen that completely spin-independent on-site Coulomb interaction and quantum mechanics for many fermions together can generate strong order in electron spins. It is also clear, on the other hand, that the mechanism that generates ferromagnetism is rather singular; the only motion allowed in the whole system is that of the single hole, and this motion generates the ferromagnetic order in the whole system. One expects that the resulting ferromagnetic state is physically pathological.

The pathology is clearly seen in the properties of low energy excitations. Kusakabe and Aoki studied spin-wave excitations above the ground state and found unusual behaviors [25]. Most notably it was shown that the width of the energy band (of the spin-wave excitation) shrinks to zero as the system size is increased. This result also

[14] This point is relevant to the extension of Nagaoka's ferromagnetism to the SU(n) Hubbard model [4, 20].

suggests that the Nagaoka's ferromagnetism does not emerge in a model with large but finite U which is independent of the system size. See also [3].

The pathology may be removed if the Nagaoka's ferromagnetism can be extended to models which have multiple holes with nonzero density. If each hole contributes in aligning spins in a finite region then it might be possible that healthy ferromagnetism in the whole system is generated. Unfortunately, the Perron–Frobenius argument which works for the one-hole case fails even for models with two holes. In fact it has been shown, e.g., in [7, 56, 76] that ferromagnetism does not emerge when there are two holes.

There is a considerable number of rigorous works (including that in Nagaoka's original work [42]) which establish that saturated ferromagnetism does not take place when one relaxes the strict conditions necessary for Nagaoka's theorem. See, for example, [14, 15, 52, 54]. Most of these works are essentially based on variational arguments where one constructs sophisticated variational states which have lower energies than the ferromagnetic state. See also [27, 47, 48] for results which indicate the instability of Nagaoka's ferromagnetism. We also recommend Sect. 8.4 of [10], which contains extensive discussion about the instability of Nagaoka's ferromagnetism. As far as we know, there are no rigorous results about the stability of Nagaoka's ferromagnetism in the Hubbard model.

11.3 Flat-Band Ferromagnetism

In the present section, we discuss versions of the Hubbard model which exhibit a type of ferromagnetism known as flat-band ferromagnetism. Flat-band ferromagnetism takes place in particularly designed systems in which the single-electron ground states have macroscopic degeneracy. Recall that Nagaoka's ferromagnetism satisfies the Stoner criterion $D_{\mathrm{F}} U \gtrsim 1$ because of the large Coulomb interaction U. In flat-band ferromagnetism, the criterion is satisfied for the opposite reason that the density of states D_{F} is infinitely large. Unlike Nagaoka's ferromagnetism, which is likely to be unstable against perturbation, flat-band ferromagnetism is believed to be stable against various perturbation. There are indeed some rigorous results about stability, as we shall discuss in Sect. 11.4.

The first class of examples of flat-band ferromagnetism was discovered in 1991 by Mielke [34], whose elegant construction makes use of graph theoretic notions. Later, Tasaki [67], who had been independently working on a similar problem, found a different class of models which exhibit flat-band ferromagnetism.[15]

We start by discussing Tasaki's model in detail in Sect. 11.3.1 since the theory is more elementary. We emphasize that the proof of the emergence of ferromagnetism in this model clearly illustrates the mechanism by which ferromagnetic exchange interaction is generated from the Coulomb repulsion and quantum mechanics for fermions. Then we describe in Sect. 11.3.2 the class of flat-band models discovered

[15] It was very early days of arXiv, and neither Mielke nor myself were posting papers. I learned about Mielke's work from my colleague some time after it was published in the journal. I was at that time working on a draft of my paper [67].

by Mielke, whose construction is based on the notion of line graphs. After discussing a general method for constructing models with flat-bands in Sect. 11.3.3, we finally discuss the general theory of flat-band ferromagnetism due to Mielke in Sect. 11.3.4. We note that the topics treated in Sects. 11.3.3 and 11.3.4 are somewhat advanced. The reader may skip these subsections and proceed directly to Sect. 11.4.

After the works of Mielke and Tasaki, various versions of the Hubbard model that exhibit flat-band ferromagnetism have been found.[16] See, e.g., [6, 13, 29, 31, 32, 51, 58, 60, 77]. We should always keep in mind that the Hubbard model is a highly simplified theoretical model. To find the implications of results for the Hubbard model in realistic many-electron systems is an extremely difficult but a challenging problem. See, e.g., [1, 11, 17, 26, 28, 44, 55] for some interesting proposals about experimental realization of flat-band ferromagnetism.

11.3.1 Tasaki's Flat-Band Ferromagnetism

We shall discuss Tasaki's flat-band ferromagnetism in detail. We define the simplest version of the model, give a complete proof, and discuss the band structure and the mechanism of the ferromagnetism. We also describe a general procedure, called the cell construction, to define a class of models that exhibit flat-band ferromagnetism.

The model on the decorated hypercubic lattice and the main theorem Let $\mathscr{E}$ be the set of sites in the d-dimensional $L \times L$ hypercubic lattice with unit lattice spacing and periodic boundary conditions. It is exactly the same as Λ_L defined in (3.1.2). We take a new site in the middle of each bond (i.e., a pair of sites separated by distance 1) of the hypercubic lattice, and denote by $\mathscr{I}$ the collection of all such sites. We study the Hubbard model on the decorated hypercubic lattice $\Lambda = \mathscr{E} \cup \mathscr{I}$. Sites in $\mathscr{E}$ are called external sites, and in $\mathscr{I}$ are called internal sites, for a reason to become clear when we discuss the general construction at the end of the section. One may regard the lattice structure as crudely mimicking that of a metallic oxide, where sites in $\mathscr{E}$ and $\mathscr{I}$ are identified with metallic atoms and oxygen atoms, respectively. The two-dimensional version of Λ is the same as the Lieb lattice. See Fig. 10.2 in p. 355 and Fig. 11.10.

Let us define two types of localized states in the single-electron Hilbert space $\mathfrak{h} \cong \mathbb{C}^{|\Lambda|}$. Let $\nu > 0$ be a fixed parameter. For each $p \in \mathscr{E}$, we define $\boldsymbol{\alpha}_p = (\alpha_p(x))_{x\in\Lambda} \in \mathfrak{h}$ by

$$\alpha_p(x) = \begin{cases} 1 & \text{if } x = p, \\ -\nu & \text{if } |x - p| = 1/2, \\ 0 & \text{otherwise,} \end{cases} \tag{11.3.1}$$

[16] We believe it fair to say that rigorous results preceded numerical works in the study of ferromagnetism in the Hubbard model. There also appeared numerical works in various versions of the Hubbard model, but we shall not try to list them.

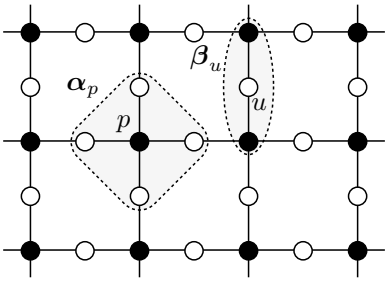

Fig. 11.10 The decorated hypercubic lattice with $d = 2$, which is the same as the Lieb lattice (Fig. 10.2). Black dots represent sites in $\mathscr{E}$ (which may be identified with metallic atoms) and white dots represent sites in $\mathscr{I}$ (which may be identified with oxygen atoms). Single-electron states $\boldsymbol{\alpha}_p$ and $\boldsymbol{\beta}_u$ are localized around sites $p \in \mathscr{E}$ and $u \in \mathscr{I}$, respectively ()

and, for each $u \in \mathscr{I}$, we define $\boldsymbol{\beta}_u = (\beta_u(x))_{x\in\Lambda} \in \mathfrak{h}$ by

$$\beta_u(x) = \begin{cases} 1 & \text{if } x = u, \\ \nu & \text{if } |x-u| = 1/2, \\ 0 & \text{otherwise.} \end{cases} \tag{11.3.2}$$

See Fig. 11.10. Although ν is completely arbitrary here, it is useful to imagine that $0 < \nu \ll 1$. Then $\boldsymbol{\alpha}_p$ represents a state in which the electron is mostly localized at a metallic site p with small components on the neighboring sites, and likewise $\boldsymbol{\beta}_u$ represents a state nearly localized at an oxygen site u. We will see that the ferromagnetic ground states consist only of electrons in the $\boldsymbol{\alpha}$ states as in (11.3.9).

Note that $\langle \boldsymbol{\alpha}_p, \boldsymbol{\beta}_u \rangle = 0$ for any $p \in \mathscr{E}$ and $u \in \mathscr{I}$. The following lemma, which should be expected, is essential.

Lemma 11.10 $\{\boldsymbol{\alpha}_p\}_{p\in\mathscr{E}} \cup \{\boldsymbol{\beta}_u\}_{u\in\mathscr{I}}$ *is a basis of* $\mathfrak{h}$.

Proof $\boldsymbol{\alpha}_p$ with $p \in \mathscr{E}$ are linearly independent since only $\boldsymbol{\alpha}_p$ has nonzero component on site p. Likewise $\boldsymbol{\beta}_u$ with $u \in \mathscr{I}$ are linearly independent. Noting that $\{\boldsymbol{\alpha}_p\}_{p\in\mathscr{E}}$ and $\{\boldsymbol{\beta}_u\}_{u\in\mathscr{I}}$ span mutually orthogonal spaces with dimensions $|\mathscr{E}|$ and $|\mathscr{I}|$, respectively, and that the dimension of $\mathfrak{h}$ is $|\Lambda| = |\mathscr{E}| + |\mathscr{I}|$, we see that $\{\boldsymbol{\alpha}_p\}_{p\in\mathscr{E}} \cup \{\boldsymbol{\beta}_u\}_{u\in\mathscr{I}}$ forms a basis of $\mathfrak{h}$. ∎

Let us define fermion operators corresponding to $\boldsymbol{\alpha}_p$ and $\boldsymbol{\beta}_u$ by

$$\hat{a}_{p,\sigma} := \hat{C}_\sigma(\boldsymbol{\alpha}_p) = \hat{c}_{p,\sigma} - \nu \sum_{\substack{u\in\mathscr{I} \\ (|u-p|=1/2)}} \hat{c}_{u,\sigma}, \tag{11.3.3}$$

for $p \in \mathscr{E}$, and

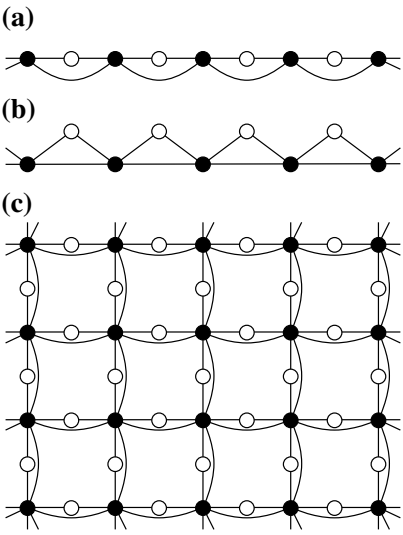

Fig. 11.11 Hopping in the Tasaki model in **a** $d = 1$ and **c** $d = 2$. Note that the lattice for $d = 1$ can be modified (without changing the connection) into the Delta chain in **b**. In addition to the hopping amplitude indicated by the lines, we have on-site potential which is fine tuned. See (11.3.22). Note that on each bond we have a structure with three sites that resembles the toy model for ferromagnetism described in Fig. 11.1 (p. 377) ()

$$\hat{b}_{u,\sigma} := \hat{C}_\sigma(\boldsymbol{\beta}_u) = \hat{c}_{u,\sigma} + \nu \sum_{\substack{p\in\mathscr{E} \\ (|p-u|=1/2)}} \hat{c}_{p,\sigma}, \tag{11.3.4}$$

for $u \in \mathscr{I}$. We then consider the Hubbard model with the Hamiltonian $\hat{H} = \hat{H}_{\text{hop}} + \hat{H}_{\text{int}}$, where the hopping Hamiltonian is defined as

$$\hat{H}_{\text{hop}} = t \sum_{\substack{u\in\mathscr{I} \\ \sigma=\uparrow,\downarrow}} \hat{b}^\dagger_{u,\sigma}\hat{b}_{u,\sigma}, \tag{11.3.5}$$

with $t > 0$, and the interaction Hamiltonian as

$$\hat{H}_{\text{int}} = U \sum_{x\in\Lambda} \hat{n}_{x,\uparrow}\hat{n}_{x,\downarrow}. \tag{11.3.6}$$

Note that our hopping Hamiltonian has a particular form while the interaction Hamiltonian is standard. Recalling the definition (11.3.4) of $\hat{b}_{u,\sigma}$, one sees that $\hat{H}_{\text{hop}}$ contains hopping between a pair of sites in $\mathscr{E}$ separated by distance 1 as well as a pair of sites in $\mathscr{E}$ and $\mathscr{I}$ separated by distance 1/2 as in Fig. 11.11. See also (11.3.22) below for an explicit expression of the hopping amplitude.

The following theorem in [40, 67] establishes the emergence of ferromagnetism in the present model.

Theorem 11.11 (Tasaki's flat-band ferromagnetism) *Consider the above Hubbard model with electron number $N = |\mathscr{E}| = L^d$. Then for any $\nu > 0$, $t > 0$, and $U > 0$,*

the ground states have $S_{\rm tot} = S_{\rm max} = N/2$*, and are unique apart from the trivial* $2S_{\rm max} + 1 = N + 1$ *fold degeneracy.*

Before proving the theorem, let us construct ground states of the model. Note that $\langle \boldsymbol{\alpha}_p, \boldsymbol{\beta}_u \rangle = 0$ and (9.2.64) imply

$$\{\hat{b}_{u,\sigma}, \hat{a}^\dagger_{p,\tau}\} = 0, \tag{11.3.7}$$

for any $u \in \mathscr{I}$, $p \in \mathscr{E}$, and $\sigma, \tau = \uparrow, \downarrow$. This in particular means $[\hat{b}^\dagger_{u,\sigma}\hat{b}_{u,\sigma}, \hat{a}^\dagger_{p,\tau}] = 0$, and hence

$$\hat{H}_{\rm hop}|\Phi_{\boldsymbol{\alpha}\ {\rm all}\uparrow}\rangle = 0, \tag{11.3.8}$$

where

$$|\Phi_{\boldsymbol{\alpha}\ {\rm all}\uparrow}\rangle = \Big(\prod_{p\in\mathscr{E}} \hat{a}^\dagger_{p,\uparrow}\Big)|\Phi_{\rm vac}\rangle \tag{11.3.9}$$

is a ferromagnetic state where all the $\boldsymbol{\alpha}$ states are filled with up-spin electrons. It is also obvious that $\hat{H}_{\rm int}|\Phi_{\boldsymbol{\alpha}\ {\rm all}\uparrow}\rangle = 0$, and we find that $\hat{H}|\Phi_{\boldsymbol{\alpha}\ {\rm all}\uparrow}\rangle = 0$. Noting that $\hat{H}_{\rm hop} \geq 0$, $\hat{H}_{\rm int} \geq 0$, and hence $\hat{H} \geq 0$ (see Appendix A.2.3 for inequalities for self-adjoint operators), we see that the ground state energy of $\hat{H}$ is zero, and the ferromagnetic state $|\Phi_{\boldsymbol{\alpha}\ {\rm all}\uparrow}\rangle$ is a ground state. This is indeed a straightforward consequence of the (artificial) definition (11.3.5). The main point of Theorem 11.11 is that $|\Phi_{\boldsymbol{\alpha}\ {\rm all}\uparrow}\rangle$ is essentially the unique ground state. Since only trivial $2S_{\rm tot} + 1$ fold degeneracy is allowed by the theorem, we see that the ground states are written as

$$|\Phi^{(M)}_{\rm GS}\rangle = (\hat{S}^-_{\rm tot})^{(N/2)-M}|\Phi_{\boldsymbol{\alpha}\ {\rm all}\uparrow}\rangle \tag{11.3.10}$$

with $M = -S_{\rm max}, -S_{\rm max}+1, \ldots, S_{\rm max}$.

Proof of Theorem 11.11 We shall prove that any ground state must be a linear combination of the ground states (11.3.10). Here each step in the proof highlights essential physical mechanism for ferromagnetism. We shall make clear the physical meaning of each argument.

Frustration free properties: Let $|\Phi_{\rm GS}\rangle$ be an arbitrary ground state of $\hat{H}$ with $N = |\mathscr{E}|$ electrons. Since the ground state energy is zero, we have $\hat{H}|\Phi_{\rm GS}\rangle = 0$, and hence $\hat{H}_{\rm hop}|\Phi_{\rm GS}\rangle = 0$ and $\hat{H}_{\rm int}|\Phi_{\rm GS}\rangle = 0$. Recalling the definitions (11.3.5) and (11.3.6), we find from Lemma A.10 (p. 469) about frustration-free Hamiltonians that $\hat{b}^\dagger_{u,\sigma}\hat{b}_{u,\sigma}|\Phi_{\rm GS}\rangle = 0$ for each u, σ, and $\hat{n}_{x,\uparrow}\hat{n}_{x,\downarrow}|\Phi_{\rm GS}\rangle = 0$ for each x. We further see from Lemma A.11 (p. 469) about positive semidefinite operators that

$$\hat{b}_{u,\sigma}|\Phi_{\rm GS}\rangle = 0 \text{ for any } u \in \mathscr{I} \text{ and } \sigma = \uparrow, \downarrow, \tag{11.3.11}$$

and

$$\hat{c}_{x,\downarrow}\hat{c}_{x,\uparrow}|\Phi_{\rm GS}\rangle = 0 \text{ for any } x \in \Lambda, \tag{11.3.12}$$

where we noted that $\hat{n}_{x,\uparrow}\hat{n}_{x,\downarrow} = (\hat{c}_{x,\downarrow}\hat{c}_{x,\uparrow})^\dagger\, \hat{c}_{x,\downarrow}\hat{c}_{x,\uparrow}$. The conditions (11.3.11) and (11.3.12), which we shall call the zero-energy conditions, will turn out to be quite useful.

Restriction to the lowest band: From Lemma 9.4 (p. 321) about general basis of the Hubbard model and Lemma 11.10 above, we see that our ground state is (indeed, any state is) expanded as

$$|\Phi_{\rm GS}\rangle = \sum_{\substack{A_\uparrow, A_\downarrow \subset \mathscr{E} \\ B_\uparrow, B_\downarrow \subset \mathscr{I} \\ (|A_\uparrow|+|A_\downarrow|+|B_\uparrow|+|B_\downarrow|=N)}} f(A_\uparrow, A_\downarrow, B_\uparrow, B_\downarrow)\Big(\prod_{p\in A_\uparrow}\hat{a}^\dagger_{p,\uparrow}\Big)\Big(\prod_{p\in A_\downarrow}\hat{a}^\dagger_{p,\downarrow}\Big)\Big(\prod_{u\in B_\uparrow}\hat{b}^\dagger_{u,\uparrow}\Big)\Big(\prod_{u\in B_\downarrow}\hat{b}^\dagger_{u,\downarrow}\Big)|\Phi_{\rm vac}\rangle, \tag{11.3.13}$$

where $f(A_\uparrow, A_\downarrow, B_\uparrow, B_\downarrow)$ is a certain coefficient. It should be clear that the zero-energy condition (11.3.11) shows that $|\Phi_{\rm GS}\rangle$ does not contain any $\hat{b}^\dagger_{u,\sigma}$, i.e., one has $f(A_\uparrow, A_\downarrow, B_\uparrow, B_\downarrow) = 0$ unless $B_\uparrow = B_\downarrow = \emptyset$.[17] Thus the ground state is written as

$$|\Phi_{\rm GS}\rangle = \sum_{\substack{A_\uparrow, A_\downarrow \subset \mathscr{E} \\ (|A_\uparrow|+|A_\downarrow|=N)}} g(A_\uparrow, A_\downarrow)\Big(\prod_{p\in A_\uparrow}\hat{a}^\dagger_{p,\uparrow}\Big)\Big(\prod_{p\in A_\downarrow}\hat{a}^\dagger_{p,\downarrow}\Big)|\Phi_{\rm vac}\rangle, \tag{11.3.14}$$

where $g(A_\uparrow, A_\downarrow) = f(A_\uparrow, A_\downarrow, \emptyset, \emptyset)$.

As we shall see in the next part, the states created by the $\hat{a}^\dagger$ operators belong to the lowest flat-band of the single-electron spectrum. That we can discuss the low energy properties of the model within the space spanned by the lowest band is of essential importance for the rest of the proof (and in the physical picture of nearly-flat-band ferromagnetism).

Repulsion in the state space: We next make use of the zero-energy condition (11.3.12), which represents the effect of local Coulomb repulsion. Note that $[\hat{c}_{p,\downarrow}\hat{c}_{p,\uparrow}, \hat{a}^\dagger_{q,\sigma}] = 0$ for any $p, q \in \mathscr{E}$ such that $p \neq q$, and that

$$\hat{c}_{p,\downarrow}\hat{c}_{p,\uparrow}\hat{a}^\dagger_{p,\uparrow}\hat{a}^\dagger_{p,\downarrow}|\Phi_{\rm vac}\rangle = |\Phi_{\rm vac}\rangle, \tag{11.3.15}$$

for any $p \in \mathscr{E}$. These relations imply that the condition (11.3.12) with $x = p \in \mathscr{E}$ cannot be valid if the ground state (11.3.14) contains $\hat{a}^\dagger_{p,\uparrow}\hat{a}^\dagger_{p,\downarrow}$. This means that one has $g(A_\uparrow, A_\downarrow) = 0$ whenever $A_\uparrow \cap A_\downarrow \neq \emptyset$. We have thus found, not too surprisingly, that repulsion in the real space leads to repulsion in the state space (described by $\hat{a}^\dagger$ operators). Of course this is not the only effect of the repulsive interaction, as we shall see below.

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[17] This is in fact not entirely obvious because $\boldsymbol{\beta}_u$ with $u \in \mathscr{I}$ are not mutually orthogonal. Let us give a careful proof. Define the Gramm matrix G by $(\mathsf{G})_{u,v} = \langle \boldsymbol{\beta}_u, \boldsymbol{\beta}_v\rangle = \{\hat{b}_{u,\sigma}, \hat{b}^\dagger_{v,\sigma}\}$ for $u, v \in \mathscr{I}$. The linear independence of $\{\boldsymbol{\beta}_u\}_{u\in\mathscr{I}}$ implies that G is invertible. We define the dual operators by $\hat{b}'_{u,\sigma} = \sum_{v\in\mathscr{I}}(\mathsf{G}^{-1})_{u,v}\hat{b}_{v,\sigma}$, which clearly satisfy $\{\hat{b}'_{u,\sigma}, \hat{b}^\dagger_{v,\tau}\} = \delta_{u,v}\delta_{\sigma,\tau}$. We also have $\{\hat{b}'_{u,\sigma}, \hat{a}^\dagger_{p,\tau}\} = 0$ for any $u \in \mathscr{I}$ and $p \in \mathscr{E}$. Since (11.3.11) implies $\hat{b}'_{u,\sigma}|\Phi_{\rm GS}\rangle = 0$ for any $u \in \mathscr{I}$ and $\sigma = \uparrow, \downarrow$, we get the desired property.

Since $|A_\uparrow| + |A_\downarrow| = N = |\mathscr{E}|$, we find that $A_\uparrow \cap A_\downarrow = \emptyset$ implies $A_\uparrow \cup A_\downarrow = \mathscr{E}$. We therefore see that the ground state (11.3.14) is further rewritten as

$$|\Phi_{\rm GS}\rangle = \sum_{\boldsymbol{\sigma}} C(\boldsymbol{\sigma}) \Big(\prod_{p\in\mathscr{E}} \hat{a}^\dagger_{p,\sigma_p} \Big) |\Phi_{\rm vac}\rangle, \tag{11.3.16}$$

where $\boldsymbol{\sigma} = (\sigma_p)_{p\in\mathscr{E}}$ (with $\sigma_p = \uparrow, \downarrow$) is summed over all possible spin configurations on $\mathscr{E}$, and $C(\boldsymbol{\sigma})$ is a coefficient determined from $g(A_\uparrow, A_\downarrow)$. We have fixed an arbitrary ordering of the elements of $\mathscr{E}$, and assume that any product respects the ordering. The expression (11.3.16) may be called the spin system representation.

Ferromagnetic exchange interaction: Let us examine the implication of the zero-energy condition (11.3.12) when x is in $\mathscr{I}$. Take $p, q \in \mathscr{E}$ separated by distance 1, and let $u \in \mathscr{I}$ be the unique site in between them. Then we see from the definition (11.3.3) that

$$\hat{c}_{u,\downarrow}\hat{c}_{u,\uparrow}\hat{a}^\dagger_{p,\sigma}\hat{a}^\dagger_{q,\tau}|\Phi_{\rm vac}\rangle = \begin{cases} |\Phi_{\rm vac}\rangle & \text{if } (\sigma,\tau) = (\uparrow,\downarrow), \\ -|\Phi_{\rm vac}\rangle & \text{if } (\sigma,\tau) = (\downarrow,\uparrow), \\ 0 & \text{if } (\sigma,\tau) = (\uparrow,\uparrow), (\downarrow,\downarrow). \end{cases} \tag{11.3.17}$$

Note that the sign changes when the spins are exchanged because of the fermionic anticommuation relation.

For the same p, q, let us rewrite the spin system representation (11.3.16) as

$$|\Phi_{\rm GS}\rangle = \sum_{\boldsymbol{\sigma}} \mathrm{sgn}(p,q)\, C(\boldsymbol{\sigma})\, \hat{a}^\dagger_{p,\sigma_p}\hat{a}^\dagger_{q,\sigma_q} \Big(\prod_{p'\in\mathscr{E}\setminus\{p,q\}} \hat{a}^\dagger_{p',\sigma_{p'}} \Big) |\Phi_{\rm vac}\rangle, \tag{11.3.18}$$

where $\mathrm{sgn}(p,q) = \pm 1$ is a fermionic sign factor which depends only on p and q. Noting that $\hat{c}_{u,\downarrow}\hat{c}_{u,\uparrow}$ commutes with $(\prod_{p'\in\mathscr{E}\setminus\{p,q\}} \hat{a}^\dagger_{p',\sigma_{p'}})$, we see from (11.3.17) that

$$\begin{aligned} &\hat{c}_{u,\downarrow}\hat{c}_{u,\uparrow}|\Phi_{\rm GS}\rangle \\ &\quad = \sum_{\boldsymbol{\sigma}'} \mathrm{sgn}(p,q) \big\{ C\big((\uparrow,\downarrow,\boldsymbol{\sigma}')\big) - C\big((\downarrow,\uparrow,\boldsymbol{\sigma}')\big) \big\} \Big(\prod_{p'\in\mathscr{E}\setminus\{p,q\}} \hat{a}^\dagger_{p',\sigma_{p'}} \Big) |\Phi_{\rm vac}\rangle. \end{aligned} \tag{11.3.19}$$

We here wrote $\boldsymbol{\sigma}$ as $(\sigma_p, \sigma_q, \boldsymbol{\sigma}')$, where $\boldsymbol{\sigma}'$ is the spin configuration on $\mathscr{E}\setminus\{p,q\}$. Since the states in the sum are linearly independent, we see that the zero-energy condition $\hat{c}_{u,\downarrow}\hat{c}_{u,\uparrow}|\Phi_{\rm GS}\rangle = 0$ implies $C\big((\uparrow,\downarrow,\boldsymbol{\sigma}')\big) = C\big((\downarrow,\uparrow,\boldsymbol{\sigma}')\big)$ for any $\boldsymbol{\sigma}'$. In other words, we have found

$$C(\boldsymbol{\sigma}) = C(\boldsymbol{\sigma}_{p\leftrightarrow q}), \tag{11.3.20}$$

for any spin configuration $\boldsymbol{\sigma}$. Here $\boldsymbol{\sigma}_{p\leftrightarrow q}$ is the new spin configuration obtained from $\boldsymbol{\sigma}$ by swapping σ_p and σ_q. This is the exchange interaction that generates the ferromagnetism in the present model. Note that it is crucial here that the two $\boldsymbol{\alpha}$ states on the neighboring $\mathscr{E}$ sites share a common site in between them. See Fig. 11.12. We

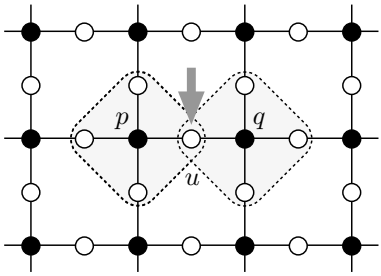

Fig. 11.12 A schematic picture of the mechanism which generates the exchange interaction (11.3.20). The two states $\boldsymbol{\alpha}_p$ and $\boldsymbol{\alpha}_q$ on the adjacent sites $p, q \in \mathscr{E}$ shares a common site $u \in \mathscr{I}$. When we take into account the effect of on-site repulsion at site u, we find that the spins localized around p and q, respectively, interact ferromagnetically. This is essentially the same as the direct exchange mechanism discussed by Heisenberg [16] ()

also note that this mechanism is essentially the same as Heisenberg's direct exchange interaction, which was originally discussed within a perturbative theory [16]. See also Sect. 11.4.1, in particular Fig. 11.19.

By using (11.3.20) repeatedly we see that $C(\boldsymbol{\sigma}) = C(\boldsymbol{\sigma}')$ whenever $\sum_{p\in\mathscr{E}} \sigma_p = \sum_{p\in\mathscr{E}} \sigma'_p$. This is because all the spin configurations with common $S^{(3)}_{\mathrm{tot}}$ are connected through swapping of spins on neighboring sites.[18] We thus find that the ground state within the space of fixed $S^{(3)}_{\mathrm{tot}}$ is unique. Since we already know that there is a ferromagnetic ground state (11.3.10) in this space, we see that the unique ground state has $S_{\mathrm{tot}} = S_{\mathrm{max}}$.[19]

We have thus proved that the ground state (11.3.16) is linear combination of the states (11.3.10).

Hopping amplitude, the band structure, and the role of the flat band We have represented the hopping Hamiltonian compactly as in (11.3.5) by using the $\hat{b}$ operators. By using the definition (11.3.4) of $\hat{b}_{u,\sigma}$, one can write (11.3.5) in the standard form

$$\hat{H}_{\mathrm{hop}} = \sum_{\substack{x,y\in\Lambda \\ \sigma=\uparrow,\downarrow}} t_{x,y}\, \hat{c}^{\dagger}_{x,\sigma}\hat{c}_{y,\sigma}, \tag{11.3.21}$$

with hopping amplitude given by

[18] This should be obvious, but see "Proof of the property (iii)" in p. 41 for a rigorous proof.

[19] By recalling (2.4.11), one can directly show that the superposition of basis states (with a common $S^{(3)}_{\mathrm{tot}}$) with equal weights leads to a ferromagnetic state.

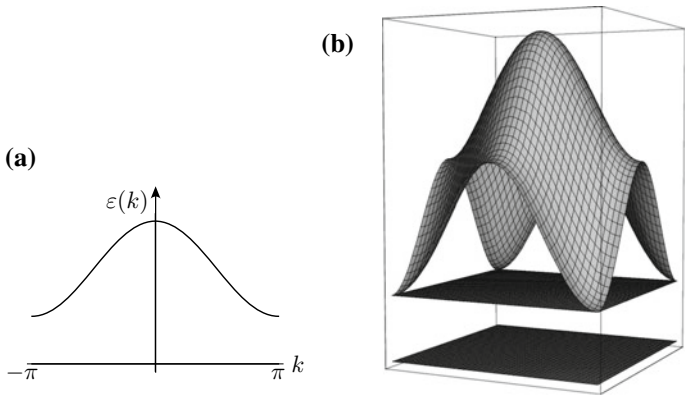

Fig. 11.13 The dispersion relations (11.3.23) of the Tasaki model on the decorated d-dimensional hypercubic lattice. **a** There are two bands in the one-dimensional model. A completely flat lower band is separated by a nonzero gap from the upper band with a cosine dispersion relation. **b** There are two flat-bands and one band with a cosine dispersion in the two-dimensional model. The lowest band is again separated by a nonzero gap from the rest of the spectrum. (The horizontal axes represent $k_1, k_2 \in [-\pi, \pi]$ and the vertical axis represents $\varepsilon(k_1, k_2)$.) ()

$$t_{x,y} = \begin{cases} v t & \text{if } |x-y| = 1/2, \\ v^2 t & \text{if } x, y \in \mathscr{E} \text{ and } |x-y| = 1, \\ t & \text{if } x = y \in \mathscr{I}, \\ 2d v^2 t & \text{if } x = y \in \mathscr{E} \\ 0 & \text{otherwise.} \end{cases} \tag{11.3.22}$$

See Fig. 11.11.

One can then solve the corresponding single-electron Schrödinger equation (9.3.3) to find the band structure. It is found that the model has $d+1$ bands with dispersion relations

$$\varepsilon_\mu(k) = \begin{cases} 0 & \mu = 1, \\ t & \mu = 2, \dots, d, \\ t + 2v^2 t \sum_{j=1}^{d} (1 + \cos k_j) & \mu = d+1, \end{cases} \tag{11.3.23}$$

where $k \in \mathscr{K}_L$ is a wave vector defined in (4.1.17). See Fig. 11.13. Rather pathologically, d bands are flat (or dispersion-less) and only the highest band has a cosine dispersion. See below for the derivation.

Clearly the lowest flat-band is most important for the present study of ferromagnetism. There are $|\mathscr{K}_L| = L^d$ states with zero energy, and are separated from other single-electron energy eigenstates by the energy gap $t > 0$. In fact the presence of the degenerate zero-energy states is obvious because the definition (11.3.5) and the anticommutation relation (11.3.7) readily imply

$$\hat{H}_{\rm hop}\,\hat{a}^{\dagger}_{p,\sigma}|\Phi_{\rm vac}\rangle = 0, \tag{11.3.24}$$

for any $p \in \mathscr{E}$. Note that the number of the zero-energy states $\hat{a}^{\dagger}_{p,\sigma}|\Phi_{\rm vac}\rangle$, which is $|\mathscr{E}|$, is the same as the degeneracy of the flat-band.

The presence of the macroscopic degeneracy in the single-electron ground states leads to a pathological degeneracy in the many-electron problem without interaction. To see this, note that, in the non-interacting model with Hamiltonian $\hat{H}_{\rm hop}$ and electron number $N = |\mathscr{E}|$, any state

$$\Big(\prod_{p\in A_\uparrow}\hat{a}^{\dagger}_{p,\uparrow}\Big)\Big(\prod_{p\in A_\downarrow}\hat{a}^{\dagger}_{p,\downarrow}\Big)|\Phi_{\rm vac}\rangle, \tag{11.3.25}$$

which appeared in (11.3.14), with arbitrary subsets $A_\uparrow, A_\downarrow \subset \mathscr{E}$ with $|A_\uparrow| + |A_\downarrow| = N$ is an exact ground state with energy zero. The ground states are highly degenerate, and, in particular, can take any total spin $S_{\rm tot}$ ranging from 0 to $S_{\rm max} = N/2$. This is a kind of paramagnetism. Then the role of U in the interacting model is to lift the degeneracy and to select those states with maximum $S_{\rm tot}$ as the only ground states. This is why Theorem 11.11 is valid for any positive value of U (rather than for U larger than a certain critical value). In this sense one can say that, in the flat-band ferromagnetism, there is no true competition (see Sect. 9.1) between the hopping Hamiltonian and the interaction Hamiltonian. We shall come back to this issue in Sect. 11.4.

Recall also that we have set the electron number N identical to the number of sites in $\mathscr{E}$. This choice enabled us to write down the spin system representation (11.3.16), in which each site in $\mathscr{E}$ (i.e., metallic atom) carries a spin. In the language of single-electron band structure, the choice $N = |\mathscr{E}|$ corresponds to the half-filling of the lowest flat-band. This feature is common for other examples of flat-band ferromagnetism, including that by Mielke. Very interestingly we observed in Sect. 10.2.3 that Lieb's ferrimagnetism also takes place when the flat-band (in the middle of the spectrum) is half-filled.

We finally comment on the derivation of the dispersion relations (11.3.23) for $\mu \geq 2$, i.e., the higher bands. The derivation is easy for $d = 1$. It is convenient to set $\mathscr{E} = \{1, 2, \ldots, L\}$ and $\mathscr{I} = \{\frac{1}{2}, \frac{3}{2}, \ldots, L - \frac{1}{2}\}$. Note that the definition (11.3.4) implies the anticommutation relation

$$\{\hat{b}_{v,\tau}, \hat{b}^{\dagger}_{u,\sigma}\} = \begin{cases} (1+2\nu^2)t\,\delta_{\sigma,\tau} & \text{if } v = u, \\ \nu^2 t\,\delta_{\sigma,\tau} & \text{if } |v-u| = 1, \\ 0 & \text{otherwise.} \end{cases} \tag{11.3.26}$$

We then find for any $\varphi_u \in \mathbb{C}$ (with $u \in \mathscr{I}$) that

$$\hat{H}_{\rm hop}\sum_{u\in\mathscr{I}}\varphi_u\,\hat{b}^{\dagger}_{u,\sigma}|\Phi_{\rm vac}\rangle = t\sum_{u\in\mathscr{I}}\varphi_u\big\{(1+2\nu^2)\hat{b}^{\dagger}_{u,\sigma} + \nu^2(\hat{b}^{\dagger}_{u+1,\sigma} + \hat{b}^{\dagger}_{u-1,\sigma})\big\}|\Phi_{\rm vac}\rangle. \tag{11.3.27}$$

This means that the Schrödinger equation $\hat{H}_{\rm hop} \sum_{u\in\mathscr{I}} \varphi_u \hat{b}^\dagger_{u,\sigma}|\Phi_{\rm vac}\rangle = \varepsilon \sum_{u\in\mathscr{I}} \varphi_u \hat{b}^\dagger_{u,\sigma}|\Phi_{\rm vac}\rangle$ reduces to

$$\nu^2 t(\varphi_{u+1} + \varphi_{u-1}) + (1 + 2\nu^2)t\,\varphi_u = \varepsilon\varphi_u, \tag{11.3.28}$$

which is essentially the same as the simplest tight-binding Schrödinger equation (9.3.7). One readily finds that the energy eigenvalues are given by $\varepsilon(k) = t + 2\nu^2 t(1 + \cos k)$, which is the desired dispersion relation for $\mu = 2$ in (11.3.23). The case with $d \geq 2$ may also be treated using the $\hat{b}^\dagger$ operators, but a straightforward calculation also works as we see in the following problem.

Problem 11.3.1.a Derive the dispersion relations (11.3.23) for general d by computing the effective hopping matrix given by (9.3.13) explicitly and then obtaining its eigenvalues. [solution→p.517]

The origin of the ferromagnetism Let us briefly discuss how the origin of the ferromagnetism in the present model can be understood intuitively. We shall see that at least three different physical pictures are possible.

First, as we have already discussed in the proof, our proof suggests that the "first order" effect of the Coulomb interaction at internal sites is relevant for ferromagnetic order. One may say that the spins of electrons nearly localized at sites in $\mathscr{E}$ (i.e., metallic sites) align with each other because of the direct exchange interaction. In this sense the model may be regarded as realizing Heisenberg's original picture of ferromagnetism. See also Sect. 11.4.1, in particular Fig. 11.19.

Secondly, one may view the present model as an assembly of the toy model with three sites discussed Sect. 11.1.3. One can then imagine that the ring exchange process in Fig. 11.1 is taking place in each part of the system and maintaining global ferromagnetism.

The third interpretation, which is most heuristic, is based on the band picture. The model has a flat-band at the bottom of the single-electron spectrum, which is exactly half-filled because we set $N = |\mathscr{E}|$. As we have discussed above, the model with $U = 0$ has highly degenerate ground states with all possible $S_{\rm tot}$. The Stoner criterion (see Sect. 11.1.4) then suggests that the degeneracy is lifted and one gets ferromagnetism for any $U > 0$ because we have $U D_{\rm F} = \infty$ for any nonzero U.

Cell construction Before closing this long subsection, we briefly discuss a general procedure, called the cell construction [73], to define models which have a flat-band and exhibit flat-band ferromagnetism. We note that, before Tasaki's work [67], Brandt and Giesekus [5] had proposed a class of Hubbard models which have a very similar cell structure. The Brandt-Giesekus model has interesting exact ground states with RVB (resonating valence-bond) structure, and exhibits paramagnetism. See also [68, 69].[20] In [59], Tanaka uses a similar construction to define a class of Hubbard models in which flat-band ferromagnetism is proved with a more sophisticated argument.

[20] In [68] we conjectured that a version of the Brandt-Giesekus model may exhibit superconductivity. We now believe that this is (unfortunately) not the case.

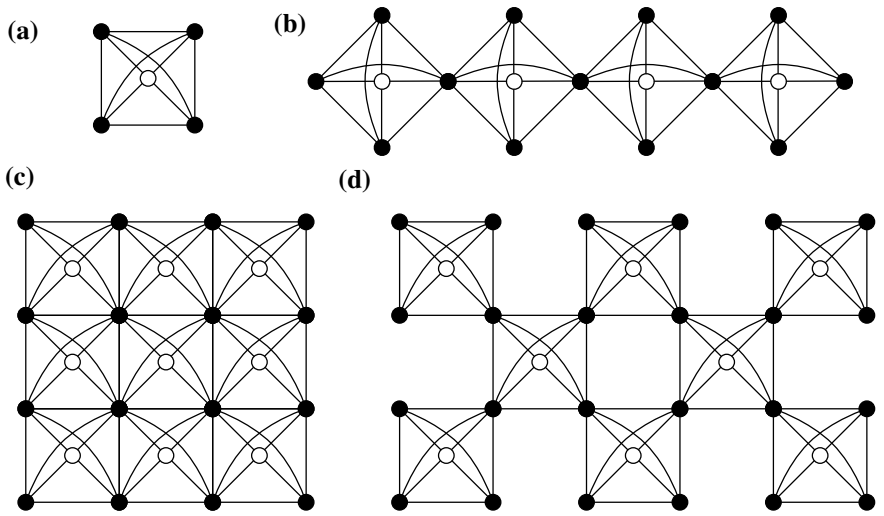

Fig. 11.14 **a** A cell with one internal site and four external sites, and **b** one dimensional and **c**, **d** two dimensional lattices constructed by assembling it ()

By a cell, we mean a set of site $C = \{u, p_1, \dots, p_n\}$, where u is called the internal site, and $p_1, \dots, p_n$ with $n \geq 2$ are called the external sites. We construct our lattice Λ by assembling a finite number of cells (which may or may not be identical), and identifying some external sites from different cells to regard them as a single site in Λ. There can be external sites which remain unidentified with other sites. We do not make such identifications for the internal sites. We assume that Λ thus constructed is connected. The lattice Λ is naturally decomposed as $\Lambda = \mathscr{E} \cup \mathscr{I}$, where $\mathscr{E}$ is the set of external sites and $\mathscr{I}$ the set of internal sites. For each $u \in \mathscr{I}$, we denote by C_u the unique cell to which u belongs.

We consider an electron system on the lattice Λ as usual, and define

$$\hat{a}_{p,\sigma} = \hat{c}_{p,\sigma} - v \sum_{\substack{u \in \mathscr{I} \\ (C_u \ni p)}} \hat{c}_{u,\sigma}, \tag{11.3.29}$$

for $p \in \mathscr{E}$, and

$$\hat{b}_{u,\sigma} = \hat{c}_{u,\sigma} + v \sum_{p \in C_u \cap \mathscr{E}} \hat{c}_{p,\sigma}, \tag{11.3.30}$$

for $u \in \mathscr{I}$, where $v > 0$ is a constant. Then the Hubbard Hamiltonian $\hat{H} = \hat{H}_{\text{hop}} + \hat{H}_{\text{int}}$ is defined as before by (11.3.5) and (11.3.6). Then Theorem 11.11 (p. 392) is valid as it is. The proof is not very much different, but see [73] for details.

Note that the models we have mainly studied in this subsection are constructed from cells with one internal site and two external sites. In particular the Delta chain

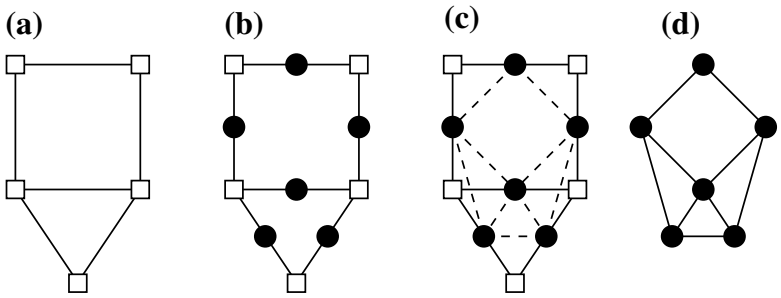

Fig. 11.15 The procedure to construct the line graph from a given connected graph. **a** The original graph $(\tilde{\Lambda}, \tilde{\mathscr{B}})$. **b** One adds a new site (drawn as a black dot) at the middle of each bond. The collection of such sites are denoted as Λ. **c** One connects two black dots by a new bond if they are directly connected to a common original site in $\tilde{\Lambda}$ (white square). **d** Leaving only the black dots and the bonds in between them, one gets the line graph $(\Lambda, \mathscr{B})$ ()

in Fig. 11.11b obviously consists of the triangular cell  . Figure 11.14 shows a cell with four external sites, and some lattices in one and two dimensions that can be constructed by assembling it.

11.3.2 Mielke's Flat-Band Ferromagnetism

We now discuss the Mielke model, which was the first example of flat-band ferromagnetism. To define the model we start by introducing the graph theoretic notion of line graph. Let $(\tilde{\Lambda}, \widetilde{\mathscr{B}})$ be a general lattice (or graph), where $\tilde{\Lambda}$ denotes the set of sites (or vertices) $\alpha, \beta \ldots$, and $\widetilde{\mathscr{B}}$ is the set of bonds (or edges) $\{\alpha, \beta\} = \{\beta, \alpha\}$ where $\alpha, \beta \in \tilde{\Lambda}$ and $\alpha \neq \beta$. We assume that the lattice $(\tilde{\Lambda}, \widetilde{\mathscr{B}})$ is connected.[21] Starting from $(\tilde{\Lambda}, \widetilde{\mathscr{B}})$, we shall construct a new lattice $(\Lambda, \mathscr{B})$, which is called the line graph of $(\tilde{\Lambda}, \widetilde{\mathscr{B}})$. We take a new site at the middle of each bond $\{\alpha, \beta\} \in \widetilde{\mathscr{B}}$, and let Λ be the collection of all such sites. Then we define the set of bonds $\mathscr{B}$ by declaring that $\{x, y\} \in \mathscr{B}$ if and only if $x, y \in \Lambda$, $x \neq y$, and x and y are directly connected to (at least) one common site $\alpha \in \tilde{\Lambda}$. See Fig. 11.15. As is shown in Fig. 11.16, the checkerboard lattice and the kagomé lattice[22] are the line graphs of the square lattice and the hexagonal lattice, respectively.

Let us consider a tight-biding electron system on the lattice Λ with the hopping Hamiltonian

[21] See footnote 28 in p. 33 for the definition of connectedness.

[22] "Kagomé" is a Japanese word that means the mesh of woven bamboo. Thus "me" is pronounced like "mesh" (without "sh").

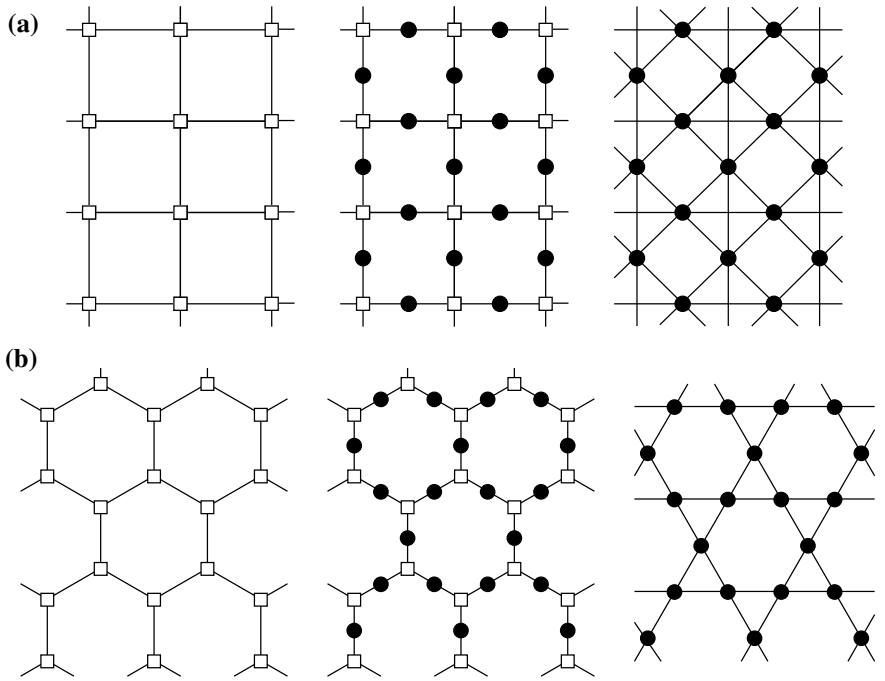

Fig. 11.16 **a** The line graph of the square lattice (left) is the checkerboard lattice (right). **b** The line graph of the hexagonal lattice (left) is the kagomé lattice (right) ()

$$\hat{H}_{\mathrm{hop}} = t \sum_{\substack{\{x,y\}\in\mathscr{B} \\ \sigma=\uparrow,\downarrow}} \hat{c}^{\dagger}_{x,\sigma}\hat{c}_{y,\sigma} + 2t \sum_{x\in\Lambda} \hat{n}_x, \tag{11.3.31}$$

with $t > 0$. The second term is added only to make the ground state energy zero. Note that there are only constant hopping between neighboring sites, and no fine tuning as in the Tasaki model (see Sect. 11.3.1) is necessary. The corresponding single-electron Schrödinger equation (9.3.3) is

$$2t\varphi(x) + t \sum_{\substack{y\in\Lambda \\ (\{x,y\}\in\mathscr{B})}} \varphi(y) = \varepsilon\,\varphi(x) \quad \text{for any } x \in \Lambda. \tag{11.3.32}$$

Let us define $D(\tilde{\Lambda}, \tilde{\mathscr{B}}) := |\tilde{\mathscr{B}}| - |\tilde{\Lambda}| + 1 = |\Lambda| - |\tilde{\Lambda}| + 1$ if the original lattice $(\tilde{\Lambda}, \tilde{\mathscr{B}})$ is bipartite, and $D(\tilde{\Lambda}, \tilde{\mathscr{B}}) := |\tilde{\mathscr{B}}| - |\tilde{\Lambda}| = |\Lambda| - |\tilde{\Lambda}|$ if $(\tilde{\Lambda}, \tilde{\mathscr{B}})$ is not bipartite.[23] Then the following preliminary but essential result was proved by Mielke [33].

[23] See p. 37 and Fig. 2.1 for the definition of bipartiteness.

Theorem 11.12 (Flat-band in a general line graph) *The single-electron Schrödinger equation (11.3.32) has exactly* $D(\tilde{\Lambda}, \widetilde{\mathscr{B}})$ *zero eigenstates with energy zero. All the other energy eigenvalues are strictly positive.*

We shall prove the theorem in Sect. 11.3.3. Thus the tight-binding electron model on a translation invariant line graph has a flat-band (or flat-bands) at the bottom of the single-electron energy spectrum. For example, the model on the d-dimensional version of the checkerboard lattice (Fig. 11.16a) with $d \geq 2$, which is the line graph of the standard d-dimensional hypercubic lattice, has d bands with the dispersion relations

$$\varepsilon_\mu(k) = \begin{cases} 0 & \mu = 1, \ldots, d-1 \\ 2t \sum_{j=1}^{d} (1 + \cos k_j) & \mu = d. \end{cases} \tag{11.3.33}$$

There are $d-1$ bands with zero energy, and one band with the cosine dispersion. Note that there is no energy gap between the flat bands and the dispersive band. The gapless nature is a generic feature of the tight-binding model on the line graph of a standard bipartite lattice, as we shall show in Sect. 11.3.3. The tight-binding model on a line graph also has strictly localized single-electron energy eigenstate with zero energy. See Problem 11.3.2.b below.

We note that the dispersion relations (11.3.33) are essentially the same as those of the higher d bands of the Tasaki model show in (11.3.23). See Fig. 11.13. This is not an accident, as the following problem shows.

Problem 11.3.2.a Examine the relation between the Tasaki model in Sect. 11.3.1 and the Mielke model on the d-dimensional checkerboard lattice. Then derive the dispersion relations (11.3.33) by using the dispersion relation (11.3.23) of the Tasaki model. (Hint: Generalize the analysis that include (11.3.26), (11.3.27), and (11.3.28) for $d = 1$ to higher dimensions.) In Sect. 11.3.3, we also show that (11.3.33) is easily obtained from (9.3.9), the dispersion relation for the simplest model on the d-dimensional hypercubic lattice. [solution→p.518]

Problem 11.3.2.b Find localized zero-energy single-electron states for the checkerboard lattice and the kagomé lattice (Fig. 11.16). [solution→p.519]

We now consider the Hubbard model on Λ with the Hamiltonian $\hat{H} = \hat{H}_{\text{hop}} + \hat{H}_{\text{int}}$, where the hopping Hamiltonian is (11.3.31) and the interaction Hamiltonian is the most standard (11.3.6) or (9.3.29).

In 1991, Mielke [34, 35] proved the following general theorem, which rigorously established, for the first time, the existence of versions of the Hubbard model which exhibit saturated ferromagnetism for finite values of the interaction U. We state it without a proof.

Theorem 11.13 (Mielke's flat-band ferromagnetism) *Assume that the original lattice* $(\tilde{\Lambda}, \widetilde{\mathscr{B}})$ *is biconnected,*[24] *and consider the above Hubbard model with electron*

[24] A lattice (or a graph) is biconnected (or two-fold connected) if and only if one cannot make it disconnected by removing a single site.

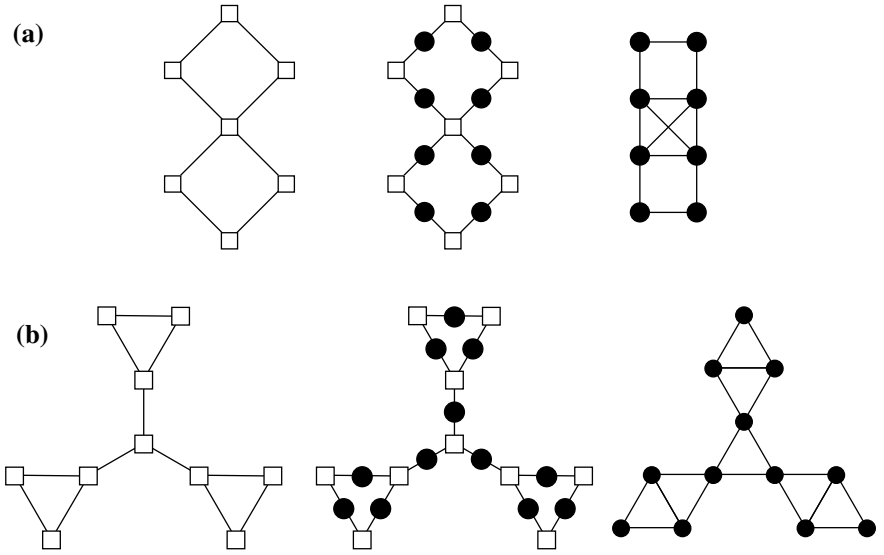

Fig. 11.17 Two lattices (whose sites are drawn as white squares) which are connected but not biconnected. Both the lattices have $D(\tilde{\Lambda}, \widetilde{\mathscr{B}}) = 2$. We consider the Hubbard model with $N = 2$ on the corresponding line graphs (whose sites are drawn as big black dots). It is found that the model on **a** does not exhibit ferromagnetism, while that on **(b)** does. See Problem 11.3.2.c. The examples are due to Akinori Tanaka (private communication) ()

number $N = D(\tilde{\Lambda}, \widetilde{\mathscr{B}})$. *Then, for any* $t > 0$ *and* $U > 0$, *the ground states have* $S_{\mathrm{tot}} = S_{\max} = N/2$, *and are unique apart from the trivial* $2S_{\max} + 1 = N + 1$ *fold degeneracy.*

Exactly as in the Tasaki model, ferromagnetism takes place when the lowest flat-bands (or, more precisely, the space of highly degenerate single-electron ground states) are half-filled. The condition of biconnectedness is satisfied in many lattices in two or higher dimensions including the checkerboard lattice and the kagomé lattice in Fig. 11.16. Mathematically speaking, biconnectedness of $(\tilde{\Lambda}, \widetilde{\mathscr{B}})$ is not a necessary condition for the Hubbard model on the line graph $(\Lambda, \mathscr{B})$ to exhibit ferromagnetism. See Fig. 11.17 and Problem 11.3.2.c below.

In Sect. 11.3.1, we have seen that one may use at least three different pictures to intuitively understand Tasaki's flat-band ferromagnetism. Note that the first picture based on the direct exchange interaction between almost localized electrons does not apply to the present model, where all the lattice sites are identical. The second picture based on the ring exchange process (see Fig. 11.2) applies as it is to the model on the kogomé lattice (Fig. 11.16b). To apply the picture to the model on the checkerboard lattice (Fig. 11.16a), we note that here the role of the triangle is played by the square

in which all the four sites are directly connected.[25] The third picture based on the Stoner criterion needs not be modified.

Problem 11.3.2.c Prove the fact stated in the caption for Fig. 11.17. This is done by first finding two linearly independent zero energy states of the corresponding single-electron Schrödinger equation, which is easy for (a) and rather nontrivial for (b). [solution→p.519]

11.3.3 Construction of Tight-Binding Models with Flat-Bands

In this section we discuss a general method for constructing tight-binding models with flat-bands. The general method allows us to understand the origin of the flat-bands in Mielke's and Tasaki's models (and even those in Lieb's model) in a unified manner.[26] We also prove Theorem 11.12 stated above, and derive some properties about the single-electron energy eigenvalues in Mileke's model. As we noted before the present and the next subsections are somewhat advanced, and may be skipped.

In the present section, we only focus on properties of the single-electron Schrödinger equation (9.3.3) or (9.3.4) corresponding to a certain hopping matrix T. The argument in this section is more or less standard, and is essentially the same as that used by Mielke in his seminal paper [33]. We here follow a general formulation in [18].

General construction Consider two sets of sites $\tilde{\Lambda}$ and Λ, whose elements are denoted as $\alpha, \beta, \ldots \in \tilde{\Lambda}$ and $x, y, \ldots \in \Lambda$. Examples include $\tilde{\Lambda}$ and Λ that appeared in the construction of line graphs. See Figs. 11.15 and 11.16.

Consider a $|\tilde{\Lambda}| \times |\Lambda|$ matrix $\mathsf{S} = (s_{\alpha,x})_{\alpha\in\tilde{\Lambda},x\in\Lambda}$ with arbitrary entries $s_{\alpha,x} \in \mathbb{C}$. We then define hopping matrices on $\tilde{\Lambda}$ and Λ by

$$\widetilde{\mathsf{T}} := \mathsf{S}\,\mathsf{S}^\dagger \quad \text{and} \quad \mathsf{T} := \mathsf{S}^\dagger\,\mathsf{S}, \tag{11.3.34}$$

respectively. More explicitly they are written as $\widetilde{\mathsf{T}} = (\tilde{t}_{\alpha,\beta})_{\alpha,\beta\in\tilde{\Lambda}}$ and $\mathsf{T} = (t_{x,y})_{x,y\in\Lambda}$ with

$$\tilde{t}_{\alpha,\beta} = \sum_{x\in\Lambda} s_{\alpha,x}(s_{\beta,x})^* \quad \text{and} \quad t_{x,y} = \sum_{\alpha\in\tilde{\Lambda}} (s_{\alpha,x})^*\, s_{\alpha,y}. \tag{11.3.35}$$

Clearly both $\widetilde{\mathsf{T}}$ and T are nonnegative matrices. We further have the following crucial property.

Lemma 11.14 *Hopping matrices* $\widetilde{\mathsf{T}}$ *and* T *have exactly identical positive eigenvalues with identical multiplicities.*

---

[25] A lattice in which all the sites are connected is called a complete graph.

[26] We note that this is by no means the unique general method to construct tight-binding models with flat-bands.

Proof Assume that $\mathsf{T}\boldsymbol{\varphi} = \lambda\boldsymbol{\varphi}$ with $\lambda > 0$, where $\boldsymbol{\varphi} = (\varphi(x))_{x\in\Lambda}$ is a nonzero $|\Lambda|$-dimensional vector (or a wave function on Λ). We define $\widetilde{\boldsymbol{\varphi}} = \mathsf{S}\boldsymbol{\varphi}$, where $\widetilde{\boldsymbol{\varphi}} = (\widetilde{\varphi}(\alpha))_{\alpha\in\tilde{\Lambda}}$ is a $|\tilde{\Lambda}|$-dimensional vector (or a wave function on $\tilde{\Lambda}$). We first note that $\langle\widetilde{\boldsymbol{\varphi}}, \widetilde{\boldsymbol{\varphi}}\rangle = \langle\boldsymbol{\varphi}, \mathsf{S}^\dagger\mathsf{S}\boldsymbol{\varphi}\rangle = \langle\boldsymbol{\varphi}, \mathsf{T}\boldsymbol{\varphi}\rangle = \lambda\langle\boldsymbol{\varphi}, \boldsymbol{\varphi}\rangle > 0$, and hence $\widetilde{\boldsymbol{\varphi}}$ is nonzero. We then observe that $\widetilde{\mathsf{T}}\widetilde{\boldsymbol{\varphi}} = \mathsf{S}\,\mathsf{S}^\dagger\mathsf{S}\boldsymbol{\varphi} = \mathsf{S}\,\mathsf{T}\boldsymbol{\varphi} = \lambda\mathsf{S}\boldsymbol{\varphi} = \lambda\widetilde{\boldsymbol{\varphi}}$, and hence $\widetilde{\boldsymbol{\varphi}}$ is an eigenvector of $\widetilde{\mathsf{T}}$ with eigenvalue λ. Finally suppose that there is a nonzero vector $\boldsymbol{\varphi}'$ orthogonal to $\boldsymbol{\varphi}$ which also satisfies $\mathsf{T}\boldsymbol{\varphi}' = \lambda\boldsymbol{\varphi}'$ with the same λ, and define $\widetilde{\boldsymbol{\varphi}}' = \mathsf{S}\boldsymbol{\varphi}'$. We then see that $\widetilde{\boldsymbol{\varphi}}$ and $\widetilde{\boldsymbol{\varphi}}'$ are orthogonal because $\langle\widetilde{\boldsymbol{\varphi}}', \widetilde{\boldsymbol{\varphi}}\rangle = \langle\boldsymbol{\varphi}', \mathsf{S}^\dagger\mathsf{S}\boldsymbol{\varphi}\rangle = \lambda\langle\boldsymbol{\varphi}', \boldsymbol{\varphi}\rangle = 0$. By repeating the same argument switching the roles of $\tilde{\Lambda}$ and Λ, we get the desired statement. ∎

Let us assume $|\tilde{\Lambda}| < |\Lambda|$, and see how flat bands emerge. We first note that the number of independent eigenvectors of $\widetilde{\mathsf{T}}$ with positive eigenvalues cannot exceed the dimension $|\tilde{\Lambda}|$. We thus find from Lemma 11.14 that the hopping matrix T must have at least $|\Lambda| - |\tilde{\Lambda}|$ independent eigenvectors with eigenvalue zero. We conclude that the tight-binding Schrödinger equation with the hopping matrix T has flat bands provided that $|\Lambda| - |\tilde{\Lambda}|$ is proportional to the system size (and the system has translation invariance).

Relation to Lieb's flat-band models Consider the composite lattice $\Lambda^{\mathrm{tot}} = \Lambda \cup \tilde{\Lambda}$. (Examples are found in Fig. 11.15b, the figures at the middle of Figs. 11.16, and 11.18.) With the matrix S given above, we define the hopping matrix $\mathsf{T}^{\mathrm{tot}} = (t^{\mathrm{tot}}_{u,v})_{u,v\in\Lambda^{\mathrm{tot}}}$ as

$$t^{\mathrm{tot}}_{u,v} = \begin{cases} s_{u,v} & \text{if } u \in \tilde{\Lambda},\, v \in \Lambda, \\ (s_{v,u})^* & \text{if } u \in \Lambda,\, v \in \tilde{\Lambda}, \\ 0 & \text{otherwise,} \end{cases} \tag{11.3.36}$$

or, in the matrix form, as

$$\mathsf{T}^{\mathrm{tot}} = \begin{pmatrix} 0 & \mathsf{S}^\dagger \\ \mathsf{S} & 0 \end{pmatrix}. \tag{11.3.37}$$

The matrix $\mathsf{T}^{\mathrm{tot}}$ describes bipartite hopping amplitude on the lattice Λ^{tot}. Note that the situation is similar to that in Sect. 10.2.3, where we discussed Lieb's ferrimagnetism.

Let $\boldsymbol{\varphi} = (\varphi(x))_{x\in\Lambda}$ be such that $\mathsf{T}\boldsymbol{\varphi} = \mathbf{0}$. Then it also holds (from Lemma A.11 in p. 469) that $\mathsf{S}\boldsymbol{\varphi} = \mathbf{0}$, and hence $\mathsf{T}^{\mathrm{tot}}(\boldsymbol{\varphi} \oplus \mathbf{0}) = \mathbf{0}$. We thus see that a zero-energy eigenstate of the hopping matrix T on Λ always corresponds to a zero-energy eigenstate of $\mathsf{T}^{\mathrm{tot}}$ on Λ^{tot}. In other words the flat-band (at the bottom of the spectrum) for T correspond to a flat-band (in the middle of the spectrum) for $\mathsf{T}^{\mathrm{tot}}$. Recall that the latter played a central role in Sect. 10.2.3. See also Proposition 10.7 (p. 356).

Mielke's flat-band model We now apply the present general formalism to Mielke's model on line graphs. As in Sect. 11.3.2, let $(\tilde{\Lambda}, \tilde{\mathscr{B}})$ be an arbitrary connected lattice, and $(\Lambda, \mathscr{B})$ be the corresponding line graph. We define the matrix $\mathsf{S} = (s_{\alpha,x})_{\alpha\in\tilde{\Lambda},x\in\Lambda}$ by

$$s_{\alpha,x} = \begin{cases} \sqrt{t} & \text{if } \alpha \in \tilde{\Lambda} \text{ and } x \in \Lambda \text{ are directly connected,} \\ 0 & \text{otherwise,} \end{cases} \tag{11.3.38}$$

with $t > 0$. Then we immediately see from (11.3.35) that

$$t_{x,y} = \begin{cases} 2t & \text{if } x = y, \\ t & \text{if } \{x, y\} \in \mathscr{B}, \\ 0 & \text{otherwise,} \end{cases} \tag{11.3.39}$$

which precisely corresponds to the hopping Hamiltonian (11.3.31) of the Mielke model.

It is also useful to consider the hopping matrix $\widetilde{\mathsf{T}} = (\tilde{t}_{\alpha,\beta})_{\alpha,\beta\in\tilde{\Lambda}}$ on the original lattice $\tilde{\Lambda}$. Again from (11.3.35), we find

$$\tilde{t}_{\alpha,\beta} = \begin{cases} z(\alpha)\, t & \text{if } \alpha = \beta, \\ t & \text{if } \{\alpha, \beta\} \in \widetilde{\mathscr{B}}, \\ 0 & \text{otherwise,} \end{cases} \tag{11.3.40}$$

where $z(\alpha)$ is the number of $\beta \in \tilde{\Lambda}$ such that $\{\alpha, \beta\} \in \widetilde{\mathscr{B}}$. Let $\widetilde{\boldsymbol{\varphi}} = (\widetilde{\varphi}(\alpha))_{\alpha\in\tilde{\Lambda}}$ be a normalized eigenstate of $\widetilde{\mathsf{T}}$ with eigenvalue λ. Since $\tilde{t}_{\alpha,\beta} \in \mathbb{R}$, we can assume $\widetilde{\varphi}(\alpha) \in \mathbb{R}$. Then we see from (11.3.40) that

$$\lambda = \langle \widetilde{\boldsymbol{\varphi}}, \widetilde{\mathsf{T}}\widetilde{\boldsymbol{\varphi}} \rangle = \sum_{\alpha,\beta\in\tilde{\Lambda}} \widetilde{\varphi}(\alpha)\, \tilde{t}_{\alpha,\beta} \widetilde{\varphi}(\beta) = t \sum_{\{\alpha,\beta\}\in\widetilde{\mathscr{B}}} (\widetilde{\varphi}(\alpha) + \widetilde{\varphi}(\beta))^2. \tag{11.3.41}$$

See (2.4.14) and Problem 2.4.d (p. 35) for essentially the same relation. Let us examine whether $\widetilde{\mathsf{T}}$ has zero as an eigenvalue. By setting $\lambda = 0$ in (11.3.41), we see that $\widetilde{\varphi}(\alpha) = -\widetilde{\varphi}(\beta)$ for any $\{\alpha, \beta\} \in \widetilde{\mathscr{B}}$. Since $(\tilde{\Lambda}, \widetilde{\mathscr{B}})$ is connected, this condition is satisfied by a unique $\widetilde{\boldsymbol{\varphi}}$ only when $(\tilde{\Lambda}, \widetilde{\mathscr{B}})$ is bipartite. We thus find that $\widetilde{\mathsf{T}}$ has exactly one eigenstate with eigenvalue zero when $(\tilde{\Lambda}, \widetilde{\mathscr{B}})$ is bipartite, and does not have zero as its eigenvalue when $(\tilde{\Lambda}, \widetilde{\mathscr{B}})$ is not bipartite. Equivalently, the number of independent eigenstates with positive eigenvalues of $\widetilde{\mathsf{T}}$ is $|\tilde{\Lambda}| - 1$ when $(\tilde{\Lambda}, \widetilde{\mathscr{B}})$ is bipartite, and is $|\tilde{\Lambda}|$ when $(\tilde{\Lambda}, \widetilde{\mathscr{B}})$ is not bipartite. This observation, with Lemma 11.14, proves Theorem 11.12 about the number of zero-energy single-electron states in Mielke's flat-band model, whose hopping matrix is T.

From Lemma 11.14, we further see that nonzero eigenvalues of T are exactly the same as nonzero eigenvalues of $\widetilde{\mathsf{T}}$, which are in general much easier to study. For example let $(\tilde{\Lambda}, \widetilde{\mathscr{B}})$ be the d-dimensional hypercubic lattice with nearest neighbor bonds. Then $(\Lambda, \mathscr{B})$ is the d-dimensional checkerboard lattice in Fig. 11.16a. Then, instead of solving the Schrödinger equation on the checkerboard lattice, which is rather complicated, one only needs to solve the equation for the simple hypercubic lattice. This is easy, and is indeed already done in (9.3.9). We thus readily obtain the dispersion relation for $\varepsilon_d(k)$ in (11.3.33), by switching the sign of t and shifting the

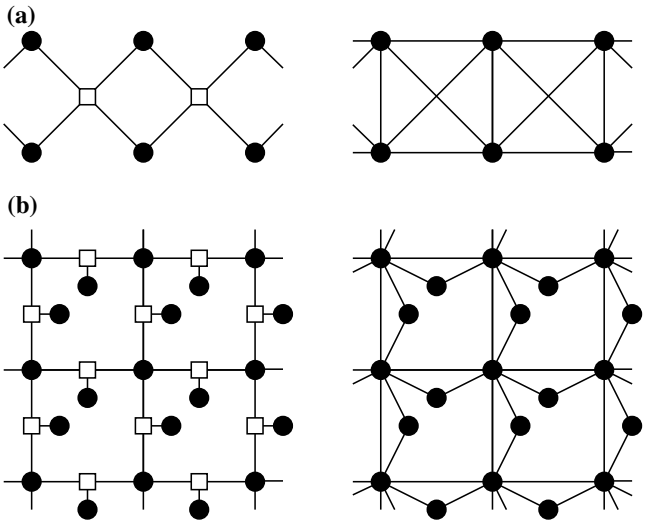

Fig. 11.18 On the left, we show the lattice $\Lambda \cup \tilde{\Lambda}$, where white squares denote sites in $\tilde{\Lambda}$ and black dots denote sites in Λ. The lines correspond to nonvanishing $s_{\alpha,x}$. On the right we show the resulting lattice $(\Lambda, \mathscr{B})$, on which we have an electron model with flat-bands (or, more precisely, highly degenerate single-electron ground states). **a** The diamond chain $\Lambda \cup \tilde{\Lambda}$ reduces to the crossed ladder. **b** Starting from a decorated square lattice with dangling bonds, one gets the decorated square lattice for the Tasaki model in Fig. 11.11c (© Hal Tasaki 2020. All Rights Reserved)

energy by $2dt$ in (9.3.9). Likewise the band structure of the model on the kagomé lattice can be determined from the band structure of the tight-binding model on the hexagonal lattice.

Let us finally comment on the gapless nature of the single-electron spectrum in the Mielke model. Assume that $(\tilde{\Lambda}, \tilde{\mathscr{B}})$ is a general connected bipartite lattice. Then one can transform the hopping matrix $\tilde{\mathsf{T}}$ as $\mathsf{U}\tilde{\mathsf{T}}\mathsf{U} = -t\Delta$, where Δ is the lattice Laplacian defined in (2.4.13). Here U is the unitary matrix for gauge transformation defined by $(\mathsf{U})_{\alpha,\beta} = (-1)^{\alpha}\,\delta_{\alpha,\beta}$, where the sign factor $(-1)^{\alpha} = \pm 1$ distinguishes the two sublattices (see, e.g., Sect. 9.3.3). It is known that, for most translation invariant lattices with periodic boundary conditions, the Laplacian has an almost continuous band of nonpositive eigenvalues including zero. This means that the hopping matrix T has a continuum of positive eigenvalues just above the highly degenerate eigenvalue zero. One also sees that when $(\tilde{\Lambda}, \tilde{\mathscr{B}})$ is a non-bipartite lattice like the triangular lattice, then there is a nonzero gap above the eigenvalue zero in the spectrum of the corresponding T on the line graph.

Other models The above construction certainly works for models not related to line graphs. If one starts from the lattice $\Lambda \cup \tilde{\Lambda}$ as in the left of Fig. 11.18a, then one obtains the crossed ladder as in the right of Fig. 11.18a. This corresponds to the flat-band model studied in [60], where, interestingly, the existence of saturated

ferromagnetism is proved when there are one more electrons than the half-filling of the flat-band.

Consider the lattice in the left of Fig. 11.18b, which has dangling bonds. The resulting lattice $(\Lambda, \mathscr{B})$ depicted in the right of Fig. 11.18b is nothing but the decorated square lattice of the Tasaki model. See Fig. 11.11c. Furthermore by setting $s_{\alpha,x} = \sqrt{t}$ for dangling bonds $\{\alpha, x\}$, and $s_{\alpha,x} = \sqrt{t}\,\nu$ for other bonds, the hopping matrix T precisely recovers the hopping amplitude (11.3.22) of the Tasaki model. (This construction appear in [18].)

11.3.4 General Theory of Flat-Band Ferromagnetism

In the present section we discuss the general theory of flat-band ferromagnetism developed by Mielke in 1993 [36, 38]. We treat a general Hubbard model with a flat lowest band (or, more precisely, degenerate single-electron ground states), and prove Theorem 11.15, which states a compact necessary and sufficient condition for the emergence of saturated ferromagnetism when the number of electrons is equal to the degree of degeneracy. Although it is usually not necessary to resort to the general condition when working on concrete models, it is important to see that there is a clear necessary and sufficient condition. In the proof we shall see another important necessary and sufficient condition stated in Theorem 11.17, which is also due to Mielke.

Setting and main theorem Let Λ be a finite lattice. As before we denote by $\mathfrak{h} = \{\boldsymbol{\varphi} = (\varphi(x))_{x\in\Lambda} \,|\, \varphi(x) \in \mathbb{C}\}$ the single-electron Hilbert space for Λ. We consider a general hopping matrix $\mathsf{T} = (t_{x,y})_{x,y\in\Lambda}$ with complex hopping amplitude $t_{x,y} \in \mathbb{C}$ such that $\mathsf{T}^\dagger = \mathsf{T}$ (i.e., $(t_{x,y})^* = t_{y,x}$ for any $x, y, \in \Lambda$) and $\mathsf{T} \geq 0$. Let $\mathfrak{h}_0 := \ker \mathsf{T}$ be the subspace which consists of $\boldsymbol{\varphi} \in \mathfrak{h}$ such that $\mathsf{T}\boldsymbol{\varphi} = \mathbf{0}$. We assume that $\mathfrak{h}_0$ is not empty, and write $D_0 := \dim \mathfrak{h}_0$. We denote by P_0 the orthogonal projection matrix onto the space $\mathfrak{h}_0$, and define $\Lambda_0 := \{x \in \Lambda \,|\, (\mathsf{P}_0)_{x,x} \neq 0\}$.

We consider a Hubbard model on Λ with the standard Hamiltonian $\hat{H} = \hat{H}_{\mathrm{hop}} + \hat{H}_{\mathrm{int}}$, where $\hat{H}_{\mathrm{hop}}$ is the hopping Hamiltonian (9.3.17) corresponding to the hopping matrix T, and $\hat{H}_{\mathrm{int}}$ is the interaction Hamiltonian (11.3.6) or (9.3.29) with arbitrary $U > 0$. As in the Mielke model and the Tasaki model, we set the electron number as $N = D_0$, which corresponds to the exact half-filling of the flat-band (or, more precisely, the space of degenerate single-electron ground states). The following theorem of Mieleke's [36, 38] is the main result of the present section.

Theorem 11.15 *The above Hubbard model exhibits ferromagnetism, i.e., has $N + 1$ fold degenerate ground states with $S_{\mathrm{tot}} = N/2$, if and only if the $|\Lambda_0| \times |\Lambda_0|$ matrix $((\mathsf{P}_0)_{x,y})_{x,y\in\Lambda_0}$ is irreducible.*

To be precise we say that the matrix $((\mathsf{P}_0)_{x,y})_{x,y\in\Lambda_0}$ is reducible if and only if Λ_0 is decomposed as $\Lambda_0 = \Lambda_1 \cup \Lambda_2$ with $\Lambda_1 \cap \Lambda_2 = \emptyset$, $\Lambda_1 \neq \emptyset$, and $\Lambda_2 \neq \emptyset$, and it holds

that $(\mathsf{P}_0)_{x,y} = 0$ for any $x \in \Lambda_1$ and $y \in \Lambda_2$. We say $((\mathsf{P}_0)_{x,y})_{x,y\in\Lambda_0}$ is irreducible when it is not reducible.

The theorem provides us with a simple and elegant criterion, which is based only on the subspace $\mathfrak{h}_0$, for the emergence of flat-band ferromagnetism. However, as we have mentioned already, it rarely happens that one really needs to invoke this condition to establish the existence of ferromagnetism. An example in which the above condition is applied can be found in [19]. Needless to say the existence of a flat-band does not necessarily imply ferromagnetism. Mielke constructed flat-band models with reducible $((\mathsf{P}_0)_{x,y})_{x,y\in\Lambda_0}$, which do not exhibit ferromagnetism [39].

One can represent the matrix element $(\mathsf{P}_0)_{x,y}$ by using an off-diagonal correlation function; it is indeed the way Mielke first formulated the theorem. Let $|\Phi_{\text{ferro GS}}\rangle$ be the unique lowest-energy state within the states consisting only of N up-spin electrons. Then one has

$$(\mathsf{P}_0)_{x,y} = \langle \Phi_{\text{ferro GS}} | \hat{c}^\dagger_{y,\uparrow} \hat{c}_{x,\uparrow} | \Phi_{\text{ferro GS}} \rangle. \tag{11.3.42}$$

To see this let $\{\boldsymbol{\psi}_j\}_{j=1,\dots,D_0}$ be an arbitrary orthonormal basis of the zero-energy space $\mathfrak{h}_0$. We then have

$$|\Phi_{\text{ferro GS}}\rangle = \Big(\prod_{j=1}^{D_0} \hat{C}^\dagger_\uparrow(\boldsymbol{\psi}_j)\Big)|\Phi_{\text{vac}}\rangle. \tag{11.3.43}$$

This, with the anticommutation relation (9.2.64), implies

$$\langle \Phi_{\text{ferro GS}} | \hat{c}^\dagger_{y,\uparrow} \hat{c}_{x,\uparrow} | \Phi_{\text{ferro GS}} \rangle = \sum_{j=1}^{D_0} \psi_j(x)\{\psi_j(y)\}^*, \tag{11.3.44}$$

where the right-hand side is nothing but $(\mathsf{P}_0)_{x,y}$.

Proof of the Main Theorem We shall give a complete and detailed Proof of Theorem 11.15.[27] In Theorem 11.17 below, we state another necessary and sufficient condition for flat-band ferromagnetism.

We start by proving the following lemma due to Mielke [36, 38], which we believe to be of essential importance in the study of flat-band systems.[28]

Lemma 11.16 *Assume that the hopping matrix* T *satisfies* $\mathsf{T}^\dagger = \mathsf{T}$ *and* $\mathsf{T} \geq 0$*, and let* $\mathfrak{h}_0 = \ker \mathsf{T}$ *and* $D_0 = \dim \mathfrak{h}_0$*. Then one can take a subset* $I \subset \Lambda$ *with* $|I| = D_0$ *and a basis* $\{\boldsymbol{\mu}_z\}_{z\in I}$ *of* $\mathfrak{h}_0$*. Here, for each* $z \in I$*, the basis state* $\boldsymbol{\mu}_z = (\mu_z(x))_{x\in\Lambda}$ *satisfies* $\mu_z(z) \neq 0$ *and* $\mu_z(z') = 0$ *for any* $z' \in I\backslash\{z\}$*.*

This means that, among the basis states, $\boldsymbol{\mu}_z$ is characterized as the only one with a nonzero component on the index site z. Recall that the Tasaki model (Sect. 11.3.1) is

[27] A large part of the present proof is due to Akinori Tanaka (private communication).

[28] Unfortunately the lemma, as far as we know, has not been applied much to concrete problems. It is possible that the lemma will be useful when one studies totally different aspects of flat-band systems.

designed so that the basis $\{\boldsymbol{\alpha}_p\}_{p\in\mathscr{E}}$ in (11.3.1) or (11.3.29) precisely has this property. An essential point of the above Lemma is that such a basis can always be taken in a flat-band system. We note that the basis states $\boldsymbol{\mu}_z$ may not be local in general.

Proof The present proof is a nice example which shows that elementary linear algebra sometimes enables us to prove nontrivial (and useful) results quite easily. Let A be a general square matrix with rank r. It is known that there exists an $r \times r$ submatrix of A with nonzero determinant, and that any $(r+1) \times (r+1)$ submatrix of A has determinant zero.[29] Since rank $\mathsf{T} = |\Lambda| - D_0$ by assumption, there exists a subset $\Lambda' \subset \Lambda$ with $|\Lambda'| = |\Lambda| - D_0$ such that the submatrix $(t_{x,y})_{x,y\in\Lambda'}$ has nonzero determinant. We set $I = \Lambda\backslash\Lambda'$. Take any $z \in I$. Then the $(|\Lambda'|+1) \times (|\Lambda'|+1)$ matrix $(t_{x,y})_{x,y\in\Lambda'\cup\{z\}}$ has determinant zero, and hence has zero as an eigenvalue. Let $\tilde{\boldsymbol{\mu}}_z = (\tilde{\mu}_z(x))_{x\in\Lambda'\cup\{z\}}$ be the corresponding eigenvector. We note that $\tilde{\mu}_z(z) \neq 0$ since, otherwise, $(t_{x,y})_{x,y\in\Lambda'}$ would have zero as an eigenvalue. Let us define a $|\Lambda|$-dimensional vector $\boldsymbol{\mu}_z = (\mu_z(x))_{x\in\Lambda}$ by

$$\mu_z(x) = \begin{cases} \tilde{\mu}_z(x) & \text{if } x \in \Lambda' \cup \{z\}, \\ 0 & \text{otherwise.} \end{cases} \tag{11.3.45}$$

We then have $\langle \boldsymbol{\mu}_z, \mathsf{T}\boldsymbol{\mu}_z \rangle = \sum_{x,y\in\Lambda'\cup\{z\}} (\tilde{\mu}_z(x))^* t_{x,y}\, \tilde{\mu}_z(y) = 0$. Since $\mathsf{T} \geq 0$, we find from the variational principle that $\mathsf{T}\boldsymbol{\mu}_z = \mathbf{0}$. Since $\boldsymbol{\mu}_z$ with $z \in I$ are obviously linearly independent, $\{\boldsymbol{\mu}_z\}_{z\in I}$ is a basis of $\mathfrak{h}_0$. ∎

For any $z, z' \in I$, we write $\boldsymbol{\mu}_z \sim \boldsymbol{\mu}_{z'}$ (and say that $\boldsymbol{\mu}_z$ and $\boldsymbol{\mu}_{z'}$ are directly connected) if there is $x \in \Lambda$ such that $\mu_z(x) \neq 0$ and $\mu_{z'}(x) \neq 0$. The whole basis $\{\boldsymbol{\mu}_z\}_{z\in I}$ is said to be connected if, for any $z, z' \in I$, there is a sequence $z_0, \ldots, z_n$ such that $z_0 = z$, $z_n = z'$, and $\boldsymbol{\mu}_{z_{j-1}} \sim \boldsymbol{\mu}_{z_j}$ for all $j = 1, \ldots, n$. We then have the following necessary and sufficient condition for flat-band ferromagnetism, which is also due to Mielke.

Theorem 11.17 *The above Hubbard model exhibits ferromagnetism, i.e., has $N+1$ fold degenerate ground states with $S_{\mathrm{tot}} = N/2$, if and only if the basis $\{\boldsymbol{\mu}_z\}_{z\in I}$ is connected.*

Note that the theorem also implies that whether a basis (characterized by Lemma 11.16) is connected or not does not depend on the choice of the index set I or the basis. It is a property determined solely by the structure of the zero-energy state $\mathfrak{h}_0$.

Proof The proof is essentially the same as that of Theorem 11.11 (p. 392) for the Tasaki model. We shall not repeat the detailed argument, and shall be sketchy. For each $z \in I$, we define the fermion operator $\hat{a}^\dagger_{z,\sigma} = \hat{C}^\dagger_\sigma(\boldsymbol{\mu}_z)$.

[29] This characterization of r is known as the determinantal rank. Its equivalence to the standard characterization in terms of the dimension of $\ker \mathsf{A}$ is a well-known theorem.

Let $|\Phi_{\rm GS}\rangle$ be an arbitrary ground state with $N = D_0$ electrons. Then, exactly as in (11.3.14), the condition $\hat{H}_{\rm hop}|\Phi_{\rm GS}\rangle = 0$ implies that the ground state is written only in terms of the $\hat{a}^\dagger$ operators as

$$|\Phi_{\rm GS}\rangle = \sum_{\substack{I_\uparrow, I_\downarrow \subset I \\ (|I_\uparrow|+|I_\downarrow|=D_0)}} g(I_\uparrow, I_\downarrow)\Big(\prod_{z\in I_\uparrow} \hat{a}^\dagger_{z,\uparrow}\Big)\Big(\prod_{z\in I_\downarrow} \hat{a}^\dagger_{z,\downarrow}\Big)|\Phi_{\rm vac}\rangle. \tag{11.3.46}$$

Next, by using the zero-energy condition $\hat{c}_{z,\downarrow}\hat{c}_{z,\uparrow}|\Phi_{\rm GS}\rangle = 0$ (which follows from $\hat{H}_{\rm int}|\Phi_{\rm GS}\rangle = 0$) for $z \in I$, we find that there can be no double occupancies of the $\hat{a}^\dagger$ states, and the ground state admits, as in (11.3.16), the spin system representation

$$|\Phi_{\rm GS}\rangle = \sum_{\boldsymbol{\sigma}} C(\boldsymbol{\sigma})\Big(\prod_{z\in I} \hat{a}^\dagger_{z,\sigma_z}\Big)|\Phi_{\rm vac}\rangle, \tag{11.3.47}$$

where $\boldsymbol{\sigma} = (\sigma_z)_{z\in I}$ with $\sigma_z = \uparrow, \downarrow$ is a spin configuration on I. Finally, take $x \in \Lambda\backslash I = \Lambda'$. We then find by inspection that

$$\begin{aligned}\hat{c}_{x,\downarrow}\hat{c}_{x,\uparrow}|\Phi_{\rm GS}\rangle = \sum_{\boldsymbol{\sigma}} \sum_{\substack{z_1,z_2\in I \\ (z_1<z_2)}} {\rm sgn}(z_1, z_2)\{C(\boldsymbol{\sigma}) - C(\boldsymbol{\sigma}_{z_1\leftrightarrow z_2})\}\times \\ \times\, \mu_{z_1}(x)\,\mu_{z_2}(x)\Big(\prod_{z\in I\backslash\{z_1,z_2\}} \hat{a}^\dagger_{z,\sigma_z}\Big)|\Phi_{\rm vac}\rangle. \end{aligned} \tag{11.3.48}$$

See (11.3.19). Since $(\prod_{z\in I\backslash\{z_1,z_2\}} \hat{a}^\dagger_{z,\sigma_z})|\Phi_{\rm vac}\rangle$ with different (z_1, z_2) are linearly independent, we find that the zero-energy condition $\hat{c}_{x,\downarrow}\hat{c}_{x,\uparrow}|\Phi_{\rm GS}\rangle = 0$ for $x \in \Lambda\backslash I$ implies $C(\boldsymbol{\sigma})=C(\boldsymbol{\sigma}_{z_1\leftrightarrow z_2})$ for any $z_1, z_2\in I$ such that $z_1 \neq z_2$ and $\mu_{z_1}(x)\,\mu_{z_2}(x) \neq 0$. Recalling the definition that two basis states are directly connected, we finally find

$$C(\boldsymbol{\sigma}) = C(\boldsymbol{\sigma}_{z_1\leftrightarrow z_2}) \quad \text{if} \quad \boldsymbol{\mu}_{z_1} \sim \boldsymbol{\mu}_{z_2}. \tag{11.3.49}$$

We see that the spins associated with directly connected basis states are coupled ferromagnetically. Since these are the conditions which completely determine the ground state, we find that there can be only ferromagnetic ground states if the whole basis is connected, and there can be non-ferromagnetic ground states if it is not connected. ∎

As far as its mathematical structure is concerned, Theorem 11.17 may be regarded a straightforward generalization of Theorem 11.11 (p. 392). We should stress however that the Proof of Theorem 11.11 is after all an ad hoc argument devised for a very specific model, while it is guaranteed by Lemma 11.16 that Theorem 11.17 applies to any model that exhibits flat-band ferromagnetism. In this sense, we should understand that Lemma 11.16 and Theorem 11.17 together form an essential statement that characterizes flat-band ferromagnetism. Lemma 11.16 and Theorem 11.17 are useful in proving the emergence of flat-band ferromagnetism in concrete models. See, e.g.,

[19, 58, 59], where the uniqueness of ferromagnetic ground states is proved by using similar ideas.

We are now ready to prove the main result of the present section.

Proof of Theorem 11.15, given Theorem 11.17 We only need to prove the equivalence of irreducibility of $((\mathsf{P}_0)_{x,y})_{x,y\in\Lambda_0}$ and connectivity of the basis $\{\boldsymbol{\mu}_z\}_{z\in I}$. Note that the set $\Lambda_0 = \{x \in \Lambda \mid (\mathsf{P}_0)_{x,x} \neq 0\}$ is also written as[30] $\Lambda_0 = \{x \in \Lambda \mid \mu_z(x) \neq 0 \text{ for some } z \in I\}$.

We first show that non-connectivity of the basis $\{\boldsymbol{\mu}_z\}_{z\in I}$ implies reducibility of $((\mathsf{P}_0)_{x,y})_{x,y\in\Lambda_0}$. This is easy.

Let I and $\{\boldsymbol{\mu}_z\}_{z\in I}$ be arbitrary subset and basis characterized by Lemma 11.16. Assume that the index set I is decomposed as $I = I_1 \cup I_2$ with $I_1 \cap I_2 = \emptyset$, $I_1 \neq \emptyset$, and $I_2 \neq \emptyset$, in such a way that $\boldsymbol{\mu}_{z_1} \nsim \boldsymbol{\mu}_{z_2}$ for any $z_1 \in I_1$ and $z_2 \in I_2$. For $j = 1, 2$, let $\Lambda_j = \{x \in \Lambda \mid \mu_z(x) \neq 0 \text{ for some } z \in I_j\}$. This leads to a decomposition $\Lambda_0 = \Lambda_1 \cup \Lambda_2$ with $\Lambda_1 \cap \Lambda_2 = \emptyset$. Note that both Λ_1 and Λ_2 are nonempty because $\Lambda_j \supset I_j \neq \emptyset$.

Now, from Lemma 9.3 in p. 320 about Slater determinant states, we find that the ferromagnetic ground state (11.3.43) can also be written as

$$|\Phi_{\text{ferro GS}}\rangle = c\Big(\prod_{z\in I} \hat{a}^\dagger_{z,\uparrow}\Big)|\Phi_{\text{vac}}\rangle, \tag{11.3.50}$$

where $\hat{a}^\dagger_{z,\sigma} = \hat{C}^\dagger_\sigma(\boldsymbol{\mu}_z)$ as before and $c \in \mathbb{C}$ is a normalization constant. We define $\hat{N}_1 := \sum_{x\in\Lambda_1} \hat{n}_x$. We see from the commutation relation (9.2.31) that

$$[\hat{N}_1, \hat{a}^\dagger_{z,\uparrow}] = \begin{cases} \hat{a}^\dagger_{z,\uparrow} & \text{if } z \in I_1 \\ 0 & \text{if } z \in I_2. \end{cases} \tag{11.3.51}$$

Take arbitrary $x \in \Lambda_1$ and $y \in \Lambda_2$, and let $|\Psi_x\rangle = \hat{c}_{x,\uparrow}|\Phi_{\text{ferro GS}}\rangle$ and $|\Psi_y\rangle = \hat{c}_{y,\uparrow}|\Phi_{\text{ferro GS}}\rangle$. From (11.3.51), it obviously holds that $\hat{N}_1|\Psi_x\rangle = (|I_1| - 1)|\Psi_x\rangle$ and $\hat{N}_1|\Psi_y\rangle = |I_1||\Psi_y\rangle$, which implies $(\mathsf{P}_0)_{x,y} = \langle\Phi_{\text{ferro GS}}|\hat{c}^\dagger_{y,\uparrow}\hat{c}_{x,\uparrow}|\Phi_{\text{ferro GS}}\rangle = \langle\Psi_y|\Psi_x\rangle = 0$.

We next prove that reducibility of $((\mathsf{P}_0)_{x,y})_{x,y\in\Lambda_0}$ implies non-connectivity of the basis $\{\boldsymbol{\mu}_z\}_{z\in I}$.

Assume that Λ_0 is decomposed as $\Lambda_0 = \Lambda_1 \cup \Lambda_2$ with $\Lambda_1 \cap \Lambda_2 = \emptyset$, $\Lambda_1 \neq \emptyset$, and $\Lambda_2 \neq \emptyset$, in such a way that $(\mathsf{P}_0)_{x,y} = 0$ for any $x \in \Lambda_1$ and $y \in \Lambda_2$. We then decompose the projection matrix as $\mathsf{P}_0 = \mathsf{P}_1 + \mathsf{P}_2$, where

[30] This may be obvious, but let us see a proof. If $\mu_z(x) = 0$ for some $x \in \Lambda$ and all $z \in I$, then it is obvious that $\psi_j(x) = 0$ for all $j = 1, \ldots, D_0$, where $\{\boldsymbol{\psi}_j\}_{j=1,\ldots,D_0}$ is an orthonormal basis of $\mathfrak{h}_0$. (See (11.3.44).) Thus $(\mathsf{P}_0)_{x,x} = \sum_{j=1}^{D_0} (\psi_j(x))^* \psi_j(x) = 0$. Next, suppose that $\mu_z(x) \neq 0$ for some $x \in \Lambda$ and some $z \in I$. Let us denote by P_z the projection matrix onto the unit vector proportional to $\boldsymbol{\mu}_z$. Then since $\mathsf{P}_0 \geq \mathsf{P}_z$, we have $(\mathsf{P}_0)_{x,x} \geq (\mathsf{P}_z)_{x,x} \neq 0$.

$$(\mathsf{P}_j)_{x,y} = \begin{cases} (\mathsf{P}_0)_{x,y} & \text{if } x, y \in \Lambda_j, \\ 0 & \text{otherwise,} \end{cases} \tag{11.3.52}$$

for $j = 1, 2$. Note that $\mathsf{P}_1\mathsf{P}_2 = \mathsf{P}_2\mathsf{P}_1 = \mathsf{O}$, and both P_1 and P_2 are projection matrices.

Let I and $\{\boldsymbol{\mu}_z\}_{z\in I}$ be arbitrary subset and basis characterized by Lemma 11.16. We then claim that $\mathsf{P}_1\boldsymbol{\mu}_z = \boldsymbol{\mu}_z$, $\mathsf{P}_2\boldsymbol{\mu}_z = \mathbf{0}$ if $z \in \Lambda_1$, and $\mathsf{P}_1\boldsymbol{\mu}_z = \mathbf{0}$, $\mathsf{P}_2\boldsymbol{\mu}_z = \boldsymbol{\mu}_z$ if $z \in \Lambda_2$. This clearly implies that $\boldsymbol{\mu}_{z_1} \nsim \boldsymbol{\mu}_{z_2}$ for any $z_1 \in \Lambda_1 \cap I$ and $z_2 \in \Lambda_2 \cap I$, and hence the basis $\{\boldsymbol{\mu}_z\}_{z\in I}$ is not connected.

To show the claim, let $j(x) = 1$ if $x \in \Lambda_1$ and $j(x) = 2$ if $x \in \Lambda_2$. Noting that $(\mathsf{P}_1\boldsymbol{\varphi})(x) = 0$ if $x \in \Lambda_2$ and $(\mathsf{P}_2\boldsymbol{\varphi})(x) = 0$ if $x \in \Lambda_1$ for any $\boldsymbol{\varphi} \in \mathfrak{h}$, we have

$$(\mathsf{P}_{j(z)}\,\boldsymbol{\mu}_z)(x) = \begin{cases} ((\mathsf{P}_1 + \mathsf{P}_2)\boldsymbol{\mu}_z)(x) = \mu_z(x) & \text{if } x \in \Lambda_{j(z)}, \\ 0 & \text{otherwise,} \end{cases} \tag{11.3.53}$$

for any $z \in I$. Since P_0 and P_j $(j = 1, 2)$ commute, we also have $\mathsf{P}_0\mathsf{P}_{j(z)}\,\boldsymbol{\mu}_z = \mathsf{P}_{j(z)}\mathsf{P}_0\,\boldsymbol{\mu}_z = \mathsf{P}_{j(z)}\,\boldsymbol{\mu}_z$, which implies $\mathsf{P}_{j(z)}\,\boldsymbol{\mu}_z \in \mathfrak{h}_0$. We can then expand $\mathsf{P}_{j(z)}\,\boldsymbol{\mu}_z$ in terms of the basis $\{\boldsymbol{\mu}_z\}_{z\in I}$ as $\mathsf{P}_{j(z)}\,\boldsymbol{\mu}_z = \sum_{z'\in I}\gamma_{z'}\boldsymbol{\mu}_{z'}$. Note that (11.3.53) with $z \in \Lambda_{j(z)}$ implies $(\mathsf{P}_{j(z)}\,\boldsymbol{\mu}_z)(z) = \mu_z(z)$ and $(\mathsf{P}_{j(z)}\,\boldsymbol{\mu}_z)(z') = 0$ for $z' \in I\backslash\{z\}$. This uniquely determines the coefficients as $\gamma_{z'} = \delta_{z,z'}$. ∎

11.4 Ferromagnetism in Non-singular Hubbard Models

In the foregoing sections, we discussed two essentially different classes of models which exhibit ferromagnetism. In Sect. 11.2 we have seen that some Hubbard models with $U = \infty$ and exactly one hole exhibit ferromagnetism, i.e., Nagaoka's ferromagnetism. In Sect. 11.3, we have seen that special Hubbard models with a flat lowest band exhibit ferromagnetism for any $U > 0$ when the flat-band is half-filled. One sees that the Stoner criterion $D_{\mathrm{F}}\,U \gtrsim 1$ (see Sect. 11.1.4) is satisfied because $U = \infty$ in Nagaoka's ferromagnetism, and because $D_{\mathrm{F}} = \infty$ in the flat-band ferromagnetism. It is certainly desirable to have models which exhibit ferromagnetism and in which both D_{F} and U are finite. We shall see in the present section that one gets such non-singular Hubbard models by perturbing models exhibiting flat-band ferromagnetism, especially the Tasaki model (Sect. 11.3.1).

Let us recall that, in Lieb's ferrimagnetism (Sect. 10.2.3), Mielke's flat-band ferromagnetism (Sect. 11.3.2), and in Tasaki's flat-band ferromagnetism (Sect. 11.3.1), ferrimagnetism or ferromagnetism emerges for any value of $U > 0$. As we have discussed before, this is because the corresponding models with $U = 0$ have highly degenerate ground states with a wide range of values of S_{tot}, and the only role of the interaction U is to lift the degeneracy and to select those states with the largest S_{tot} as the only ground states. We have emphasized in Sect. 9.1 that a theoretical challenge in the Hubbard model is to control the competition between the hopping

Hamiltonian, which leads to the wave-like nature of electrons, and the interaction Hamiltonian, which leads to the particle-like nature of electrons. But we should say that there is no true such competition in those models with a flat-band which exhibit magnetic ordering for any $U > 0$.

In order to study more realistic and challenging situations without pathological degeneracy, and with true competition between wave-like and particle-like natures, we shall focus on models obtained by adding a translation invariant perturbation to the hopping Hamiltonian of the flat-band models. For a generic perturbation, the degeneracy in the single-electron ground states is lifted, and the lowest band becomes dispersive. The essential question is whether ferromagnetism realized in the flat-band models is stable against such perturbations. Note that Theorem 11.3 in p. 375 shows that a Hubbard model without a flat-band never exhibits ferromagnetism when the interaction $U > 0$ is too small. Thus the question is whether a perturbed model with a near-flat-band exhibits ferromagnetism when U is sufficiently large. Note that possible ferromagnetism is a purely non-perturbative phenomenon in such a situation.

It was conjectured in [40, 67] that Tasaki's flat-band ferromagnetism is stable against small perturbations to the hopping Hamiltonian. Kusakabe and Aoki [23, 24] made a systematic study on the stability of flat-band ferromagnetism. They argued that the flat-band models possess spin-wave excitations which have healthy dispersions, and this fact guarantees the robustness of the flat-band ferromagnetism. They also found numerical evidences for the stability of ferromagnetism in a model with a nearly-flat-band model. See also [45] for a further study on the stability. Later, as we shall discuss in detail below, the local stability for general perturbations and the global stability for a special class of perturbations were proved by Tasaki in [70, 71] and in [72, 74], respectively.

In the present section we focus on the stability of Tasaki's flat-band ferromagnetism against perturbations to the hopping Hamiltonian. In Sect. 11.4.1, we describe a non-rigorous perturbative argument, which should shed light on the physical mechanism of stability and instability. Then in Sect. 11.4.2 we treat models obtained by adding general translation invariant perturbations to the flat-band models, and discuss rigorous results on the local stability of ferromagnetism and on low energy excitations. In Sect. 11.4.3, we introduce a class of models with nearly-flat-band obtained by adding special perturbations to Tasaki's flat-band models, and prove that the models exhibit ferromagnetism provided that the Coulomb interaction U is sufficiently large. The results in Sects. 11.4.2 and 11.4.3 are among the most advanced rigorous results on ferromagnetism in itinerant electron systems.

11.4.1 Wannier State Perturbation Theory

We start with a preliminary heuristic analysis of a model obtained by adding a simple perturbation to the Tasaki model in Sect. 11.3.1. We shall see from a non-rigorous

perturbative argument that the ferromagnetism found for the flat-band model survives when the band is nearly flat and the interaction U is large enough.

Model and the band structure As a simple illustrative example we shall consider a model obtained by shifting the on-site potential in the one-dimensional version of the Tasaki model. As in Sect. 11.3.1, we set $\mathscr{E} = \{1, 2, \ldots, L\}$, $\mathscr{I} = \{\frac{1}{2}, \frac{3}{2}, \ldots, L - \frac{1}{2}\}$, and $\Lambda = \mathscr{E} \cup \mathscr{I}$ with periodic boundary conditions. We then consider the hopping matrix $\mathsf{T} = (t_{x,y})_{x,y\in\Lambda}$ with

$$t_{x,y} = \begin{cases} \nu t & \text{if } |x - y| = 1/2, \\ \nu^2 t & \text{if } x, y \in \mathscr{E} \text{ and } |x - y| = 1, \\ (1 + \gamma)\, t & \text{if } x = y \in \mathscr{I}, \\ 2\nu^2 t & \text{if } x = y \in \mathscr{E} \\ 0 & \text{otherwise,} \end{cases} \tag{11.4.1}$$

where $t > 0$ and $\nu > 0$. Here $\gamma \geq 0$[31] is a new parameter which shifts the on-site potential for sites in $\mathscr{I}$. The hopping amplitude (11.4.1) reduces to (11.3.22) when $\gamma = 0$. See also Fig. 11.11 in p. 392. In the present section we shall assume that $0 < \nu \ll 1$.

By solving the single-electron Schrödinger equation corresponding to (11.4.1) as we explained in Sect. 9.3.1, one finds that there are two bands with dispersion relations

$$\varepsilon_{\pm}(k) = \frac{t}{2}\Big\{1 + \gamma + C(k) \pm \sqrt{\big\{1 + \gamma + C(k)\big\}^2 - 4\gamma\, C(k)}\Big\}, \tag{11.4.2}$$

where $k \in (-\pi, \pi]$, and $C(k) = 2\nu^2(1 + \cos k)$. Note that (11.4.2) recovers the dispersion relations (11.3.23) with a flat-band when $\gamma = 0$. Since we assumed $0 < \nu \ll 1$, it is useful to expand (11.4.2) in ν as

$$\varepsilon_{+}(k) = t\Big\{1 + \gamma + \frac{2\nu^2}{1 + \gamma}(1 + \cos k)\Big\} + O(\nu^4), \tag{11.4.3}$$

$$\varepsilon_{-}(k) = \frac{2\nu^2\gamma}{1 + \gamma}\, t\,(1 + \cos k) + O(\nu^4). \tag{11.4.4}$$

The lower band is nearly-flat when $\gamma > 0$ is small.

Wannier state basis It is convenient for our heuristic discussion to describe single-electron states in terms of the Wannier state basis, which is a standard tool for analyzing multi-band systems. In the present model, the Wannier state basis is an orthonormal basis $\{\boldsymbol{\omega}_y\}_{y\in\Lambda}$, where each basis state $\boldsymbol{\omega}_y = (\omega_y(x))_{x\in\Lambda}$ is exponentially localized at site y. The collection $\{\boldsymbol{\omega}_p\}_{p\in\mathscr{E}}$ spans the lower band, and $\{\boldsymbol{\omega}_u\}_{u\in\mathscr{I}}$ spans the upper band. Wannier states are usually defined through Fourier transformation,

[31] In fact we only need to assume that γ is sufficiently away from -1.

but in this case we find by inspection (see footnote 32 below) that

$$\omega_p(x) = \left(1 + \frac{2\nu^2}{(1+\gamma)^2}\right)^{-1/2} \times \begin{cases} 1 + O(\nu^3) & \text{if } x = p, \\ -\dfrac{\nu}{1+\gamma} + O(\nu^3) & \text{if } |x-p| = \frac{1}{2}, \\ -\dfrac{1}{2}\left(\dfrac{\nu}{1+\gamma}\right)^2 + O(\nu^3) & \text{if } |x-p| = 1, \\ O(\nu^3) & \text{otherwise,} \end{cases} \tag{11.4.5}$$

for any $p \in \mathscr{E}$. We see that the state $\boldsymbol{\omega}_p$ is sharply localized at site p because $0 < \nu \ll 1$. It should be noted that $\boldsymbol{\omega}_p$ is different from $\boldsymbol{\alpha}_p$ defined in (11.3.1) even when $\gamma = 0$. The basis states $\boldsymbol{\alpha}_p$ are strictly localized at three sites, but are not orthogonal with each other. The Wannier states $\boldsymbol{\omega}_p$ are only exponentially localized, but are orthogonal with each other.

That $\{\boldsymbol{\omega}_p\}_{p\in\mathscr{E}}$ spans the lower band can be seen from the relation

$$\mathsf{T}\boldsymbol{\omega}_p = \tau\,\{2\boldsymbol{\omega}_p + \boldsymbol{\omega}_{p-1} + \boldsymbol{\omega}_{p+1}\} + O(\nu^3), \tag{11.4.6}$$

for any $p \in \mathscr{E}$, where the effective hopping amplitude is

$$\tau = \frac{\nu^2\gamma}{1+\gamma}\,t + O(\nu^3). \tag{11.4.7}$$

The relations (11.4.6) and (11.4.7) can be checked by a straightforward calculation using (11.4.1) and (11.4.5).[32] Note that this hopping amplitude τ is consistent with the dispersion relation (11.4.4) of the lower band.

We define fermion operators corresponding to the Wannier states as

$$\hat{d}^\dagger_{x,\sigma} := \hat{C}^\dagger_\sigma(\boldsymbol{\omega}_x). \tag{11.4.8}$$

Since the Wannier state basis is orthonormal, we find from (9.2.64) that

$$\{\hat{d}^\dagger_{x,\sigma}, \hat{d}_{y,\tau}\} = \delta_{x,y}\delta_{\sigma,\tau}, \tag{11.4.9}$$

for any $x, y \in \Lambda$ and $\sigma, \tau = \uparrow, \downarrow$.

Problem 11.4.1.a Find, to the second order in ν, the Wannier state $\boldsymbol{\omega}_u$ for the upper band, and the corresponding relation like (11.4.6). This is indeed easy when (11.4.5) is given. [solution→p.519]

First order perturbation We consider the Hubbard model on the one-dimensional lattice $\Lambda = \{\frac{1}{2}, 1, \ldots, L - \frac{1}{2}, L\}$ with $N = L$ electrons and Hamiltonian $\hat{H} = \hat{H}_{\rm hop} + \hat{H}_{\rm int}$. The hopping Hamiltonian $\hat{H}_{\rm hop}$ is defined by the standard formula (9.3.17)

[32] In fact we obtained (11.4.5) by demanding that $\langle\boldsymbol{\omega}_p, \boldsymbol{\omega}_{p+1}\rangle = 0$ and that $\mathsf{T}\boldsymbol{\omega}_p = \tau_0\,\boldsymbol{\omega}_p + \tau_1\{\boldsymbol{\omega}_{p-1} + \boldsymbol{\omega}_{p+1}\} + O(\nu^3)$ holds for some τ_0 and τ_1.

with the hopping amplitude (11.4.1), and $\hat{H}_{\rm int}$ is the standard interaction Hamiltonian (11.3.6) or (9.3.29) with $U > 0$. We decompose the interaction Hamiltonian as $\hat{H}_{\rm int} = \hat{H}_{\rm int}^{\mathscr{E}} + \hat{H}_{\rm int}^{\mathscr{I}}$, where

$$\hat{H}_{\rm int}^{\mathscr{E}} = U \sum_{p \in \mathscr{E}} \hat{n}_{p,\uparrow} \hat{n}_{p,\downarrow}, \quad \hat{H}_{\rm int}^{\mathscr{I}} = U \sum_{u \in \mathscr{I}} \hat{n}_{u,\uparrow} \hat{n}_{u,\downarrow}. \tag{11.4.10}$$

We shall now regard $\hat{H}_0 = \hat{H}_{\rm hop} + \hat{H}_{\rm int}^{\mathscr{E}}$ as the unperturbed Hamiltonian, and develop a non-rigorous perturbation theory. We first see from the assumption $0 < \nu \ll 1$ that the band gap between the two bands, which is roughly $(1+\gamma)\,t$, is much larger than the band width of the lower band, which is $4\nu^2 t\,\gamma/(1+\gamma)$. See (11.4.3) and (11.4.4). It might be reasonable to assume that low energy states of the N electron system are approximately described only in terms of the $\hat{d}_{p,\sigma}^\dagger$ operators with $p \in \mathscr{E}$. We next assume that the Coulomb interaction energy U is much larger than the band width $4\nu^2 t\,\gamma/(1+\gamma)$, so that double occupancy of $\hat{d}^\dagger$ states is inhibited. We then find that (near) degenerate ground states of the unperturbed Hamiltonian $\hat{H}_0$ are given by

$$|\Omega^{\boldsymbol{\sigma}}\rangle = \Big(\prod_{p \in \mathscr{E}} \hat{d}_{p,\sigma_p}^\dagger\Big)|\Phi_{\rm vac}\rangle, \tag{11.4.11}$$

where $\boldsymbol{\sigma} = (\sigma_1, \ldots, \sigma_L)$ with $\sigma_p = \uparrow, \downarrow$ is a spin configuration on $\mathscr{E}$. Note that the anticommutation relations (11.4.9) imply

$$\langle \Omega^{\boldsymbol{\sigma}} | \Omega^{\boldsymbol{\sigma}'} \rangle = \delta_{\boldsymbol{\sigma},\boldsymbol{\sigma}'} \tag{11.4.12}$$

for any spin configurations $\boldsymbol{\sigma}$ and $\boldsymbol{\sigma}'$. This simple relation makes the following calculations easy. Although the foregoing discussion is very similar to the Proof of Theorem 11.11, one should note that here we have been making several uncontrolled approximations.

Since we have encountered (near) degenerate unperturbed ground states, we shall follow the standard procedure, and examine how the degeneracy is lifted by the first order perturbation theory. We thus need to evaluate matrix elements

$$\langle \Omega^{\boldsymbol{\sigma}} | \hat{H}_{\rm int}^{\mathscr{I}} | \Omega^{\boldsymbol{\sigma}'} \rangle = U \sum_{u \in \mathscr{I}} \langle \Omega^{\boldsymbol{\sigma}} | \hat{n}_{u,\uparrow} \hat{n}_{u,\downarrow} | \Omega^{\boldsymbol{\sigma}'} \rangle, \tag{11.4.13}$$

for any spin configurations $\boldsymbol{\sigma}$ and $\boldsymbol{\sigma}'$. Since $\hat{n}_{u,\uparrow}\hat{n}_{u,\downarrow} = (\hat{c}_{u,\downarrow}\hat{c}_{u,\uparrow})^\dagger\, \hat{c}_{u,\downarrow}\hat{c}_{u,\uparrow}$, we see that $\langle \Omega^{\boldsymbol{\sigma}} | \hat{n}_{u,\uparrow}\hat{n}_{u,\downarrow} | \Omega^{\boldsymbol{\sigma}'} \rangle$ is the inner product of $\hat{c}_{u,\downarrow}\hat{c}_{u,\uparrow}|\Omega^{\boldsymbol{\sigma}}\rangle$ and $\hat{c}_{u,\downarrow}\hat{c}_{u,\uparrow}|\Omega^{\boldsymbol{\sigma}'}\rangle$. From (11.4.11), we have

$$\hat{c}_{u,\downarrow}\hat{c}_{u,\uparrow}|\Omega^{\boldsymbol{\sigma}}\rangle \simeq \begin{cases} (\omega_{1/2})^2\Big(\prod_{p\in\mathscr{E}\setminus\{u-\frac{1}{2},u+\frac{1}{2}\}} \hat{d}^{\dagger}_{p,\sigma_p}\Big)|\Phi_{\mathrm{vac}}\rangle & \text{if } (\sigma_{u-\frac{1}{2}},\sigma_{u+\frac{1}{2}})=(\uparrow,\downarrow), \\ -(\omega_{1/2})^2\Big(\prod_{p\in\mathscr{E}\setminus\{u-\frac{1}{2},u+\frac{1}{2}\}} \hat{d}^{\dagger}_{p,\sigma_p}\Big)|\Phi_{\mathrm{vac}}\rangle & \text{if } (\sigma_{u-\frac{1}{2}},\sigma_{u+\frac{1}{2}})=(\downarrow,\uparrow), \\ 0 & \text{otherwise}, \end{cases} \tag{11.4.14}$$

where $\omega_{1/2}=\omega_p(p\pm\frac{1}{2})\simeq -\nu/(1+\gamma)$. Here, and in what follows, near equality $\simeq$ indicates that we omit contributions of $O(\nu^3)$. We thus find that

$$\langle\Omega^{\boldsymbol{\sigma}}|\hat{n}_{u,\uparrow}\hat{n}_{u,\downarrow}|\Omega^{\boldsymbol{\sigma}'}\rangle \simeq \begin{cases} (\omega_{1/2})^4 & \text{if } \sigma_{u-\frac{1}{2}}\neq\sigma_{u+\frac{1}{2}} \text{ and } \boldsymbol{\sigma}'=\boldsymbol{\sigma}, \\ -(\omega_{1/2})^4 & \text{if } \sigma_{u-\frac{1}{2}}\neq\sigma_{u+\frac{1}{2}} \text{ and } \boldsymbol{\sigma}'=\boldsymbol{\sigma}_{u-\frac{1}{2}\leftrightarrow u+\frac{1}{2}}, \\ 0 & \text{otherwise}. \end{cases} \tag{11.4.15}$$

As before, $\boldsymbol{\sigma}_{u-\frac{1}{2}\leftrightarrow u+\frac{1}{2}}$ denotes the configuration obtained from $\boldsymbol{\sigma}$ by swapping $\sigma_{u-\frac{1}{2}}$ and $\sigma_{u+\frac{1}{2}}$.

We now recall that, in a system of two spins with $S=1/2$, one has

$$\langle\Psi^{(\sigma_1,\sigma_2)}|\Big(\frac{1}{2}-2\,\hat{\boldsymbol{S}}_1\cdot\hat{\boldsymbol{S}}_2\Big)|\Psi^{(\sigma_1',\sigma_2')}\rangle = \begin{cases} 1 & \text{if } \sigma_1\neq\sigma_2 \text{ and } (\sigma_1',\sigma_2')=(\sigma_1,\sigma_2), \\ -1 & \text{if } \sigma_1\neq\sigma_2 \text{ and } (\sigma_1',\sigma_2')=(\sigma_2,\sigma_1), \\ 0 & \text{otherwise}, \end{cases} \tag{11.4.16}$$

where $\sigma_1,\sigma_2=\uparrow,\downarrow$. See (2.2.16). By comparing (11.4.15) and (11.4.16), we find that the effect of the first order perturbation is described by the effective spin Hamiltonian

$$\hat{H}^{(1)}_{\mathrm{eff}} = J_1\sum_{p=1}^{L}\Big(\frac{1}{4}-\hat{\hat{\boldsymbol{S}}}_p\cdot\hat{\hat{\boldsymbol{S}}}_{p+1}\Big), \tag{11.4.17}$$

where $\hat{\hat{\boldsymbol{S}}}_p$ is the spin operator corresponding to the Wannier state $\boldsymbol{\omega}_p$, defined by replacing $\hat{c}_{x,\sigma}$ in (9.2.38) with $\hat{d}_{p,\sigma}$. The exchange interaction constant is given by

$$J_1 = 2(\omega_{1/2})^4U \simeq \frac{2\nu^4}{(1+\gamma)^4}U, \tag{11.4.18}$$

and is always positive. The effective Hamiltonian (11.4.17) is nothing but that of the ferromagnetic Heisenberg model. We note that this argument is essentially the same as Heisenberg's perturbative derivation of the direct exchange interaction [16]. Although the above perturbation theory is rather ad hoc, we know from rigorous bounds for the spin-wave excitation energy that (11.4.17) and (11.4.18) are quantitatively reliable, provided that $\gamma\ll 1$. See Sect. 11.4.2, in particular, (11.4.36).

"Second order" perturbation The above perturbation theory suggests that the present Hubbard model, whose effective Hamiltonian (11.4.17) is ferromagnetic, universally exhibits ferromagnetism, no matter whether the lower band is flat (i.e.,

$\gamma = 0$) or non-flat (i.e., $\gamma \neq 0$). Furthermore, by examining the argument, we see that it is only essential for the emergence of the ferromagnetic interaction that the Wannier states on neighboring $\mathscr{E}$ sites share a common $\mathscr{I}$ site in between them. Should we then conclude that one always gets ferromagnetism in the Hubbard model on the lattice with two sublattices, such as our $\Lambda = \mathscr{E} \cup \mathscr{I}$?

Of course this is not the case; we are definitely overestimating the tendency toward ferromagnetism, as Heisenberg was doing in his seminal work on the direct exchange interaction [16]. In the present model we also have to look at the "second order" effect, which may become comparable to the above first order effect. The contribution we have been overlooking comes from the effective hopping process (11.4.6) for the Wannier states of the lower band. Indeed if we concentrate only on states formed by $\hat{d}^{\dagger}_{p,\sigma}$ with $p \in \mathscr{E}$ (which are in the lower band), the situation is exactly the same as that in Sect. 10.1, where we examined the second order perturbation effect in the half-filled Hubbard model. We have seen that the super-exchange interaction emerges, and the low energy properties of the model are described by the antiferromagnetic Heisenberg model (10.1.12). Here we only need to replace the hopping amplitude $t_{x,y}$, which appears in the expression (10.1.11) of the exchange interaction constant, by the effective hopping amplitude τ in (11.4.7). We thus see that the effective Hamiltonian from the "second order" perturbation is[33]

$$\hat{H}^{(2)}_{\text{eff}} = J_2 \sum_{p=1}^{L} \Big(\hat{\tilde{\boldsymbol{S}}}_p \cdot \hat{\tilde{\boldsymbol{S}}}_{p+1} - \frac{1}{4} \Big), \tag{11.4.19}$$

with

$$J_2 \simeq \frac{4\tau^2}{U} \simeq \frac{4\gamma^2 \nu^2}{(1+\gamma)^2} \frac{t^2}{U}. \tag{11.4.20}$$

Since $J_2 \geq 0$, we always get antiferromagnetic interaction from this process.

Stability and instability of ferromagnetism We have seen that there are two essentially different mechanisms which generate effective Heisenberg-type interaction between electronic spins in the present Hubbard model. The direct exchange interaction, which comes from the first order perturbation, leads to ferromagnetism, and the super-exchange interaction, which comes from the "second order" process, leads to antiferromagnetism. See Fig. 11.19. The overall effective spin Hamiltonian

$$\hat{H}_{\text{eff}} = (J_1 - J_2) \sum_{p=1}^{L} \Big(\frac{1}{4} - \hat{\tilde{\boldsymbol{S}}}_p \cdot \hat{\tilde{\boldsymbol{S}}}_{p+1} \Big), \tag{11.4.21}$$

where $J_1 > 0$ and $J_2 \geq 0$, is ferromagnetic if $J_1 - J_2 > 0$ and is antiferromagnetic if $J_1 - J_2 < 0$. For the flat-band model with $\gamma = 0$, we have $J_2 = 0$, and the model always exhibits ferromagnetism. This conclusion is consistent with the rigorous

[33] This is not really the second order perturbation which corresponds to the first order that we saw above. Here we are treating τ as a perturbation.

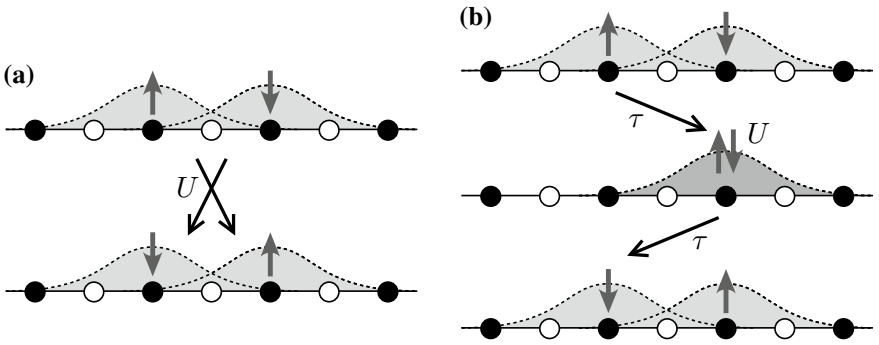

Fig. 11.19 The two exchange mechanisms in the nearly-flat-band model found from the non-rigorous Wannier state perturbation theory. **a** The direct exchange interaction due to Heisenberg leads to ferromagnetism. **b** The super-exchange interaction due to Anderson leads to antiferromagnetism. The magnetic property of the model is determined by the competition between the two effects ()

result, namely, Theorem 11.11 in p. 392. If $\gamma > 0$, we find by comparing (11.4.18) for J_1 and (11.4.20) for J_2 that $J_1 - J_2$ is negative for sufficiently small $U > 0$. We expect that the model exhibits antiferromagnetism. As we increase U (with γ fixed) the sign of $J_1 - J_2$ changes at a critical value of U, which is estimated as

$$U_{\mathrm{c}} \simeq \frac{\sqrt{2}\gamma(1+\gamma)t}{\nu}. \tag{11.4.22}$$

We expect that the model exhibits ferromagnetism when U is larger than U_{c}. In this sense ferromagnetism in a non-flat band model is a purely non-perturbative phenomenon. In conclusion the perturbative analysis in the present section suggests that the model exhibits ferromagnetism when the lower band is nearly flat, and the interaction is large enough.

11.4.2 Local Stability and the Spin Wave Excitation

We shall discuss the local stability of ferromagnetism in models obtained by adding an arbitrary translation invariant perturbation to the hopping Hamiltonian of the Tasaki model [70, 71]. We also discuss rigorous upper and lower bounds for the spin-wave excitation energy. These rigorous results provide strong support to the belief (or the conjecture) that the nearly-flat-band models exhibit physically realistic ferromagnetism.

Local stability theorem We consider the Hubbard model on the d-dimensional decorated hypercubic lattice $\Lambda = \mathscr{E} \cup \mathscr{I}$ as in Sect. 11.3.1. See, in particular, Figs. 11.10

and 11.11.[34] We again fix the electron number as $N = |\mathscr{E}| = L^d$. The Hamiltonian is $\hat{H} = \hat{H}_{\rm hop} + \hat{H}_{\rm int}$, with $\hat{H}_{\rm int}$ being the standard interaction Hamiltonian (11.3.6). The hopping Hamiltonian in the present model is

$$\hat{H}_{\rm hop} = t \sum_{\substack{u\in\mathscr{I}\\ \sigma=\uparrow,\downarrow}} \hat{b}^\dagger_{u,\sigma}\hat{b}_{u,\sigma} + \zeta \sum_{\substack{x,y\in\Lambda\\ \sigma=\uparrow,\downarrow}} t'_{x,y}\hat{c}^\dagger_{x,\sigma}\hat{c}_{x,\sigma}, \tag{11.4.23}$$

with $t > 0$, where $\hat{b}^\dagger$ operator is defined in (11.3.4). Here $\zeta \in \mathbb{R}$ is the perturbation parameter. Note that, when $\zeta = 0$, (11.4.23) reduces to the hopping Hamiltonian (11.3.5) for the flat-band model. The new hopping amplitude is real symmetric, i.e., $t'_{x,y} = t'_{y,x} \in \mathbb{R}$, and satisfies the translation invariance

$$t'_{x+z,y+z} = t'_{x,y}, \tag{11.4.24}$$

for any $z \in \mathbb{Z}^d$ (where we use periodic boundary conditions), and the summability

$$\sum_{y\in\Lambda} |t'_{x,y}| \le t, \quad \sum_{y\in\Lambda} |x-y|\,|t'_{x,y}| \le tR, \tag{11.4.25}$$

for any $x \in \Lambda$ with a constant $R > 0$, which may be interpreted as the range of the hopping. We thus allow any translation invariant hopping (which decays sufficiently fast) as a perturbation. The lowest band in the corresponding single-electron problem is generally no longer flat when $\zeta \neq 0$. The model with (11.4.1) studied in Sect. 11.4.1 is an example.

To state the first theorem, we define the minimum energy among the states with total spin S as

$$E_{\rm min}(S) := \min\Big\{\langle\Phi|\hat{H}|\Phi\rangle \,\Big|\, (\hat{\boldsymbol{S}}_{\rm tot})^2|\Phi\rangle = S(S+1)|\Phi\rangle,\ \|\Phi\| = 1\Big\}, \tag{11.4.26}$$

where $S = 0, 1, \ldots, S_{\rm max}$. The ground state energy is written as $E_{\rm GS} = \min_S E_{\rm min}(S)$. The model exhibits (saturated) ferromagnetism if and only if $E_{\rm min}(S_{\rm max}) < E_{\rm min}(S)$ for any S such that $S \neq S_{\rm max}$. It is not (yet) possible to prove that the model exhibits ferromagnetism, but the following local stability theorem was proved by Tasaki [70, 71]. The proof is based on an elementary but rigorous perturbation theory.

Theorem 11.18 (Local stability of ferromagnetic ground states) *There are constants ν_0, η_0, and ξ_0 which depend only on the dimension d and the range R. If the model parameters satisfy*

$$0 < \nu \le \nu_0, \quad |\zeta| \le \nu^3\eta_0, \tag{11.4.27}$$

and

$$U \ge \frac{\xi_0\, t}{\nu^2}|\zeta|, \tag{11.4.28}$$

[34] In [71] general models obtained by the cell construction (see the end of Sect. 11.3.1) are treated.

then we have

$$E_{\min}(S_{\max}) < E_{\min}(S_{\max} - 1). \tag{11.4.29}$$

Note that $E_{\min}(S_{\max} - 1)$ is the minimum energy in the subspace where a single spin is flipped from the ferromagnetic state and coupled antiferromagnetically to the rest of the spins. Thus the inequality (11.4.29) shows that ferromagnetic ground states are stable against a single-spin flip. Such a local stability is a necessary but not a sufficient condition for the emergence (or the global stability) of ferromagnetism. Physically speaking, however, it is strongly believed (based on numerous examples) that the local stability generally implies the global stability in the case of ferromagnetism. See [37, 38] for related rigorous results. In this sense Theorem 11.18 provides a strong support for the emergence of saturated ferromagnetism in the perturbed model with a nearly-flat band.

The most important condition for the above local stability theorem is (11.4.28), which requires the Coulomb interaction to be sufficiently large. This is natural since we never have ferromagnetism in a generic model with $\zeta \neq 0$ if $U > 0$ is too small, as is stated in Theorem 11.3 in p. 375. We can say that the above local stability theorem establishes a truly nonperturbative result in which the "competition" between hopping and interaction is properly taken into account.

Let us stress that the problem of stability against a single-spin flip is already a highly nontrivial many-body problem. The restriction to the sector with $S_{\text{tot}} = S_{\max} - 1$ does not reduce the problem to that of a single-particle (such as a magnon) since there are plenty of spaces for the electrons to move around. Moreover there is no hope of expressing general energy eigenstates as Slater determinant states since there are both up-spin and down-spin electrons interacting via local Coulomb repulsion.

Spin-wave excitation energy By using the same rigorous perturbation theory, rigorous upper and lower bounds for the spin-wave excitation energies in the above model was obtained in [70, 71].

For $z \in \mathbb{Z}^d$, we define the translation operator $\hat{\tau}_z : \mathscr{H}_N \to \mathscr{H}_N$ by

$$\hat{\tau}_z \hat{c}^\dagger_{x_1,\sigma_1} \hat{c}^\dagger_{x_2,\sigma_2} \cdots \hat{c}^\dagger_{x_N,\sigma_N} |\Phi_{\text{vac}}\rangle = \hat{c}^\dagger_{x_1+z,\sigma_1} \hat{c}^\dagger_{x_2+z,\sigma_2} \cdots \hat{c}^\dagger_{x_N+z,\sigma_N} |\Phi_{\text{vac}}\rangle \tag{11.4.30}$$

for any $x_1, \ldots, x_N \in \Lambda$ and $\sigma_1, \ldots, \sigma_N = \uparrow, \downarrow$, and by assuming the linearity. We use periodic boundary conditions. The operator $\hat{\tau}_z$ is unitary, and its eigenvalues are written as $e^{-ik\cdot z}$ with $k \in \mathscr{K}_L$. Here $\mathscr{K}_L$ is the k-space defined in (4.1.17), and $k \cdot z = \sum_{\mu=1}^d k_\mu z_\mu$ with $k = (k_1, \ldots, k_d)$ and $z = (z_1, \ldots, z_d)$. Since both $\hat{H}$ and $\hat{S}^{(3)}_{\text{tot}}$ are translation invariant, we can look for simultaneous eigenstates of $\hat{H}$, $\hat{S}^{(3)}_{\text{tot}}$, and $\hat{\tau}_z$.[35] We then let $E_{\text{SW}}(k)$ be the smallest energy eigenvalue among the states satisfying $\hat{S}^{(3)}_{\text{tot}}|\Phi\rangle = (S_{\max} - 1)|\Phi\rangle$ and $\hat{\tau}_z|\Phi\rangle = e^{-ik\cdot z}|\Phi\rangle$ for any $z \in \mathbb{Z}^d$. This is the most general definition of the energy of the elementary spin-wave excitation with momentum k.

[35] $\hat{A}$ is translation invariant if $(\hat{\tau}_z)^{-1}\hat{A}\hat{\tau}_z = \hat{A}$, which means $[\hat{\tau}_z, \hat{A}] = 0$.

Theorem 11.19 (Bounds on the spin-wave excitation energy) *There are constants ν_1, η_1, ξ_1, and ξ_2 which depend only on the dimension d and the range R. If the model parameters satisfy*

$$0 < \nu \le \nu_1, \quad |\zeta| \le \nu^2 \eta_1, \tag{11.4.31}$$

and

$$\frac{\xi_1 t}{\nu^2}|\zeta| \le U \le \xi_2 t \nu, \tag{11.4.32}$$

then it holds that

$$F_1 \, 2\nu^4 U \sum_{\mu=1}^{d} (1 - \cos k_\mu) \ge E_{\mathrm{SW}}(k) - E_{\min}(S_{\max}) \ge F_2 \, 2\nu^4 U \sum_{\mu=1}^{d} (1 - \cos k_\mu), \tag{11.4.33}$$

for any $k \in \mathscr{K}_L$. Here the constants F_1 and F_2 are written as

$$F_1 = 1 + a_1 \nu + a_2 \frac{|\zeta|}{\nu^3} + \frac{a_3 t}{\nu^4 U}|\zeta|^2, \tag{11.4.34}$$

$$F_2 = 1 - b_1 \nu - b_2 \frac{|\zeta|}{\nu^2} - \frac{b_3 t}{\nu^4 U}|\zeta|^2, \tag{11.4.35}$$

with positive constants a_1, a_2, a_3, b_1, b_2, and b_3.

Therefore when ν is small, and $|\zeta|$ is much smaller (and hence the lowest band is nearly-flat), we have an almost precise estimate

$$E_{\mathrm{SW}}(k) - E_{\mathrm{GS}} \simeq 2\nu^4 U \sum_{\mu=1}^{d} (1 - \cos k_\mu), \tag{11.4.36}$$

about the spin-wave excitation energies. We recall that this dispersion relation is what one expects for the elementary magnon excitation in a ferromagnetic Heisenberg model on the hypercubic lattice $\mathscr{E}$ with the exchange interaction $J_{\mathrm{eff}} = 2\nu^4 U$. See Sect. 2.4, in particular, (2.4.17). This partially justifies the estimate (11.4.18) for the ferromagnetic coupling in the Wannier state perturbation theory as well as the conclusion by Kusakabe and Aoki that the flat-band models have normal spin-wave excitations [23, 24]. (Note that Theorem 11.19 applies also to the flat-band model.) Theorem 11.19 thus suggests that ferromagnetism realized in Tasaki's (near-)flat-band models is "healthy" from a physical point of view.

About the proofs We are not going to prove Theorems 11.18 or 11.19 in the present book. The proofs are rather involved, as can be seen from the fact that the paper [71] has 119 pages. We nevertheless stress that the essence of the proofs is quite elementary. We encourage the interested reader to take a look at (at least) Sects. 1 and 2 of [71], which can be read as a self-contained account of the rigorous perturbation method used in this work.

The basic strategy of the proofs is somewhat similar to the Wannier state perturbation theory discussed in Sect. 11.4.1. We represent the Hubbard model by using a basis consisting of exponentially localized states, and then control all the matrix elements rigorously. This is of course a formidable task in general, but is barely doable if we restrict ourselves to the subspace with $N-1$ up-spin electrons and one down-spin electrons, and make full use of the translation invariance. We need to face a tough many-body problem even within this subspace, but the problem becomes much easier because the Coulomb energy $\hat{H}_{\rm int}$ is at most U in the subspace.

11.4.3 Ferromagnetism in Non-singular Hubbard Models

We finally discuss the result due to Tasaki [72, 74] on global stability of ferromagnetism in a Hubbard model with a nearly-flat lowest band, obtained by adding a particular perturbation to the flat-band model studied in Sect. 11.3.1. As we have already emphasized, this work established the emergence of ferromagnetism in a Hubbard model without any singularity, i.e., a model with finite density of states $D_{\rm F}$ and finite Coulomb interaction U. It is also important that the result is essentially non-perturbative in the sense that it can never be valid if the interaction $U > 0$ is too small.

The proof, which we shall describe in detail below, is again based on the properties of frustration-free Hamiltonians. In this case, however, the construction of frustration-free local Hamiltonians is highly nontrivial; one must take a local Hamiltonian that acts on $4d+1$ sites to make the argument work. See Fig. 11.23.

As far as we know, this strategy, which was proposed in [72], is still essentially the only method to prove the existence of ferromagnetism in a Hubbard model with a non-flat lowest band. There have been extensions of the method to the Hubbard model with a certain multi-band structure [62], on the kagomé lattice [65], on three coupled chains [77], on planar line graphs [30], and on certain three dimensional lattices [58]. See also [57] for an extension to the SU(n) Hubbard model.

The model and the main result We consider the Hubbard model on the d-dimensional decorated hypercubic lattice $\Lambda = \mathscr{E} \cup \mathscr{I}$ as in Sect. 11.3.1. See, in particular, Figs. 11.10 and 11.11. We again make use of the operators $\hat{a}_{p,\sigma}$ and $\hat{b}_{u,\sigma}$ defined in (11.3.3) and (11.3.4), respectively. Our Hamiltonian is $\hat{H} = \hat{H}_{\rm hop} + \hat{H}_{\rm int}$, where

$$\hat{H}_{\rm int} = U \sum_{x \in \Lambda} \hat{n}_{x,\uparrow} \hat{n}_{x,\downarrow}, \tag{11.4.37}$$

with $U > 0$, is the standard interaction Hamiltonian (9.3.29). We consider a particular hopping Hamiltonian

$$\hat{H}_{\rm hop} = t \sum_{\substack{u \in \mathscr{I} \\ \sigma = \uparrow,\downarrow}} \hat{b}^{\dagger}_{u,\sigma} \hat{b}_{u,\sigma} - s \sum_{\substack{p \in \Lambda \\ \sigma = \uparrow,\downarrow}} \hat{a}^{\dagger}_{p,\sigma} \hat{a}_{p,\sigma}, \tag{11.4.38}$$

with two parameters $t > 0$ and $s > 0$. Note that the model reduces to the flat-band model of Sect. 11.3.1 if we set $s = 0$. Note also that this is a special case of the hopping Hamiltonian (11.4.23) of the perturbed model with a nearly-flat band treated in Sect. 11.4.2. Again the hopping Hamiltonian (11.4.38) is written in the standard form

$$\hat{H}_{\rm hop} = \sum_{\substack{x,y\in\Lambda \\ \sigma=\uparrow,\downarrow}} t_{x,y}\, \hat{c}^\dagger_{x,\sigma}\hat{c}_{y,\sigma}, \tag{11.4.39}$$

with admittedly complicated hopping amplitude given by

$$t_{x,y} = \begin{cases} v(t+s) & \text{if } |x-y| = 1/2, \\ v^2 t & \text{if } x, y \in \mathscr{E} \text{ and } |x-y| = 1, \\ -v^2 s & \text{if } x \neq y \in \mathscr{I} \text{ and } \exists p \in \mathscr{E} \text{ s.t. } |x-p| = |y-p| = 1/2, \\ t - 2v^2 s & \text{if } x = y \in \mathscr{I}, \\ 2dv^2 t - s & \text{if } x = y \in \mathscr{E} \\ 0 & \text{otherwise.} \end{cases} \tag{11.4.40}$$

See Fig. 11.20. By solving the corresponding single-electron Schrödinger equation (9.3.3), one finds the dispersion relations of $d+1$ bands

$$\varepsilon_\mu(k) = \begin{cases} -s - 2v^2 s \sum_{j=1}^d (1+\cos k_j) & \mu = 1, \\ t & \mu = 2, \dots, d, \\ t + 2v^2 t \sum_{j=1}^d (1+\cos k_j) & \mu = d+1, \end{cases} \tag{11.4.41}$$

where $k \in \mathscr{K}_L$ is a wave number vector defined in (4.1.17). See Fig. 11.21. The dispersion relations should be compared with the corresponding (11.3.23) for the flat-band model. One sees that the flat lowest band has become dispersive because of the nonzero hopping parameter s. This dispersion relation is indeed easily understood. From the anticommutation relations $\{\hat{b}_{u,\sigma}, \hat{a}^\dagger_{p,\tau}\} = 0$, which is (11.3.7), and

$$\{\hat{a}_{p,\sigma}, \hat{a}^\dagger_{q,\tau}\} = \begin{cases} (1+2dv^2)\,\delta_{\sigma,\tau} & \text{if } p = q, \\ v^2\,\delta_{\sigma,\tau} & \text{if } |p-q| = 1, \\ 0 & \text{otherwise} \end{cases} \tag{11.4.42}$$

one finds

$$\hat{H}_{\rm hop}\,\hat{a}^\dagger_{p,\sigma}|\Phi_{\rm vac}\rangle = -\Big\{ s\,\hat{a}^\dagger_{p,\sigma} + v^2 s \Big(2d\,\hat{a}^\dagger_{p,\sigma} + \sum_{\substack{q\in\mathscr{E} \\ (|q-p|=1)}} \hat{a}^\dagger_{q,\sigma} \Big) \Big\} |\Phi_{\rm vac}\rangle, \tag{11.4.43}$$

which represents nearest neighbor hopping on the d-dimensional hypercubic lattice $\mathscr{E}$. The dispersion relations for the remaining d bands are exactly the same as (11.3.23)

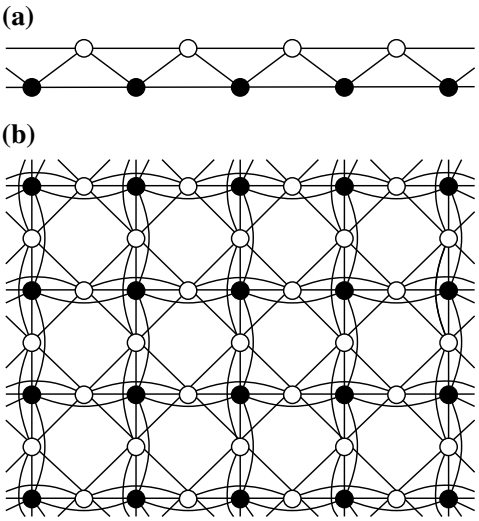

Fig. 11.20 Hopping in the non-singular model studied in Sect. 11.4.3 for **a** $d = 1$ and **b** $d = 2$. There are additional short range hopping compared with Fig. 11.11 (p. 392) for the flat-band models ()

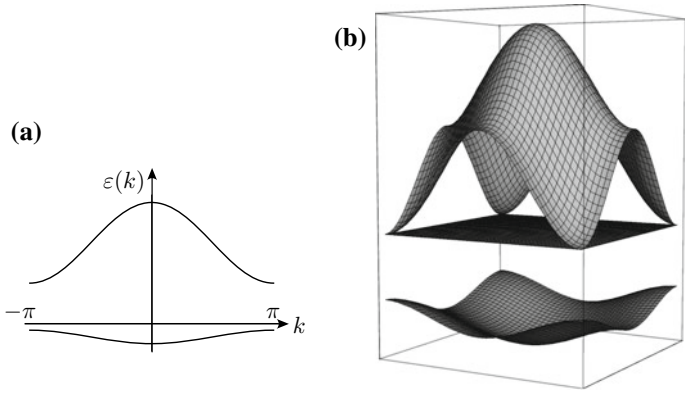

Fig. 11.21 The dispersion relations (11.4.41) of the non-singular model on the decorated d-dimensional hypercubic lattice, which should be compared with Fig. 11.13 (p. 397) for the flat-band models. **a** The two bands in the one dimensional model are now both dispersive. **b** In the two dimensional model, the lowest and the highest bands are dispersive, while the band in the middle is still flat. But the middle band has almost nothing to do with the properties of the ground states. (The horizontal axes represent $k_1, k_2 \in [-\pi, \pi]$ and the vertical axis represent $\varepsilon(k_1, k_2)$.) ()

for the flat-band model. This is because the hopping Hamiltonian (11.4.38) does not connect $\hat{a}^\dagger$ states and $\hat{b}^\dagger$ states. (Of course the interaction Hamiltonian (11.4.37) in general mixes $\hat{a}^\dagger$ states and $\hat{b}^\dagger$ states.)

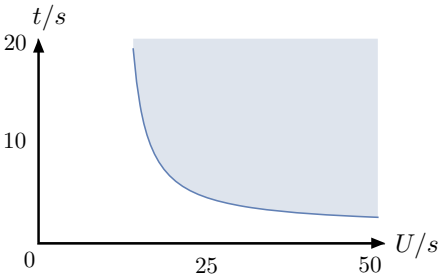

Fig. 11.22 The region in which the present Hubbard model with $d = 1$ and $\nu = 1/\sqrt{2}$ is proved to exhibit ferromagnetism. It is sufficient to chose $t/s \geq 4.5$ when $U/s = 25$, and $t/s \geq 2.6$ when $U/s = 50$ ()

One might have noticed that both the highest and the lowest bands in (11.4.41) have perfect cosine dispersions. This is a peculiar feature of the present model, and is essentially related to the tractability of the model.[36] In a general multi-band model, one encounters dispersion relations which are not a linear functions of trigonometric functions. See, e.g., (9.3.16).

Another peculiar feature in the dispersion relations (11.4.41) is that, for $d \geq 2$, there still remain $(d-1)$ flat bands with energy t. We stress however that these flat bands have almost nothing to do with the properties of the ground states. If one does not want to have a flat-band, then it is easy to perturb the model and lift the degeneracy in such a manner that the main theorem (Theorem 11.20 below) is still valid. See Sect. 6.2 of [74].

To state the theorem, let us define, for $d \geq 2$,

$$\nu_{\mathrm{c}}(d) := \sqrt{\frac{2d+1+\sqrt{4d^2+12d-7}}{4(d-1)}}. \tag{11.4.44}$$

Theorem 11.20 (Ferromagnetism in the non-singular Hubbard model) *Consider the above Hubbard model with electron number $N = |\mathscr{E}| = L^d$. Assume that $\nu > 0$ for $d = 1$, and $0 < \nu < \nu_{\mathrm{c}}(d)$ for $d \geq 2$. Then for sufficiently large $t/s > 0$ and $U/s > 0$, the ground states have $S_{\mathrm{tot}} = S_{\max} = N/2$, and are unique apart from the trivial $2S_{\max} + 1 = N + 1$ fold degeneracy.*

How large t/s and U/s should be depends only on d and ν, and not on the system size L. The theorem establishes the emergence of ferromagnetism in nearly-flat-band models, where one has $t/s \gg 1$, but it is valid even when the lower band is far from being flat. In the model with $d = 1$ and $\nu = 1/\sqrt{2}$, for example,[37] it suffices to take $t/s \geq 4.5$ when $U/s = 25$, and $t/s \geq 2.6$ when $U/s = 50$. See Fig. 11.22.

Recall that we argued in Sect. 11.4.2 that the flat-band model is stable against perturbation when $\nu \ll 1$, i.e., when $\hat{a}^\dagger$ states are almost localized at a site in $\mathscr{E}$. The

[36] We expect (or hope) that the model represents a specially tractable class of tight-binding systems, and may play the role analogous to that played by matrix product states (or the VBS state) in quantum spin chains.

[37] When $d = 1$ and $\nu = 1/\sqrt{2}$, one finds from (11.4.40) that $t_{x,x} = t - s$ for all $x \in \Lambda$. Thus the model is equivalent to that with $t_{x,x} = 0$ for all $x \in \Lambda$.

above theorem clearly covers the region where such a picture does not apply; we have $\nu_c \sim 1$ in general ($\nu_c \simeq 1.64$ for $d = 2$ and $\nu_c \simeq 1.37$ for $d = 3$), and there is no upper limit for $\nu > 0$ in $d = 1$.

Since our hopping Hamiltonian (11.4.38) is a special case of the hopping Hamiltonian (11.4.23) treated in Sect. 11.4.2, Theorem 11.19 in p. 424 on the spin-wave excitations also applies to the present model provided that $0 < \nu \ll 1$, $t/s \gg 1$, and U is in a suitable range. In particular, we have rigorous upper and lower bounds for the spin-wave excitation energy, which imply

$$E_{\mathrm{SW}}(k) - E_{\mathrm{GS}} \simeq 2\nu^4 U \sum_{\mu=1}^{d} (1 - \cos k_\mu), \tag{11.4.45}$$

where $E_{\mathrm{SW}}(k)$ is defined in p. 424. Thus for the range of ν, t, s, U, and d where both Theorems 11.19 and 11.20 are applicable, we have established rigorously that the ground states of the model exhibit saturated ferromagnetism, and the spin-wave excitations above the ground states have normal dispersion relations corresponding to the exchange interaction $\nu^4 U$. Starting from models of itinerant electrons, we have rigorously shown that their low energy properties perfectly coincide with those of physically natural insulating ferromagnets.

Reduction to a finite system In the rest of the present subsection, we give a complete Proof of Theorem 11.20. We start from a fundamental lemma, Lemma 11.21 below, which reduces our problem to that of a Hubbard model on a small lattice with $4d + 1$ sites. Although the basic idea of the lemma and its proof follows that in the original work [72], we here present a simplified version due to Hosho Katsura (private communication). See also [57].

The starting point is the decomposition of the Hamiltonian

$$\hat{H} = -L^d(1 + 2d\nu^2)\, s + \lambda\, \hat{H}_{\mathrm{flat}} + \sum_{p \in \mathscr{E}} \hat{h}_p, \tag{11.4.46}$$

where

$$\hat{H}_{\mathrm{flat}} = \sum_{\substack{u \in \mathscr{I} \\ \sigma = \uparrow, \downarrow}} \hat{b}^\dagger_{u,\sigma} \hat{b}_{u,\sigma} + \sum_{x \in \Lambda} \hat{n}_{x,\uparrow} \hat{n}_{x,\downarrow} \tag{11.4.47}$$

is nothing but the Hamiltonian of Tasaki's flat-band model studied in Sect. 11.3.1, with two parameters set as $t = U = 1$. We defined, for each $p \in \mathscr{E}$, the local Hamiltonian

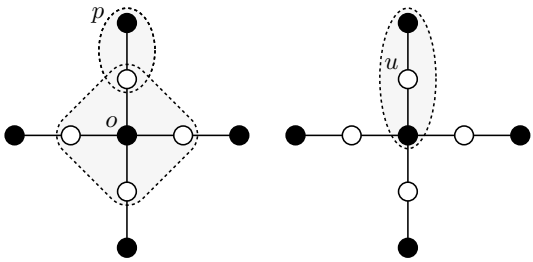

Fig. 11.23 The nine-site lattice on which the local Hamiltonian $\hat{h}_o$ for $d = 2$ acts. We have also depicted the states generated by $\hat{a}_o^\dagger$ and $\hat{a}_p^\dagger$ (left), and by $\hat{b}_u^\dagger$ (right) ()

$$\begin{aligned}\hat{h}_p =&(1+2d\nu^2)\,s - s\sum_{\sigma=\uparrow,\downarrow}\hat{a}_{p,\sigma}^\dagger\hat{a}_{p,\sigma} + \frac{t-\lambda}{2}\sum_{\substack{u\in\mathscr{I}\\(|u-p|=1/2)\\\sigma=\uparrow,\downarrow}}\hat{b}_{u,\sigma}^\dagger\hat{b}_{u,\sigma}\\ &+(1-\kappa)(U-\lambda)\hat{n}_{p,\uparrow}\hat{n}_{p,\downarrow} + \frac{U-\lambda}{2}\sum_{\substack{u\in\mathscr{I}\\(|u-p|=1/2)}}\hat{n}_{u,\uparrow}\hat{n}_{u,\downarrow}\\ &+\frac{\kappa}{2d}(U-\lambda)\sum_{\substack{q\in\mathscr{E}\\(|q-p|=1)}}\hat{n}_{q,\uparrow}\hat{n}_{q,\downarrow}. \end{aligned}\tag{11.4.48}$$

We have introduced two new parameters λ and κ, which satisfy $0 < \lambda < \min\{t, U\}$ and $0 \le \kappa < 1$. Note that the local Hamiltonian $\hat{h}_p$ acts nontrivially only on the site p and its $4d$ neighbors. See Fig. 11.23. The expression (11.4.48) looks complicated, but the construction is simple; we included the $\hat{a}_{p,\sigma}^\dagger\hat{a}_{p,\sigma}$ part into $\hat{h}_p$, divided the $\hat{b}_{u,\sigma}^\dagger\hat{b}_{u,\sigma}$ into two and included in $\hat{h}_p$ with two neighboring p, and decomposed the Coulomb interaction so that there is nonzero interaction $\hat{n}_{x,\uparrow}\hat{n}_{x,\downarrow}$ on each site. Although this local lattice (on which $\hat{h}_p$ acts) may seem to be rather large, we know that this is the minim size necessary for our proof to work.

We recall that Theorem 11.11 in p. 392 for the flat-band ferromagnetism shows that the ground states of $\hat{H}_{\text{flat}}$ with $N = L^d$ electrons have maximum total spin and are exactly $N + 1$ fold degenerate. Among the ground states is the all-up state

$$|\Phi_{\boldsymbol{\alpha}\,\text{all}\uparrow}\rangle = \Big(\prod_{p\in\mathscr{E}}\hat{a}_{p,\uparrow}^\dagger\Big)|\Phi_{\text{vac}}\rangle,\tag{11.4.49}$$

which is (11.3.9). It is crucial to note that $\hat{h}_p|\Phi_{\boldsymbol{\alpha}\,\text{all}\uparrow}\rangle = 0$ for all $p \in \mathscr{E}$. To see this, one notes that the Coulomb interaction obviously vanishes in an all-up state, and also that $\hat{b}_{u,\sigma}^\dagger\hat{b}_{u,\sigma}|\Phi_{\boldsymbol{\alpha}\,\text{all}\uparrow}\rangle = 0$ because of the anticommutation relations (11.3.7). For the action of $\hat{a}_{p,\sigma}^\dagger\hat{a}_{p,\sigma}$, we use the anticommutation relations (11.4.42) to note $\hat{a}_{p,\uparrow}^\dagger\hat{a}_{p,\uparrow} = (1+2d\nu^2) - \hat{a}_{p,\uparrow}\hat{a}_{p,\uparrow}^\dagger$. We then see that $\hat{a}_{p,\uparrow}^\dagger\hat{a}_{p,\uparrow}|\Phi_{\boldsymbol{\alpha}\,\text{all}\uparrow}\rangle = (1+2d\nu^2)|\Phi_{\boldsymbol{\alpha}\,\text{all}\uparrow}\rangle$ since $(\hat{a}_{p,\uparrow}^\dagger)^2 = 0$. Since we clearly have $\hat{a}_{p,\downarrow}^\dagger\hat{a}_{p,\downarrow}|\Phi_{\boldsymbol{\alpha}\,\text{all}\uparrow}\rangle = 0$, we find $(\sum_{\sigma=\uparrow,\downarrow}\hat{a}_{p,\sigma}^\dagger\hat{a}_{p,\sigma})|\Phi_{\boldsymbol{\alpha}\,\text{all}\uparrow}\rangle = (1+2d\nu^2)|\Phi_{\boldsymbol{\alpha}\,\text{all}\uparrow}\rangle$.

Recall that Theorem 11.11 shows that any ground state of $\hat{H}_{\text{flat}}$ is obtained by applying an SU(2) rotation to $|\Phi_{\boldsymbol{\alpha}\,\text{all}\uparrow}\rangle$. Since $\hat{h}_p$ is SU(2) invariant, this means that

$$\hat{h}_p|\Phi_{\text{GS}}^{\text{flat}}\rangle = 0, \tag{11.4.50}$$

for any ground state $|\Phi_{\text{GS}}^{\text{flat}}\rangle$ of $\hat{H}_{\text{flat}}$ with $N = L^d$, and for any $p \in \mathscr{E}$.

Lemma 11.21 *Consider the above Hubbard model with Hamiltonian $\hat{H}$ and electron number $N = |\mathscr{E}| = L^d$. If $\hat{h}_p \geq 0$ for all $p \in \mathscr{E}$, then the ground states have $S_{\text{tot}} = S_{\max} = N/2$, and are unique apart from the trivial $2S_{\max} + 1 = N + 1$ fold degeneracy.*

Proof Let $|\Phi_{\text{GS}}^{\text{flat}}\rangle$ be an arbitrary ground state with $N = |\mathscr{E}| = L^d$ of $\hat{H}_{\text{flat}}$ defined in (11.4.47). From (11.4.50) and $\hat{h}_p \geq 0$, we see that $|\Phi_{\text{GS}}^{\text{flat}}\rangle$ is a simultaneous ground state of $\hat{H}_{\text{flat}}$ and $\hat{h}_p$ for all $p \in \mathscr{E}$. This shows that the ground state energy of $\hat{H}$ is $-L^d(1 + 2dv^2)\,s$, and that any ground state should be a simultaneous ground state of $\hat{H}_{\text{flat}}$ and $\hat{h}_p$ for all $p \in \mathscr{E}$. (We have used Lemma A.10 in p. 469.) Then the desired uniqueness follows from Theorem 11.11 for the flat-band model. ∎

It should be noted that $\hat{h}_p$ is here regarded as an operator on the whole Hilbert space. This means that the number of electrons within the support of $\hat{h}_p$ (i.e., the $4d + 1$ sites on which $\hat{h}_p$ acts nontrivially) is not fixed. It can be anything between 0 and $2(4d + 1)$.

As is clear from the short proof, the above lemma is trivial. What is less trivial is the fact that $\hat{h}_p$ has zero eigenvalue as in (11.4.50), and what is essentially nontrivial is that there indeed exists a range of model parameters in which $\hat{h}_p$ is nonnegative.

Since $\hat{h}_p$ is after all a finite dimensional matrix, whether $\hat{h}_p \geq 0$ or not for given values of parameters may be determined numerically. In fact the region of parameters for $d = 1$ depicted in Fig. 11.22 was obtained in the original work [72] by numerically diagonalizing $\hat{h}_p$ with $\kappa = 0$.[38] Shen also performed such a computer-aided proof for higher dimensional models [53]. See also [30].

We can of course establish the nonnegativity of $\hat{h}_p$ without resorting to a computer. The following lemma will be proved below.

Lemma 11.22 *Assume that $v > 0$ if $d = 1$, and $0 < v < v_{\text{c}}(d)$ if $d \geq 2$, where $v_{\text{c}}(d)$ is defined in (11.4.44). Then for sufficiently large $t/s > 0$ and $U/s > 0$, one has $\hat{h}_p \geq 0$. (We take λ and κ to be proportional to s.)*

Proof of Theorem 11.20 *(p. 428),* ***given Lemmas*** 11.21 ***and*** 11.22: By simply combining the two lemmas, we get the desired main theorem. ∎

[38] One needs to set $\kappa > 0$ in Lemma 11.22. Numerical results for $d = 1$ indicate that one should set $\kappa = 0$ to get the largest range in the parameter space $(v, t/s, U/s)$ in which the existence of ferromagnetism is provable. (Kensuke Tamura and Hosho Katsura, private communication. See also [57].)

Why does the proof work? At this stage we wish to briefly discuss the reason why the present strategy of the proof works, especially because we ourselves still do not completely understand the reason.

The basic strategy is to first establish that ferromagnetism is realized in each small system described by the local Hamiltonian $\hat{h}_p$, and then see (by using the result for the flat-band model) that the local ferromagnetic ground states can be consistently combined to give global ferromagnetic ground states. It is rather unexpected that such a method works in an itinerant electron system with dispersive bands, since one expects that electrons behave as "waves" which are extended over the whole lattice. It is quite likely that our method relies essentially on the fact that the model behaves as insulating ferromagnet, and also on certain specific features of our model.

It seems also clear that we here have a situation similar to that in matrix product states (Sect. 7.2.2) or tensor network states (p. 213). Recall that, for a given injective matrix product state, one can always construct a parent Hamiltonian. The parent Hamiltonian is a sum of local Hamiltonians, chosen in such a way that the given MPS is a simultaneous ground state of all the local Hamiltonians. In other words, the model is frustration-free. As is noted in footnote 34 in p. 203, one has to choose the support of the local Hamiltonian large enough for the above construction to work. This is analogous to the present proof, where we needed to introduce local Hamiltonians that act on $4d + 1$ sites in order to realize a frustration-free situation. We should recall, however, that the present model is gapless and the ground states are highly degenerate because of the SU(2) symmetry. It may be interesting to understand the similarity and difference between our model and matrix product states or tensor network states, and look for the possibility of generalized theories.

Proof of Lemma 11.22 We shall prove Lemma 11.22, which is a core of our result on ferromagnetism in non-singular Hubbard models. The lemma was proved in [74] in a more general setting.[39] We here present a new transparent proof (which works only for the present model) due to Hosho Katsura and Akinori Tanaka (private communication). See also [57].

Since the system has translation invariance, it suffices to examine the local Hamiltonian $\hat{h}_o \geq 0$, where $o = (0, \ldots, 0)$ is the origin of $\mathbb{Z}^d$. We here regard $\hat{h}_o$ as an operator of the electron system on a small lattice Λ_o with $4d + 1$ sites. The lattice is written as $\Lambda_o = \{o\} \cup \mathscr{E}_o \cup \mathscr{I}_o$, where $\mathscr{E}_o$ consists of $2d$ sites of the form $(0, \ldots, 0, \pm 1, 0, \ldots, 0)$, and $\mathscr{I}_o$ consists of $2d$ sites of the form $(0, \ldots, 0, \pm 1/2, 0, \ldots, 0)$. See Fig. 11.23. Then the local Hamiltonian is

[39] In [74], general models obtained by the cell construction (see the end of Sect. 11.3.1) are also treated. The Proof of Lemma 6.1 in [74] (which corresponds to our Lemma 11.23) is highly technical. We still do not know any simplifications of the proof for models other than the simplest models that we are studying here.

$$\begin{aligned}\hat{h}_o =&(1+2d\nu^2)\,s - s\sum_{\sigma=\uparrow,\downarrow}\hat{a}^\dagger_{o,\sigma}\hat{a}_{o,\sigma} + \frac{t-\lambda}{2}\sum_{\substack{u\in\mathscr{I}_o\\ \sigma=\uparrow,\downarrow}}\hat{b}^\dagger_{u,\sigma}\hat{b}_{u,\sigma}\\ &+(1-\kappa)(U-\lambda)\hat{n}_{o,\uparrow}\hat{n}_{o,\downarrow} + \frac{U-\lambda}{2}\sum_{u\in\mathscr{I}_o}\hat{n}_{u,\uparrow}\hat{n}_{u,\downarrow}\\ &+\frac{\kappa}{2d}(U-\lambda)\sum_{p\in\mathscr{E}_o}\hat{n}_{p,\uparrow}\hat{n}_{p,\downarrow},\end{aligned} \tag{11.4.51}$$

where we assume $0<\kappa<1$ here. The fermion operators are defined by

$$\hat{a}_{o,\sigma} = \hat{c}_{o,\sigma} - \nu\sum_{u\in\mathscr{I}_o}\hat{c}_{u,\sigma}, \tag{11.4.52}$$

and

$$\hat{b}_{u,\sigma} = \hat{c}_{u,\sigma} + \nu(\hat{c}_{o,\sigma}+\hat{c}_{2u,\sigma}), \tag{11.4.53}$$

for each $u\in\mathscr{I}_o$. Note that, by definition, $2u$ denotes a site in $\mathscr{E}_o$. These definitions are the same as previous (11.3.3) and (11.3.4). It is convenient to also define for each $p\in\mathscr{E}_o$ the operator

$$\hat{a}_{p,\sigma} := \frac{1}{\sqrt{1+\nu^2}}(\hat{c}_{p,\sigma} - \nu\,\hat{c}_{p/2,\sigma}), \tag{11.4.54}$$

where $p/2$ is a site in $\mathscr{I}_o$. (Note that this is different from (11.3.3). We have also normalized the operator for later convenience.) See Fig. 11.23. Clearly the $4d+1$ single-electron states corresponding to the above $4d+1$ operators are linearly independent, and thus form a basis for the single-electron Hilbert space on Λ_o. We can thus represent any many-electron state on Λ_o by using $\hat{a}^\dagger$ and $\hat{b}^\dagger$ operators. We finally note that the fermion operators satisfy the anticommutation relations

$$\{\hat{a}_{o,\sigma},\hat{a}^\dagger_{o,\tau}\} = (1+2d\nu^2)\,\delta_{\sigma,\tau}\,,\quad \{\hat{a}_{o,\sigma},\hat{a}^\dagger_{p,\tau}\} = \frac{\nu^2}{\sqrt{1+\nu^2}}\,\delta_{\sigma,\tau}\,, \tag{11.4.55}$$

$$\{\hat{a}_{p,\sigma},\hat{a}^\dagger_{q,\tau}\} = \delta_{p,q}\,\delta_{\sigma,\tau}\,, \tag{11.4.56}$$

for any $p,q\in\mathscr{E}_o$, and $\sigma,\tau=\uparrow,\downarrow$, and

$$\{\hat{b}_{u,\sigma},\hat{a}^\dagger_{p,\tau}\} = 0, \tag{11.4.57}$$

for any $u\in\mathscr{I}_o$ and $p\in\{o\}\cup\mathscr{E}_o$.

Our goal is to prove $\hat{h}_o\ge 0$ for any electron number when the parameters satisfy the conditions described in Lemma 11.22. We first study this problem focusing only on ferromagnetic states, i.e., states with $S_{\rm tot}=n/2$, where n denotes the electron number. Then, as we saw in the proof of Proposition 11.2 (p. 373), we only need to study the system in which all electrons have up-spin. The problem reduces to that

of a non-interacting fermion system, which can be readily solved if one knows the single-electron spectrum corresponding to $\hat{h}_o$. Since $\hat{h}_o$ contains an extra constant, it is better to look at the shifted operator $\hat{h}'_o = \hat{h}_o - (1 + 2d\nu^2)s$, whose non-interacting part is $-s \sum \hat{a}^\dagger_{o,\sigma} \hat{a}_{o,\sigma} + \{(t - \lambda)/2\} \sum \hat{b}^\dagger_{u,\sigma} \hat{b}_{u,\sigma}$. One finds that there is a "band" of single-electron eigenstates generated by the $\hat{a}^\dagger$ operators. Among them the state corresponding to $\hat{a}^\dagger_o$ has the lowest eigenvalue $-(1 + 2d\nu^2)s$, and the remaining $2d$ states have eigenvalue zero. There is another "band" consisting of $2d$ states generated by the $\hat{b}^\dagger$ operators, whose eigenvalues are proportional to $t - \lambda > 0$. Going back to (non-interacting) many-electron problem, we see that the lowest eigenvalue of $\hat{h}'_o$ is $-(1 + 2d\nu^2)s$, and the second largest eigenvalue is 0. This means that, in the ferromagnetic sector, the lowest eigenvalue of the local Hamiltonian $\hat{h}_o$ is 0, and there is an energy gap $(1 + 2d\nu^2)s$ above it. Let us call these eigenstates (of $\hat{h}_o$) with zero eigenvalue the ferromagnetic zero-energy states.

It is easy to explicitly write down the ferromagnetic zero-energy states. Take an arbitrary subset A (including the empty set) of $\mathscr{E}_o$, and let

$$|\Phi_A\rangle := \hat{a}^\dagger_{o,\uparrow} \Big(\prod_{p \in A} \hat{a}^\dagger_{p,\uparrow} \Big) |\Phi_{\mathrm{vac}}\rangle. \tag{11.4.58}$$

By using the anticommutation relations (11.4.55), (11.4.56), and (11.4.57), and the relation $(\hat{a}^\dagger_{o,\uparrow})^2 = 0$ (and recalling that the Coulomb interaction vanishes), we verify that $\hat{h}_o |\Phi_A\rangle = 0$. Since $\hat{h}_o$ is SU(2) invariant, $(\hat{S}^-_{\mathrm{tot}})^m |\Phi_A\rangle$ with $m = 1, \ldots, |A| + 1$ is also a ferromagnetic zero-energy state.

We now take the limit $t, U \uparrow \infty$ in the Hamiltonian $\hat{h}_o$, with all the other parameters fixed. Clearly the ferromagnetic zero-energy states are not affected by the limits, and remain to be zero-energy eigenstates. We then prove the following.

Lemma 11.23 *Suppose that $\nu > 0$ satisfies the condition stated in Lemma 11.22. Then, in the limit $t, U \uparrow \infty$, the ferromagnetic zero-energy states are the only zero-energy eigenstates of $\hat{h}_o$, and any other eigenstates have strictly positive eigenvalues.*

Recall that $\hat{h}_o$ is nothing more than a finite dimensional matrix independent of the system size L. Then, we see from Lemma 11.23 and continuity that all the nonzero eigenvalues of $\hat{h}_o$ are strictly positive when t/s and U/s are sufficiently large. (Recall that we take λ and κ to be proportional to s.) This proves the desired Lemma 11.22.

Proof of Lemma 11.23 The statement of the lemma has already been verified for ferromagnetic states. We shall prove that if $|\Phi\rangle$ is any normalized state (not necessarily an energy eigenstate) with $S_{\mathrm{tot}} < n/2$, then one has

$$\lim_{t, U \uparrow \infty} \langle \Phi | \hat{h}_o | \Phi \rangle > 0, \tag{11.4.59}$$

where the limiting value may be infinite, provided that ν satisfies the condition in Lemma 11.22. Note that, in the left-hand side, only $\hat{h}_o$ depends on t or U. Then the desired Lemma 11.23 follows from the variational principle.

Clearly we only need to examine states such that $\lim_{t,U\uparrow\infty}\langle\Phi|\hat{h}_o|\Phi\rangle < \infty$ (where again $|\Phi\rangle$ does not depend on t or U), which we shall call finite energy states. Since $\hat{b}^\dagger_{u,\sigma}\hat{b}_{u,\sigma}$ and $\hat{n}_{x,\uparrow}\hat{n}_{x,\downarrow}$ are nonnegative, a necessary and sufficient condition that $|\Phi\rangle$ is a finite energy state is $\hat{b}^\dagger_{u,\sigma}\hat{b}_{u,\sigma}|\Phi\rangle = 0$ for any $u \in \mathscr{I}_o$ and $\sigma = \uparrow, \downarrow$, and $\hat{n}_{x,\uparrow}\hat{n}_{x,\downarrow}|\Phi\rangle = 0$ for any $x \in \Lambda_o$. Note that these finite-energy conditions are exactly the same as the zero-energy conditions that we encountered in the Proof of Theorem 11.11 (p. 392) for Tasaki's flat-band ferromagnetism. We can thus proceed in almost the same manner as in the Proof of Theorem 11.11. By using the conditions $\hat{b}_{u,\sigma}|\Phi\rangle = 0$ for all $u \in \mathscr{I}_o$ and $\sigma = \uparrow, \downarrow$, and $\hat{c}_{p,\downarrow}\hat{c}_{p,\uparrow}|\Phi\rangle = 0$ for all $p \in \{o\} \cup \mathscr{E}_o$, we find that any finite-energy state $|\Phi\rangle$ with $n_\uparrow$ up-spin electrons and $n_\downarrow$ down-spin electrons is written as

$$|\Phi\rangle = \sum_{\substack{A_\uparrow, A_\downarrow \subset \{o\}\cup\mathscr{E}_o \\ (A_\uparrow \cap A_\downarrow = \emptyset,\ |A_\uparrow| = n_\uparrow,\ |A_\downarrow| = n_\downarrow)}} \alpha(A_\uparrow, A_\downarrow)\Big(\prod_{p\in A_\uparrow}\hat{a}^\dagger_{p,\uparrow}\Big)\Big(\prod_{p\in A_\downarrow}\hat{a}^\dagger_{p,\downarrow}\Big)|\Phi_{\mathrm{vac}}\rangle, \quad (11.4.60)$$

where $\alpha(A_\uparrow, A_\downarrow) \in \mathbb{C}$ is a coefficient. The electron number $n = n_\uparrow + n_\downarrow$ can take any value in the range $\{1, \dots, 2d+1\}$. Recall that in the case of Tasaki's flat-band ferromagnetism, the same consideration led to the spin system representation (11.3.16). Here we do not get a spin system representation since the electron number is not necessarily equal to $2d+1$. Also note that we still have not used the finite-energy condition $\hat{c}_{u,\downarrow}\hat{c}_{u,\uparrow}|\Phi\rangle = 0$ for $u \in \mathscr{I}_o$.

Let us now assume that the above state $|\Phi\rangle$ has $S_{\mathrm{tot}} < n/2$. We clearly must have $n > 1$. We also claim that, in the expansion (11.4.60), one must have $\alpha(A_\uparrow, A_\downarrow) = 0$ whenever $A_\uparrow$ or $A_\downarrow$ contains o. To see this, note that if both the states created by $\hat{a}^\dagger_o$ and $\hat{a}^\dagger_p$ for some $p \in \mathscr{E}_o$ are occupied, then the finite energy condition $\hat{c}_{u,\downarrow}\hat{c}_{u,\uparrow}|\Phi\rangle = 0$ for $u = p/2$ leads to ferromagnetic exchange interaction between the electrons at o and p, exactly as in the case of Tasaki's flat-band ferromagnetism. (See the part "Ferromagnetic exchange interaction" in the Proof of Theorem 11.11.) Thus, whenever the state $\hat{a}^\dagger_o$ is occupied, all the n electrons couple ferromagnetically, and hence the state has the maximum total spin $S_{\mathrm{tot}} = n/2$. The claim has been proved.

We have thus found that any finite-energy state with $n_\uparrow$ up-spin electrons, $n_\downarrow$ down-spin electrons (where we write $n = n_\uparrow + n_\downarrow$) and $S_{\mathrm{tot}} < n/2$ is written as[40]

$$|\Phi\rangle = \sum_{\substack{A_\uparrow, A_\downarrow \subset \mathscr{E}_o \\ (A_\uparrow \cap A_\downarrow = \emptyset,\ |A_\uparrow| = n_\uparrow,\ |A_\downarrow| = n_\downarrow)}} \alpha(A_\uparrow, A_\downarrow)\Big(\prod_{p\in A_\uparrow}\hat{a}^\dagger_{p,\uparrow}\Big)\Big(\prod_{p\in A_\downarrow}\hat{a}^\dagger_{p,\downarrow}\Big)|\Phi_{\mathrm{vac}}\rangle. \quad (11.4.61)$$

In the rest of the proof we show that

$$\langle\Phi|\hat{h}_o|\Phi\rangle \geq \frac{s}{1+\nu^2}\big\{1 + (2d+1)\nu^2 + 2(1-d)\nu^4\big\}, \quad (11.4.62)$$

[40] The converse is, of course, not true. There are states of the form (11.4.61) that have $S_{\mathrm{tot}} = n/2$.

for any normalized $|\Phi\rangle$ with $n \geq 2$ written in the form (11.4.61), and for any t and U. It is easily found that the right-hand side is strictly positive for any $\nu > 0$ if $d = 1$ and for any ν such that $0 < \nu < \nu_c(d)$ if $d \geq 2$. Since the right-hand side is independent of t or U, we get the desired (11.4.59) for any normalized $|\Phi\rangle$ with $S_{\rm tot} < n/2$.

Since it holds for any finite energy state $|\Phi\rangle$ that

$$\langle\Phi|\hat{h}_o|\Phi\rangle = (1 + 2d\nu^2)s - s\langle\Phi| \sum_{\sigma=\uparrow,\downarrow} \hat{a}^\dagger_{o,\sigma}\hat{a}_{o,\sigma}|\Phi\rangle, \tag{11.4.63}$$

our task is to evaluate the expectation value $\langle\Phi| \sum_{\sigma=\uparrow,\downarrow} \hat{a}^\dagger_{o,\sigma}\hat{a}_{o,\sigma}|\Phi\rangle$. It is convenient to define the operator

$$\hat{d}_{o,\sigma} := \hat{a}_{o,\sigma} - \frac{\nu^2}{\sqrt{1+\nu^2}} \sum_{p\in\mathscr{E}_o} \hat{a}_{p,\sigma}, \tag{11.4.64}$$

for $\sigma = \uparrow, \downarrow$. From (11.4.56), we see that $\{\hat{a}^\dagger_{p,\sigma}, \hat{d}_{o,\tau}\} = 0$ for any $p \in \mathscr{E}_o$ and σ, $\tau = \uparrow, \downarrow$. Note that the anticommutation relation and $\hat{d}_{o,\sigma}|\Phi_{\rm vac}\rangle = 0$ imply $\hat{d}_{o,\sigma}|\Phi\rangle = 0$ for any $|\Phi\rangle$ of the form (11.4.61). Then we see from (11.4.64) that

$$\hat{a}_{o,\sigma}|\Phi\rangle = \frac{\nu^2}{\sqrt{1+\nu^2}} \sum_{p\in\mathscr{E}_o} \hat{a}_{p,\sigma}|\Phi\rangle, \tag{11.4.65}$$

and hence

$$-s\langle\Phi| \sum_{\sigma=\uparrow,\downarrow} \hat{a}^\dagger_{o,\sigma}\hat{a}_{o,\sigma}|\Phi\rangle = -\frac{s\nu^4}{1+\nu^2}\langle\Phi| \sum_{\substack{p,q\in\mathscr{E}_o \\ \sigma=\uparrow,\downarrow}} \hat{a}^\dagger_{p,\sigma}\hat{a}_{q,\sigma}|\Phi\rangle, \tag{11.4.66}$$

again for any $|\Phi\rangle$ as in (11.4.61).

To evaluate the right-hand side of (11.4.66), it is convenient to map the problem to that of a simpler Hubbard model defined on $\mathscr{E}_o$. Denoting the fermion operators for the new model again as $\hat{c}_{p,\sigma}$ with $p \in \mathscr{E}_o$ and $\sigma = \uparrow, \downarrow$, we consider the effective Hamiltonian

$$\hat{h}_{\rm eff} = -s' \sum_{\substack{p,q\in\mathscr{E}_o \\ \sigma=\uparrow,\downarrow}} \hat{c}^\dagger_{p,\sigma}\hat{c}_{q,\sigma}, \tag{11.4.67}$$

where $s' = s\nu^4/(1+\nu^2) > 0$. Then, from the anticommutation relation (11.4.56), we find an identity

$$-s\langle\Phi| \sum_{\sigma=\uparrow,\downarrow} \hat{a}^\dagger_{o,\sigma}\hat{a}_{o,\sigma}|\Phi\rangle = \langle\tilde{\Phi}|\hat{h}_{\rm eff}|\tilde{\Phi}\rangle. \tag{11.4.68}$$

Here the state of the new model is defined by

$$|\tilde{\Phi}\rangle = \sum_{\substack{A_\uparrow, A_\downarrow \subset \mathscr{E}_o \\ (A_\uparrow \cap A_\downarrow = \emptyset,\ |A_\uparrow| = n_\uparrow,\ |A_\downarrow| = n_\downarrow)}} \alpha(A_\uparrow, A_\downarrow) \Big(\prod_{p \in A_\uparrow} \hat{c}^\dagger_{p,\uparrow} \Big) \Big(\prod_{p \in A_\downarrow} \hat{c}^\dagger_{p,\downarrow} \Big) |\Phi_{\mathrm{vac}}\rangle, \quad (11.4.69)$$

where the coefficients $\alpha(A_\uparrow, A_\downarrow)$ are the same as in (11.4.61).

Thus the problem reduces to that of finding a lower bound of $\hat{h}_{\mathrm{eff}}$ in the space with no doubly occupied sites. In other words we need to evaluate the ground state energy of the Hamiltonian $\hat{P}_0 \hat{h}_{\mathrm{eff}} \hat{P}_0$, where $\hat{P}_0 = \prod_{p \in \mathscr{E}_0} (1 - \hat{n}_{p,\uparrow} \hat{n}_{p,\downarrow})$ is the projection operator onto the space with no doubly occupancy, known as the Gutzwiller projection. See (11.1.10). The problem is trivial for $d = 1$, where $\mathscr{E}_o$ contains only two sites. We only need to treat basis states of the form $|\Gamma_{\sigma,\tau}\rangle = \hat{c}^\dagger_{1,\sigma} \hat{c}^\dagger_{2,\tau} |\Phi_{\mathrm{vac}}\rangle$ with $\sigma, \tau = \uparrow, \downarrow$, where we wrote $\mathscr{E}_o = \{1, 2\}$. Noting that $\hat{P}_0 \hat{h}_{\mathrm{eff}} \hat{P}_0 |\Gamma_{\sigma,\tau}\rangle = -2s' |\Gamma_{\sigma,\tau}\rangle$ for any σ, τ, we find $\hat{P}_0 \hat{h}_{\mathrm{eff}} \hat{P}_0 \geq -2s' = -2s\nu^4/(1 + \nu^2)$. Recalling (11.4.63), we see that

$$\langle \Phi | \hat{h}_o | \Phi \rangle \geq (1 + 2\nu^2)s - \frac{2s\nu^4}{1 + \nu^2}, \quad (11.4.70)$$

which is the same as the desired (11.4.62) with $d = 1$.

The case with $d > 1$ is not difficult, but we need a clever trick. As was pointed out in [78], this problem can be solved exactly by using the method found by Brandt and Giesekus [5]. By using easily verifiable relations[41]

$$-\hat{P}_0 \, \hat{c}^\dagger_{p,\sigma} \hat{c}_{q,\sigma} \, \hat{P}_0 = \hat{c}_{q,\sigma} \, \hat{P}_0 \, \hat{c}^\dagger_{p,\sigma}, \quad (11.4.71)$$

$$\hat{P}_0 \big(1 - \sum_{\tau = \uparrow, \downarrow} \hat{c}^\dagger_{p,\tau} \hat{c}_{p,\tau}\big) \hat{P}_0 = \hat{c}_{p,\sigma} \, \hat{P}_0 \, \hat{c}^\dagger_{p,\sigma}, \quad (11.4.72)$$

for any $p, q \in \mathscr{E}_o$ with $p \neq q$, and any $\sigma = \uparrow, \downarrow$, one can show that

$$\hat{P}_0 \hat{h}_{\mathrm{eff}} \hat{P}_0 = s' \sum_{\sigma = \uparrow, \downarrow} \Big(\sum_{p \in \mathscr{E}_o} \hat{c}_{p,\sigma} \Big) \hat{P}_0 \Big(\sum_{p \in \mathscr{E}_o} \hat{c}^\dagger_{p,\sigma} \Big) - 2s' |\mathscr{E}_o| \, \hat{P}_0 + s' \hat{P}_0 \Big(\sum_{\substack{p \in \mathscr{E}_o \\ \sigma = \uparrow, \downarrow}} \hat{n}_{p,\sigma} \Big) \hat{P}_0. \quad (11.4.73)$$

Noting that the first term in the right-hand side is nonnegative, and that we are working with states with more than one electrons, i.e., $\sum_{p,\sigma} \hat{n}_{p,\sigma} \geq 2$, we get[42]

$$\hat{P}_0 \hat{h}_{\mathrm{eff}} \hat{P}_0 \geq -2s' \, 2d + 2s'. \quad (11.4.74)$$

Substituting this bound back into (11.4.63), we finally get

[41] One may check these relations by applying the left-hand and right-hand sides to relevant basis states and see that they yield the same results.

[42] In fact it is also easy to write down the ground states explicitly. See [78].

$$\langle \Phi | \hat{h}_o | \Phi \rangle \geq (1 + 2dv^2)s + \frac{sv^4}{1+v^2}(2 - 4d), \tag{11.4.75}$$

which is nothing but the desired (11.4.62). ∎

11.5 Toward Metallic Ferromagnetism

Metallic ferromagnetism is a fascinating phenomenon in which electrons exhibiting ferromagnetism also contribute to electric conduction. Needless to say iron is a typical substance which exhibits metallic ferromagnetism. Whether such a simple model as the Hubbard model can describe metallic ferromagnetism is an intriguing question.[43]

Nagaoka's ferromagnetism treated in Sect. 11.2 is certainly motivated by metallic ferromagnetism, and we believe that it sheds some light on possible mechanisms of metallic ferromagnetism. But, in the situation where the theorem is proved, the only dynamical freedom comes from the motion of a single hole. We never expect that the single hole can contribute to appreciable electric current in a bulk system. Nagaoka's ferromagnetism should better be interpreted as an insulator.

In Tasaki's flat-band model discussed in Sect. 11.3.1 and the related nearly-flat band models discussed in Sect. 11.4, the existence of ferromagnetism is proved for special electron numbers. These electron numbers correspond to the half-filling of the lowest bands, but since the ground states are ferromagnetic, the lowest bands become effectively fully filled. Then the systems should behave as Mott insulators.[44]

As we shall discuss below in Sect. 11.5.1, it is expected that the nearly-flat band models of Sect. 11.4 exhibit metallic ferromagnetism when the electron number N is strictly less than $L^d = |\mathscr{E}|$. Unfortunately we still do not have any rigorous results which confirm this conjecture. We believe that to rigorously justify the conjecture is one of challenging important problems in mathematical physics of quantum many-body systems.

The first rigorous example of metallic ferromagnetism in the Hubbard model was obtained in 1999 by Tanaka and Idogaki [61]. They followed Kubo's pioneering work in 1982 [22], and applied the Perron–Frobenius argument to a one-dimensional model with infinitely large band gap and Coulomb interaction. Their proof makes full use of the one-dimensional nature of the problem, and cannot be extended to models in higher dimensions. In 2007, Tanaka and Tasaki [63] proved that a (rather complicated) Hubbard model in any dimensions exhibits metallic ferromagnetism, again when the

[43] Recall that our aim here is not to build realistic models of existing materials, but to understand fundamental and universal mechanism of various physical phenomena including metallic ferromagnetism.

[44] In the ground state of Mielke's flat-band model (Sect. 11.3.2), the empty (dispersive) second lowest band touches the lowest flat-band, which is filled by ferromagnetically coupled electrons. It is likely that the model exhibits electric conduction, but the situation is slightly different from standard metals. In what follows we only focus on metals which have a partially filled band.

band gap and the Coulomb interaction are infinitely large. In Sect. 11.5.2 we prove, in the spirit of Kubo [22] and Tanaka and Idogaki [61], that a certain one-dimensional Hubbard model exhibits metallic ferromagnetism, and also discuss the theorem by Tanaka and Tasaki [63].

We admit that this final section of the whole book is a kind of anti-climax, in which we are able to present neither strong rigorous results nor promising nontrivial physical arguments. We nevertheless wish to have this section, in order to show some preliminary mathematical results provable within currently available techniques and to let the readers know of a widely open problem.

Given the fact that we are so familiar in our daily lives with metallic ferromagnetism stable at room temperatures, to prove the existence of metallic ferromagnetism (say, in a certain version of the Hubbard model) at low enough temperatures may appear as a modest goal. From theoretical and mathematical points of views, however, the problem looks formidably difficult.[45] It seems that not only mathematical techniques but fundamental understanding of physics of itinerant electron ferromagnetism is sill lacking.

11.5.1 Heuristic Arguments

Promising candidates of simple models exhibiting metallic ferromagnetism are the nearly-flat-band models studied in Sect. 11.4 with electron number N strictly less than $L^d = |\mathscr{O}|$, or, more precisely, with density N/L^d strictly less than one.[46] A rough argument is as follows. When N is less than L^d there appear $L^d - N$ "holes" in the $\hat{a}^\dagger$ state representation similar to (11.3.16) of the ground state. Even in such a situation the mechanism which generates the ferromagnetic exchange interaction between neighboring electrons should be still present. It is also important that electrons in the $\hat{a}^\dagger$ states are never at rest since the corresponding band is dispersive. Thus if N/L^d is close to 1, it is expected that all the electrons eventually interact with other electrons to generate a ferromagnetic state, i.e., a state with the maximum possible total spin. Then the model effectively reduces to that of non-interacting spinless fermions (as we have seen in the Proof of Proposition 11.2 in p. 373), and the ground states are written as Slater determinant states. Since the effective filling factor N/L^d of the lowest band is strictly less than one, the ground states correspond to a metallic ferromagnet.[47]

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[45] Recall that we are not even able to prove the existence of ferromagnetic order in the three dimensional ferromagnetic Heisenberg model at low enough temperatures. See Sect. 4.4.4.

[46] The flat-band models of Sect. 11.3 with electron numbers less than the half-filling were also studied in [35, 40, 67], and it was proved that the models still exhibit ferromagnetism in two or higher dimensions when the electron fillings are sufficiently large. We however believe that the models (as they are) are not relevant to metallic ferromagnetism since the electrons in the lowest flat bands do not contribute to conduction.

[47] We are here relying on the standard criterion (which can be found in any textbook in condensed matter physics) that a non-interacting fermion system with a partially filled band describes a metallic

The above picture is partially supported by the Wannier state perturbation theory, as we shall discuss below. Penc, Shiba, Mila, and Tsukagoshi [45] made a detailed study of a related problem in one dimension, and found both theoretical and numerical evidences that the model exhibits metallic ferromagnetism for arbitrary filling factor $\nu = N/(2|\Lambda|)$ in the range $0 < \nu < \nu_0 = 1/4$ (where ν_0 corresponds to the half-filling of the lowest nearly-flat band). See [50] for a similar numerical results, and [79, 80] for numerical results for related models with filling factor larger than ν_0.

Wannier state perturbation theory Let us present here a heuristic perturbative argument which supports the above picture about metallic ferromagnetism in the nearly-flat band model with electron number less than L^d. We in particular show that the low-energy effective theory of the Hubbard model is a model known as the ferromagnetic t-J model.

We consider exactly the same one-dimensional model as in Sect. 11.4.1, but with electron number N strictly less than $L = |\mathscr{E}|$. Recall that in the unperturbed ground states (11.4.11) for $N = L$, every Wannier state centered at $p \in \mathscr{E}$ is occupied by a single electron, with either up or down spin. Now, as we have less electrons, there appear some unoccupied sites, which may be identified as holes. Unperturbed ground states in this case are thus given by

$$|\Omega_{A_\uparrow, A_\downarrow}\rangle = \Big(\prod_{p\in A_\uparrow} \hat{d}^\dagger_{p,\uparrow}\Big)\Big(\prod_{p\in A_\downarrow} \hat{d}^\dagger_{p,\downarrow}\Big)|\Phi_{\mathrm{vac}}\rangle, \tag{11.5.1}$$

with $A_\uparrow, A_\downarrow \subset \mathscr{E}$ such that $|A_\uparrow| + |A_\downarrow| = N$ and $A_\uparrow \cap A_\downarrow = \emptyset$. We denote by $\tilde{\mathscr{H}}_N$ the effective low energy Hilbert space spanned by the states (11.5.1). As in Sect. 11.4.1, we examine low energy properties of the model perturbatively within the space $\tilde{\mathscr{H}}_N$.

This is indeed not difficult since all necessary estimates have already been done in Sect. 11.4.1. Let us here make an additional assumption that the effective hopping amplitude τ, which appears in (11.4.6) and (11.4.7), is sufficiently small so that the "second order" exchange interaction $J_2 \simeq 4\tau^2/U$ in (11.4.20) is negligible. Therefore when two neighboring sites $p, p+1 \in \mathscr{E}$ are both occupied, we get a ferromagnetic exchange interaction exactly as in (11.4.17). When there is a vacant site adjacent to an occupied site, then the electron may hop to the vacant site with the effective hopping amplitude τ.[48]

Let $\hat{\tilde{P}}_0$ be the projection operator onto the space $\tilde{\mathscr{H}}_N$. We can write the the low-energy effective Hamiltonian, which is an operator on $\tilde{\mathscr{H}}_N$, as[49]

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state. Although we are dealing with a system of strongly interacting electrons, it behaves as a non-interacting system within the space of states with $S_{\mathrm{tot}} = N/2$. There must be electric conduction, at least within the ferromagnetic sector.

[48] When there are vacant sites there appears new contribution from the "second order" perturbation which involves three sites. See, e.g., Sect. 5.1 of [10], Appendix 2.A of [9], and Sect. 3.2 of [2]. We can neglect this term since we assumed that τ^2/U is negligible.

[49] We have subtracted a trivial term $2\tau \sum_{p=1}^{L} \hat{\tilde{n}}_p$ from the effective Hamiltonian.

$$\hat{H}_{\text{eff}} = \tau\, \hat{\hat{P}}_0 \sum_{\substack{p\in\{1,\dots,L\}\\ \sigma=\uparrow,\downarrow}} (\hat{d}^\dagger_{p,\sigma}\hat{d}_{p+1,\sigma} + \text{h.c.}) + J\sum_{p=1}^{L}\Big(\frac{\hat{\hat{n}}_p\hat{\hat{n}}_{p+1}}{4} - \hat{\hat{\boldsymbol{S}}}_p\cdot\hat{\hat{\boldsymbol{S}}}_{p+1}\Big), \tag{11.5.2}$$

where "h.c." stands for Hermitian conjugate, and $\hat{\hat{n}}_p = \sum_{\sigma=\uparrow,\downarrow}\hat{d}^\dagger_{p,\sigma}\hat{d}_{p,\sigma}$ is the number operator for the Wannier state $\boldsymbol{\omega}_p$. We here wrote $J \simeq J_1 > 0$.

We have thus obtained an effective model in which (i) double occupancy of a single site is inhibited (because of the strong Coulomb interaction), (ii) electrons may hop to neighboring sites, and (iii) the spin degrees of freedom of two electrons occupying neighboring sites interact ferromagnetically. This is in fact a standard model known as the (ferromagnetic) t-J model.

It should be clear that the above derivation works in much more general models in any dimensions. As in Sect. 11.3.1, let $\mathscr{E}$ denote the d-dimensional $L\times\cdots\times L$ hypercubic lattice with periodic boundary conditions, and consider a model obtained by slightly perturbing the hopping Hamiltonian of the flat-band Hubbard model on the decorated lattice $\Lambda = \mathscr{E}\cup\mathscr{I}$. Then by developing a similar Wannier state perturbation argument, we find that the low energy effective theory of the model with electron number N strictly less than L^d is the ferromagnetic t-J model with the Hamiltonian

$$\hat{H}_{\text{eff}} = \tau\, \hat{\hat{P}}_0 \sum_{\substack{p,q\in\mathscr{E}\\ (|p-q|=1)\\ \sigma=\uparrow,\downarrow}} \hat{d}^\dagger_{p,\sigma}\hat{d}_{q,\sigma} + \frac{J}{2}\sum_{\substack{p,q\in\mathscr{E}\\ (|p-q|=1)}}\Big(\frac{\hat{\hat{n}}_p\hat{\hat{n}}_q}{4} - \hat{\hat{\boldsymbol{S}}}_p\cdot\hat{\hat{\boldsymbol{S}}}_q\Big), \tag{11.5.3}$$

with $J > 0$. Here $\hat{d}_{p,\sigma}$ is the fermion operator for the Wannier state (of the lowest band) centered around p, and $\hat{\hat{n}}_p$ and $\hat{\hat{\boldsymbol{S}}}_p$ are the corresponding number operator and the spin operator, respectively.

Since the ferromagnetic t-J model contains both electron hopping and ferromagnetic interaction, it is quite likely that the present model exhibits metallic ferromagnetism. But the story is not that simple, as we shall see in the next section. In short, ferromagnetism is always expected in one dimension, but, in higher dimensions, ferromagnetism may appear only when the electron density N/L^d is close to 1 and J/τ is large enough.

11.5.2 Rigorous Results

We shall discuss some rigorous results related to metallic ferromagnetism. As we have already stressed we still do not have any decisive theorems. We discuss results about the ferromagnetic t-J model and two different versions of the Hubbard model.

Ferromagnetism in the ferromagnetic t-J model Before dealing with the Hubbard model, we shall take a look at the ferromagnetic t-J model, which (at least apparently) looks easier. (But we will see that the essential problem may not be any easier.)

We have seen above that the ferromagnetic t-J model appears (approximately) as a low energy effective theory of the Hubbard model with a nearly-flat-band. Here we treat it as a given theoretical model.

Let us still denote by $\mathscr{E}$ the d-dimensional $L \times \cdots \times L$ hypercubic lattice with periodic boundary conditions, which is Λ_L in (3.1.2). We consider an electron model on $\mathscr{E}$ with electron number N strictly less than $L^d = |\mathscr{E}|$. Let $\mathscr{H}_N^{\rm hc}$ be the Hilbert space of N electron states with no doubly occupied sites. More precisely $\mathscr{H}_N^{\rm hc}$ is spanned by the basis states (9.2.35) which satisfy $x_i \neq x_j$ whenever $i \neq j$. We denote by $\hat{P}_{\rm hc}$ the projection operator onto $\mathscr{H}_N^{\rm hc}$. The Hamiltonian of the ferromagnetic t-J model, which is as an operator on $\mathscr{H}_N^{\rm hc}$, is given by

$$\hat{H}_{tJ} = -\tau\, \hat{P}_{\rm hc} \sum_{\substack{x,y\in\mathscr{E} \\ (|x-y|=1) \\ \sigma=\uparrow,\downarrow}} \hat{c}^\dagger_{x,\sigma}\hat{c}_{y,\sigma} + J \sum_{\substack{x,y\in\mathscr{E} \\ (|x-y|=1)}} \Big(\frac{\hat{n}_x\hat{n}_y}{4} - \hat{\boldsymbol{S}}_x \cdot \hat{\boldsymbol{S}}_y\Big), \tag{11.5.4}$$

where $\tau > 0$ is the hopping amplitude[50] and $J > 0$ is the ferromagnetic coupling constant.

Let us first focus on the ferromagnetic sector, i.e., the space of states which have maximum total spin $S_{\rm tot} = N/2$. It is easily seen that if $|\Phi_\uparrow\rangle$ is any state which consists only of up-spin electrons, then $(\hat{n}_p\hat{n}_q/4 - \hat{\boldsymbol{S}}_q \cdot \hat{\boldsymbol{S}}_p)|\Phi_\uparrow\rangle = 0$ for any $p \neq q$. Because both $\hat{n}_p\hat{n}_q$ and $\hat{\boldsymbol{S}}_q \cdot \hat{\boldsymbol{S}}_p$ are SU(2) invariant, we see that $(\hat{n}_p\hat{n}_q/4 - \hat{\boldsymbol{S}}_q \cdot \hat{\boldsymbol{S}}_p)|\Phi\rangle = 0$ for any $|\Phi\rangle$ in the ferromagnetic sector. Since there are no doubly occupied sites in a state in the ferromagnetic sector (see the Proof of Proposition 11.2 in p. 373), the problem reduces to that of a non-interacting spinless fermions with nearest neighbor hopping.

Let $\mathscr{K}_L$ be the k-space defined in (4.1.17). For each $k = (k_1, \ldots, k_d) \in \mathscr{K}_L$, we define the plane wave state by $\boldsymbol{\eta}^{(k)} = (L^{-d/2}\, e^{ik\cdot x})_{x\in\mathscr{E}}$, where we wrote $x = (x_1, \ldots, x_d) \in \mathscr{E}$ and $k \cdot x = \sum_{j=1}^d k_j x_j$. Take an arbitrary subset $\Gamma \subset \mathscr{K}_L$ with $|\Gamma| = N$ and an aribtrary $M = -N/2, \ldots, N/2$, and define

$$|\Phi_{\Gamma,M}\rangle := (\hat{S}^-_{\rm tot})^{(N/2)-M}\Big(\prod_{k\in\Gamma} \hat{C}^\dagger_\uparrow(\boldsymbol{\eta}^{(k)})\Big)|\Phi_{\rm vac}\rangle, \tag{11.5.5}$$

which is a state in the ferromagnetic sector with $\hat{S}^{(3)}_{\rm tot}|\Phi_{\Gamma,M}\rangle = M|\Phi_{\Gamma,M}\rangle$. It is then readily verified that

$$\hat{H}_{tJ}|\Phi_{\Gamma,M}\rangle = \Big(\sum_{k\in\Gamma} \varepsilon(k)\Big)|\Phi_{\Gamma,M}\rangle, \tag{11.5.6}$$

[50] For convenience, we here use a different sign convention for the hopping term.

where the single-electron energy eigenstate corresponding to $\boldsymbol{\eta}^{(k)}$ is $\varepsilon(k) = -2\tau \sum_{j=1}^{d} \cos k_j$. Choosing the subset Γ that minimizes the energy $\sum_{k\in\Gamma} \varepsilon(k)$, we obtain the lowest energy states within the ferromagnetic sector. The essential question is whether and when theses lowest energy states also become the global ground states of the t-J model.

For $d = 1$ the situation is simple. We can show that, for any $J > 0$, the ground states are in the ferromagnetic sector when electron number N is odd. The proof is based on a simple application of the Perron–Frobenius theorem. It was Kubo who first applied the Perron–Frobenius theorem to the problem of metallic ferromagnetism in his pioneering work on the double exchange model [22].

Proposition 11.24 (Ferromagnetism in the $d = 1$ ferromagnetic t-J model) *Assume that the dimension is $d = 1$ and the electron number N satisfies $N < L = |\mathscr{E}|$ and is odd. Then the ground states of the t-J model with the Hamiltonian (11.5.4) have total spin $S_{\rm tot} = N/2$, and are non-degenerate apart from the trivial $2S_{\rm tot} + 1 = N + 1$-fold degeneracy.*

The reader might find it odd that the electron number should be odd in the above proposition. In fact if we use open boundary conditions instead of periodic boundary conditions, then the proof works for any electron number N which does not exceed L. Note that, for $N = L$, the model reduces to the ferromagnetic Heisenberg model, whose ground state is ferromagnetic both for even and odd $N = L$.

Proof of Proposition 11.24 The proof is based on an elementary observation, which may be called a rigorous "spin-charge separation" argument. (See [45] and references therein.) We consider a subspace of $\mathscr{H}_N^{\rm hc}$ which consists of states with $S_{\rm tot}^{(3)} = 1/2$. Note that Theorem A.17 in p. 473 guarantees that any eigenstate of $\hat{H}_{tJ}$ has its copy in this subspace. The subspace is spanned by the basis states (9.2.35) such that $\sum_{j=1}^{N} \sigma_j = 1/2$. (Here we identify $\uparrow$ and $\downarrow$ with $1/2$ and $-1/2$, respectively.) Without loss of generality, we can assume $1 \le x_1 < x_2 < \cdots < x_N \le L$, where we wrote $\mathscr{E} = \{1, 2, \ldots, L\}$.

We first claim that all the matrix elements of $\hat{H}_{tJ}$ in the present basis are nonpositive. For the hopping term, this is obvious since there is no exchange in electron ordering and one does not have to worry about fermion signs.[51] For the exchange term, the nonpositivity is easily verified by using the identity $\hat{\boldsymbol{S}}_x \cdot \hat{\boldsymbol{S}}_{x+1} = (\hat{S}_x^+ \hat{S}_{x+1}^- + \hat{S}_x^- \hat{S}_{x+1}^+)/2 + \hat{S}_x^{(3)} \hat{S}_{x+1}^{(3)}$. It is also verified that all the basis states are connected via nonvanishing negative matrix elements of $\hat{H}_{tJ}$. Note that the existence of the exchange term is essential for the connectivity. Therefore we can readily apply the Perron–Frobenius theorem (Theorem A.18 in p. 475) to conclude that the ground state $|\Phi_{\rm GS}\rangle$ is unique (in this sector), and it is a linear combination of all the basis states with positive coefficients. This means that the ground state has nonzero overlap

[51] A hop between sites 1 and L is exceptional, but it does not produce any sign if N is odd. When N is even, such a hop generates the "wrong" sign for the Perron–Frobenius theorem.

with the ferromagnetic state (2.4.11) (with a proper identification of sites), and hence has $S_{\rm tot} = N/2$. ∎

Unfortunately, Proposition 11.24 and its proof hardly shed light on the nature of the ground states of the higher dimensional t-J model. The one-dimensional problem is very special in the sense that no exchanges (in the spin configuration) are caused by hopping of electrons. This means that the ground states for $J = 0$ can have any values of $S_{\rm tot}$, from $1/2$ to $N/2$. This enormous degeneracy is lifted by infinitesimal $J > 0$, which produces ferromagnetism.

In higher dimensional lattices (or even in slightly more complicated one-dimensional systems, e.g., those with next-nearest neighbor hopping or on a ladder), the problem is essentially different since highly nontrivial exchange processes already take place when $J = 0$. There is no guarantee that the ground states are ferromagnetic when J is positive. In fact it is likely that, when the electron density is very low, the model in two or higher dimensions behaves essentially as an non-interacting system and the ground states exhibit Pauli paramagnetism (see Sect. 9.3.2). We believe that it is not very difficult to extend Theorem 11.4 in p. 376 to the t-J model to prove that the ground states never exhibit saturated ferromagnetism for any $J > 0$ provided that $d > 2$ and the density is sufficiently low.[52]

We of course believe that the ferromagnetic t-J model in higher dimensions also exhibits ferromagnetism when the ferromagnetic coupling $J/|t|$ is sufficiently large and the density N/L^d is sufficiently close to one. But nothing has been rigorously shown as far as we know, and we have no idea at all about how such a result can be proved, even in the singular limit $J \uparrow \infty$. Although "establishing ferromagnetism in the ferromagnetic t-J models" might sound like a tautology at first glance, it is indeed a very difficult problem, whose solution should shed light on various aspects of strongly interacting itinerant electron systems.

A version of the Hubbard model related to the t-J model Let us now turn to the Hubbard model. It would be desirable if we could treat, for example, the nearly-flat-band model studied in Sect. 11.4.3 with electron number N strictly less than $L^d = |\mathscr{E}|$. The model is of course artificial, but is probably sufficiently simple as a theoretical toy model. Unfortunately this problem is very difficult, probably much more difficult than one might expect. For the moment we cannot prove any nontrivial statements about the model.

We here study a more complicated version of the Hubbard model proposed by Tanaka and Tasaki [64], for which an exact equivalence to the t-J model can be proved in a certain limit. By using the equivalence we can establish the emergence of ferromagnetism in the ground state, provided that we restrict ourselves to the one-dimensional model.

Let us introduce the model in any dimension. Exactly as in Sect. 11.3.1, we denote by $\mathscr{E}$ the d-dimensional $L \times L$ hypercubic lattice, and by $\mathscr{I}$ the set of sites taken at the middle of bonds in $\mathscr{E}$. See Fig. 11.10. Here we follow Sekizawa [51], and consider

[52] Instead of the Gutzwiller projection, we use the projection operator on states in which an up-spin electron and a down-spin electron never come to neighboring sites.

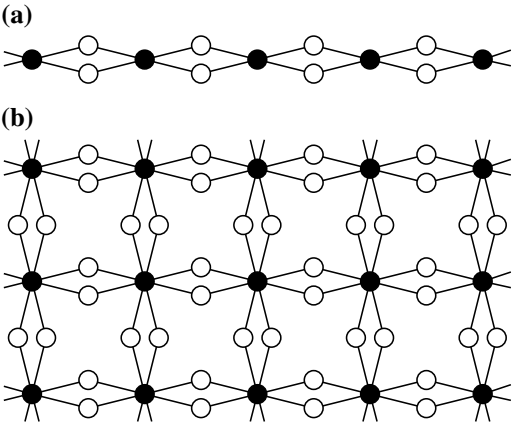

Fig. 11.24 The decorated hypercubic lattice used to define the model studied in the present section. Compared with the decorated hypercubic lattice in Fig. 11.10, the internal sites (i.e., white dots) are duplicated. The present lattice was studied by Sekizawa, who considered a version of flat-band ferromagnetism [51] ()

a decorated hypercubic lattice $\Lambda = \mathscr{E} \cup \mathscr{I} \times \{1, 2\}$. Compared with the decorated hypercubic lattice in Sect. 11.3.1, which is $\mathscr{E} \cup \mathscr{I}$, the sites in $\mathscr{I}$ are duplicated. See Fig. 11.24. We denote sites in $\mathscr{E}$ again as $p, q, \ldots$, and sites in $\mathscr{I} \times \{1, 2\}$ as $(u, 1)$ and $(u, 2)$ with $u \in \mathscr{I}$.

We shall again define localized states $\boldsymbol{\alpha}_p$ and $\boldsymbol{\beta}_{(u,\zeta)}$ on the present decorated lattice. For $j = 1, \ldots, d$, we denote by $\boldsymbol{b}_j = (0, \ldots, 0, \frac{1}{2}, 0, \ldots, 0)$ the half of the unit vector in the jth direction. For $p \in \mathscr{E}$, we define $\boldsymbol{\alpha}_p = (\alpha_p(x))_{x\in\Lambda}$ by

$$\alpha_p(x) = \begin{cases} 1 & \text{if } x = p, \\ \nu & \text{if } x = (p + \boldsymbol{b}_j, 1), \\ -\nu & \text{if } x = (p + \boldsymbol{b}_j, 2) \text{ or } (p - \boldsymbol{b}_j, \zeta), \\ 0 & \text{otherwise,} \end{cases} \tag{11.5.7}$$

where $j = 1, \ldots, d$ and $\zeta = 1, 2$. Note that $p \pm \boldsymbol{b}_j$ is a site in $\mathscr{I}$ for any $j = 1, \ldots, d$. For $u \in \mathscr{I}$ and $\zeta = 1, 2$, we define $\boldsymbol{\beta}_{(u,\zeta)} = (\beta_{(u,\zeta)}(x))_{x\in\Lambda}$ by

$$\beta_{(u,1)}(x) = \begin{cases} 1 & \text{if } x = u, \\ \nu & \text{if } x = u + \boldsymbol{b}_j, \\ -\nu & \text{if } x = u - \boldsymbol{b}_j, \\ 0 & \text{otherwise,} \end{cases} \tag{11.5.8}$$

and

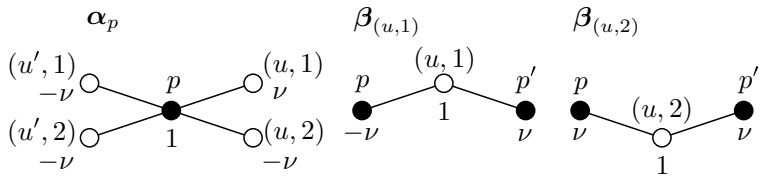

Fig. 11.25 Nonzero components of the localized states $\boldsymbol{\alpha}_p$, $\boldsymbol{\beta}_{(u,1)}$, and $\boldsymbol{\beta}_{(u,2)}$ for $d = 1$. The lattice sites are related by $u' = p - \frac{1}{2}$, $u = p + \frac{1}{2}$, and $p' = p + 1$. The particular choice of the signs of the components of $\boldsymbol{\alpha}_p$ ensures that these states with different p are orthogonal as in (11.5.11) ()

$$\beta_{(u,2)}(x) = \begin{cases} 1 & \text{if } x = u, \\ \nu & \text{if } x = u \pm \boldsymbol{b}_j, \\ 0 & \text{otherwise,} \end{cases} \tag{11.5.9}$$

where j is the unique index such that $u \pm \boldsymbol{b}_j \in \mathscr{E}$. Here $\nu > 0$ is a parameter of the model. See Fig. 11.25. It is not hard to show that these states are linearly independent and hence they altogether form a basis of the single-electron Hilbert space $\mathfrak{h}$.

We define fermion operators corresponding to these localized states by

$$\hat{a}_{p,\sigma} := \hat{C}_\sigma(\boldsymbol{\alpha}_p), \quad \hat{b}_{(u,\zeta),\sigma} := \hat{C}_\sigma(\boldsymbol{\beta}_{(u,\zeta)}), \tag{11.5.10}$$

for any $p \in \mathscr{E}$, $u \in \mathscr{I}$, $\zeta = 1, 2$, and $\sigma = \uparrow, \downarrow$. Then from the definition (11.5.7), one finds that the $\hat{a}$ operators satisfy

$$\{\hat{a}_{p,\sigma}, \hat{a}^\dagger_{q,\tau}\} = (1 + 4dv^2)\, \delta_{p,q}\, \delta_{\sigma,\tau}, \tag{11.5.11}$$

for any $p, q \in \mathscr{E}$ and $\sigma, \tau = \uparrow, \downarrow$, which, apart from the normalization, is the same as the basic anticommutation relation (9.2.28) for fermion operators. This fact makes the analysis of the present model a lot easier than that of the previous (similar) models. The main reason for the introduction of the duplicated internal sites was to guarantee the orthogonality. It is also easy to find, as in the previous models, that

$$\{\hat{b}_{(u,\zeta),\sigma}, \hat{a}^\dagger_{p,\tau}\} = 0, \tag{11.5.12}$$

for any $u \in \mathscr{I}$, $\zeta = 1, 2$, $p \in \mathscr{E}$, and $\sigma, \tau = \uparrow, \downarrow$.

We consider the Hubbard model on Λ with the Hamiltonian $\hat{H} = \hat{H}_{\text{hop}} + \hat{H}_{\text{int}}$, where the interaction Hamiltonian is

$$\hat{H}_{\text{int}} = U \sum_{x \in \Lambda} \hat{n}_{x,\uparrow} \hat{n}_{x,\downarrow}, \tag{11.5.13}$$

which is (9.3.29), and the hopping Hamiltonian is

$$\hat{H}_{\rm hop} = t \sum_{\substack{u\in\mathscr{I},\,\zeta=1,2\\ \sigma=\uparrow,\downarrow}} \hat{b}^\dagger_{(u,\zeta),\sigma}\hat{b}_{(u,\zeta),\sigma} - s \sum_{\substack{p,q\in\mathscr{E}\\ (|p-q|=1)\\ \sigma=\uparrow,\downarrow}} \hat{a}^\dagger_{p,\sigma}\hat{a}_{q,\sigma}\,, \tag{11.5.14}$$

where $s \in \mathbb{R}\backslash\{0\}$ and $t > 0$. Note that this is similar to but is different from the hopping Hamiltonian (11.4.38) of the non-singular model studied in Sect. 11.4.3. Since $\hat{a}$ operators in this model satisfy the standard anticommutation relations (11.5.11), the diagonal term $\hat{a}^\dagger_{p,\sigma}\hat{a}_{p,\sigma}$ alone does not induce any electron hopping. We thus included the off-diagonal terms $\hat{a}^\dagger_{p,\sigma}\hat{a}_{q,\sigma}$ to make the band dispersive. We should note that the hopping Hamiltonian (11.5.14) becomes quite complicated when expressed in the standard form (9.3.17).

Exactly as in Tasaki's flat-band model (Sect. 11.3.1) and the corresponding perturbed models (Sect. 11.4), the single-electron energy spectrum of the present model consists of the lowest band spanned by the $\boldsymbol{\alpha}$-states and higher bands spanned by the $\boldsymbol{\beta}$-states. The lowest band thus contains L^d states. Recalling that the model with electron number $N = L^d$, which corresponds to the half-filling of the lowest band, should describe an insulator, we here concentrate on the case where N is strictly less than L^d (or, more precisely, the density N/L^d is strictly less than one). Unfortunately none of the techniques developed for the flat-band models or the nearly-flat band models apply to the present model with $N \neq L^d$. The only way (that we know of for the moment) to proceed is to consider the model in the limit where both the band gap and the Coulomb interaction become infinitely large, i.e., $t, U \uparrow \infty$.

Fix the electron number $N < L^d$, and let the finite-energy subspace $\mathscr{H}_0$ be a collection of states $|\Phi\rangle$ such that $\lim_{t,U\uparrow\infty}\langle\Phi|\hat{H}|\Phi\rangle < \infty$. (Note that the state $|\Phi\rangle$ is independent of t or U.) The Theorem A.12 (p. 470) implies that tha model in the limit $t, U \uparrow \infty$ is precisely described by the effective Hamiltonian $\hat{H}_{\rm eff} = \hat{P}_0\hat{H}\hat{P}_0$, where $\hat{P}_0$ is the projection operator onto $\mathscr{H}_0$. We also find that a state $|\Phi\rangle$ belongs to $\mathscr{H}_0$ if and only if $\hat{b}^\dagger_{(u,\zeta),\sigma}\hat{b}_{(u,\zeta),\sigma}|\Phi\rangle = 0$ for any $u \in \mathscr{I}$, $\zeta = 1, 2$, and $\sigma = \uparrow, \downarrow$, and $\hat{n}_{x,\uparrow}\hat{n}_{x,\downarrow}|\Phi\rangle = 0$ for all $x \in \Lambda$. Lemma A.11 (p. 469) further implies that these conditions are equivalent to

$$\hat{b}_{(u,\zeta),\sigma}|\Phi\rangle = 0, \tag{11.5.15}$$

for any $u \in \mathscr{I}$, $\zeta = 1, 2$, and $\sigma = \uparrow, \downarrow$, and

$$\hat{c}_{x,\downarrow}\hat{c}_{x,\uparrow}|\Phi\rangle = 0, \tag{11.5.16}$$

for any $x \in \Lambda$. Note that these finite-energy conditions are exactly the same as the zero-energy conditions (11.3.11), (11.3.12), which played central roles in flat-band ferromagnetism. We shall therefore be sketchy, assuming that the reader has gone through the proof of Theorem 11.11. (In fact the first half of the following poof is almost identical to the proof of Lemma 11.23 in p. 434.)

Since $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$ states span the single-electron Hilbert space $\mathfrak{h}$, we can express any state by using $\hat{a}^\dagger$ and $\hat{b}^\dagger$ operators as in (11.3.13). Then from the condition (11.5.15) we see that any finite-energy state must be written only in terms of the $\hat{a}^\dagger$ operators, exactly as in (11.3.14). Next, by using the condition (11.5.16) for $x \in \mathscr{E}$, we find that

there can be no double occupancies in $\hat{a}^\dagger$ states. Therefore any finite-energy state $|\Phi\rangle$ is expanded as

$$|\Phi\rangle = \sum_{\substack{A_\uparrow, A_\downarrow \subset \mathscr{E} \\ (A_\uparrow \cap A_\downarrow = \emptyset,\, |A_\uparrow| + |A_\downarrow| = N)}} c(A_\uparrow, A_\downarrow) \Big(\prod_{p \in A_\uparrow} \hat{a}^\dagger_{p,\uparrow} \Big) \Big(\prod_{p \in A_\downarrow} \hat{a}^\dagger_{p,\downarrow} \Big) |\Phi_{\mathrm{vac}}\rangle, \qquad (11.5.17)$$

with arbitrary coefficients $c(A_\uparrow, A_\downarrow) \in \mathbb{C}$. The model has thus reduced to an electron model on $\mathscr{E}$ with hard core repulsion. The effective Hamiltonian is of course given by

$$\hat{H}_{\mathrm{eff}} = \hat{P}_0 \hat{H} \hat{P}_0 = -s \sum_{\substack{p,q \in \mathscr{E} \\ (|p-q|=1) \\ \sigma = \uparrow, \downarrow}} \hat{P}_0\, \hat{a}^\dagger_{p,\sigma} \hat{a}_{q,\sigma}\, \hat{P}_0, \qquad (11.5.18)$$

which is the simple nearest neighbor hopping Hamiltonian on $\mathscr{E}$.

It only remains to take into account the condition (11.5.16) for x in $\mathscr{I} \times \{1, 2\}$. Exactly as in the proof of Tasaki's flat-band ferromagnetism (see the part "Ferromagnetic exchange interaction" in the proof of Theorem 11.11), we get ferromagnetic exchange interaction from these conditions. In this case we see that the coefficients $c(A_\uparrow, A_\downarrow)$ are such that the spins of any pair of electrons occupying $\hat{a}^\dagger_p$ and $\hat{a}^\dagger_q$ states with $|p - q| = 1$ are coupled ferromagnetically. This means that all the spins in each connected component of $A_\uparrow \cup A_\downarrow$ (which is the set of occupied sites) must be coupled to have the maximum total spin. (But note that this fact does not imply that $|\Phi\rangle$ exhibits ferromagnetism. In general $A_\uparrow \cup A_\downarrow$ consists of several connected components.)

Now inspection shows that one gets exactly the same finite-energy conditions in the $J \uparrow \infty$ limit of the t-J model (11.5.4) on the same lattice $\mathscr{E}$ with the same electron number N. This implies the desired equivalence of the Hubbard model and the t-J model.

Lemma 11.25 *The limit $t, U \uparrow \infty$ of the above Hubbard model with electron number $N \le L^d$ is equivalent to the $J \uparrow \infty$ limit of the t-J model (11.5.4) with the same electron number N and the hopping amplitude $\tau = (1 + 4dv^2)s$.*

The equivalence does not lead to any conclusions about the Hubbard model unless we know something about the t-J model. For the one-dimensional model, we get the following from Proposition 11.24 (p. 443) and Lemma 11.25.

Theorem 11.26 (Metallic ferromagnetism in the $d = 1$ Hubbard model)
Consider the above Hubbard model in one-dimension, and let the electron number N be odd and satisfy $N \le L$. Then in the limit $t, U \uparrow \infty$, the ground states of the model have total spin $S_{\mathrm{tot}} = N/2$, and are non-degenerate apart from the trivial $2S_{\mathrm{tot}} + 1 = N + 1$-fold degeneracy.

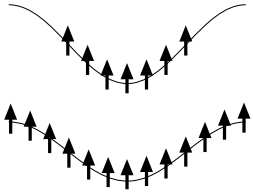

Fig. 11.26 A metallic ground state of the model by Tanaka and Tasaki. There are two dispersive bands, which we call the a-band and the b-band. One gets ferromagnetic ground states in which the a-band is fully filled and the b-band is partially filled (© Hal Tasaki 2020. All Rights Reserved)

When N/L^d is strictly less than one, the ground states describe metallic states since the lowest band is partially filled.[53] We have thus obtained a rigorous example of metallic ferromagnetism in the Hubbard model on the one-dimensional decorated lattice. We note that this result is a variant of earlier results by Kubo [22] and by Tanaka and Idogaki [61]. The proof is based on the Perron–Frobenius argument, which works only in simple one-dimensional systems.

The model and the theorem of Tanaka and Tasaki We finally discuss the work by Tanaka and Tasaki [63], which established that a certain version of (rather complicated) Hubbard model in any dimensions exhibits metallic ferromagnetism. At the time of writing, this is still the only rigorous example of Hubbard model which becomes a metallic ferromagnet in two or higher dimensions. As the reader can guess from Figs. 11.27 and 11.28, the model is artificial and complicated. We must note however that this is a fruit of our serious effort to construct the simplest possible Hubbard model in which we can rigorously control metallic ferromagnetism. It may be the case that we had gone too much into the mathematical game of designing artificial examples to prove some nontrivial phenomenon "for the first time".

Before introducing the model, we briefly discuss the nature of metallic ferromagnetism that we obtain in the present model. The model has a rather complicated band structure with two lowest dispersive bands, which we call the a-band and the b-band, and other higher bands. We take the limit in which both the Coulomb interaction U and the band gap separating the two lowest bands and the other higher bands become infinitely large. We consider the electron number which is larger than the half-filling of the lowest a-band but is smaller than the half-filling of both the a and b-bands. Then, in a suitable range of parameters, we get ferromagnetic ground states in which the a-band is fully filled and the b-band is partially filled as in Fig. 11.26. This certainly corresponds to a metallic state. (See footnote 47 above.) Very roughly speaking, in a ground state the present model, electrons filling the a-band first form a ferromagnetic state according to the mechanism familiar in the flat-band and nearly-flat band ferromagnetism, and then electrons in the b-band join the ferromagnetic state because of exchange interaction between the a-band and the b-bands.[54]

[53] Recall that the ground states can be expressed as Slater determinant states as in (11.5.5).

[54] This explanation should not be taken too literally since all electrons are exactly identical, and a ground state should be determined once and for all to minimize the total energy.

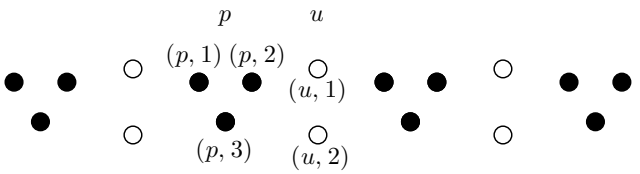

Fig. 11.27 Sites in the one-dimensional decorated lattice $\Lambda = \mathscr{E} \times \{1, 2, 3\} \cup \mathscr{I} \times \{1, 2\}$. Here $p \in \mathscr{E}$ is an integer and $u = p + \frac{1}{2} \in \mathscr{I}$ (© Hal Tasaki 2020. All Rights Reserved)

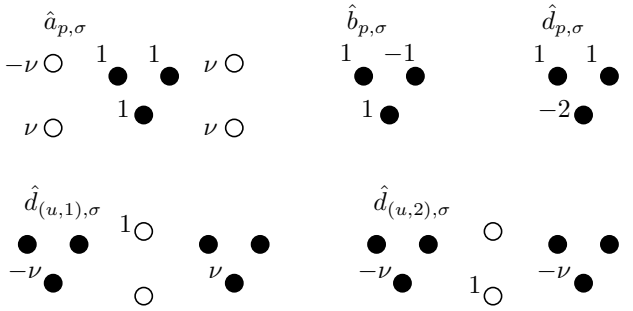

Fig. 11.28 Nonzero components of the fermion operators (11.5.19), (11.5.20), (11.5.21), and (11.5.22) for the one-dimensional model (© Hal Tasaki 2020. All Rights Reserved)

We again denote by $\mathscr{E}$ the d-dimensional $L \times L$ hypercubic lattice, and by $\mathscr{I}$ the corresponding lattice consisting of sites in the middle of bonds in $\mathscr{E}$. This time we consider a Hubbard model on a (considerably) decorated lattice $\Lambda = \mathscr{E} \times \{1, 2, 3\} \cup \mathscr{I} \times \{1, 2\}$. Now, sites in $\mathscr{I}$ are duplicated as before, and sites in $\mathscr{E}$ are triplicated. We denote lattice sites as $(p, 1)$, $(p, 2)$, $(p, 3)$, $(u, 1)$, and $(u, 2)$ with $p \in \mathscr{E}$ and $u \in \mathscr{I}$. See Fig. 11.27.

Let us define special fermion operators. We again let $\boldsymbol{b}_j = (0, \dots, 0, \frac{1}{2}, 0, \dots, 0)$ be the half of the unit vector in the jth direction, where $j = 1, \dots, d$. For any $p \in \mathscr{E}$, $\zeta = 1, 2, 3$ and $\sigma = \uparrow, \downarrow$, we define

$$\hat{a}_{p,\sigma} = \frac{1}{\sqrt{3 + 4dv^2}} \Big[\sum_{\zeta=1}^{3} \hat{c}_{(p,\zeta),\sigma} + v \sum_{\substack{j=1,\dots,d \\ \zeta=1,2}} \big\{ \hat{c}_{(p+\boldsymbol{b}_j,\zeta),\sigma} + (-1)^{\zeta} \hat{c}_{(p-\boldsymbol{b}_j,\zeta),\sigma} \big\} \Big], \tag{11.5.19}$$

$$\hat{b}_{p,\sigma} = \frac{1}{\sqrt{2}} \big\{ \hat{c}_{(p,1),\sigma} - \hat{c}_{(p,2),\sigma} \big\}, \tag{11.5.20}$$

$$\hat{d}_{p,\sigma} = \hat{c}_{(p,1),\sigma} + \hat{c}_{(p,2),\sigma} - 2\hat{c}_{(p,3),\sigma}, \tag{11.5.21}$$

and for any $u \in \mathscr{I}$, $\zeta = 1, 2$, and $\sigma = \uparrow, \downarrow$, we define

$$\hat{d}_{(u,\zeta),\sigma} = \hat{c}_{(u,\zeta),\sigma} - v\big\{\hat{c}_{(u-\boldsymbol{b}_j,3),\sigma} + (-1)^{\zeta}\,\hat{c}_{(u+\boldsymbol{b}_j,3),\sigma}\big\}, \tag{11.5.22}$$

where j is the unique index such that $u \pm \boldsymbol{b}_j \in \mathscr{E}$. Again $v > 0$ is a model parameter. See Fig. 11.28. As in the previous models, one can represent any state of the system by using the $\hat{a}^\dagger$, $\hat{b}^\dagger$, and $\hat{d}^\dagger$ operators. From (11.5.19) and (11.5.20), we see that the $\hat{a}$ and $\hat{b}$ operators satisfy the standard anticommutation relations

$$\{\hat{a}_{p,\sigma}, \hat{a}^\dagger_{q,\tau}\} = \delta_{p,q}\,\delta_{\sigma,\tau}, \quad \{\hat{b}_{p,\sigma}, \hat{b}^\dagger_{q,\tau}\} = \delta_{p,q}\,\delta_{\sigma,\tau}, \tag{11.5.23}$$

for any $p, q \in \mathscr{E}$ and $\sigma, \tau = \uparrow, \downarrow$. We also find that $\{\hat{b}, \hat{a}^\dagger\} = 0$, $\{\hat{d}, \hat{a}^\dagger\} = 0$, and $\{\hat{d}, \hat{b}^\dagger\} = 0$ for any combinations of indices.

We consider the Hubbard model on Λ with the Hamiltonian $\hat{H} = \hat{H}_{\mathrm{hop}} + \hat{H}_{\mathrm{int}}$, where the interaction Hamiltonian is the standard (11.5.13) or (9.3.29), and the hopping Hamiltonian is

$$\begin{aligned}\hat{H}_{\mathrm{hop}} = &\sum_{\substack{p,q\in\mathscr{E}\\(|p-q|=1)\\\sigma=\uparrow,\downarrow}} \big\{-s\,\hat{a}^\dagger_{p,\sigma}\hat{a}_{q,\sigma} - t\,\hat{b}^\dagger_{p,\sigma}\hat{b}_{q,\sigma}\big\} + u_1 \sum_{\substack{p\in\mathscr{E}\\\sigma=\uparrow,\downarrow}} \hat{b}^\dagger_{p,\sigma}\hat{b}_{p,\sigma}\\ &+ u_2\Bigg\{\sum_{\substack{p\in\mathscr{E}\\\sigma=\uparrow,\downarrow}} \hat{d}^\dagger_{p,\sigma}\hat{d}_{p,\sigma} + \sum_{\substack{u\in\mathscr{I},\,\zeta=1,2\\\sigma=\uparrow,\downarrow}} \hat{d}^\dagger_{(u,\zeta),\sigma}\hat{d}_{(u,\zeta),\sigma}\Bigg\},\end{aligned} \tag{11.5.24}$$

where $s, t, u_1, u_2 \in \mathbb{R}$ are model parameters. From the above anticommutation relations, we see that $\hat{a}$-states and $\hat{b}$-states form separate bands with dispersion relations $\varepsilon_a(k) = -2s\sum_{j=1}^d \cos(k_j)$ and $\varepsilon_b(k) = u_1 - 2t\sum_{j=1}^d \cos(k_j)$. We take the limit $u_2 \uparrow \infty$, in which the energies of the other bands formed by $\hat{d}^\dagger$-states become infinite. Then any finite-energy state is written only in terms of $\hat{a}^\dagger$ and $\hat{b}^\dagger$ operators. From (11.5.19) and (11.5.20) (and also from Fig. 11.28) one finds that there should be a ferromagnetic exchange interaction between neighboring $\hat{a}^\dagger$ states and also between an $\hat{a}^\dagger$ state and a $\hat{b}^\dagger$ state sharing the same p. It is then likely that the ferromagnetic state as depicted in Fig. 11.26 emerges. In fact we have the following.

Theorem 11.27 *Let the dimension $d = 1, 2, 3, \ldots$ be arbitrary and suppose that the electron number N satisfies $L^d \le N \le 2L^d$, and $u_1 > 2d(|s| + 2|t|)$. Then, in the limit $u_2, U \uparrow \infty$, the ground states of the above model exhibit ferromagnetism in the sense that they have the maximum possible total spin $S_{\mathrm{tot}} = N/2$.*

See the original paper [63] for the proof. The ground states are certainly metallic when N/L^d is strictly larger than 1 and strictly less than 2.

Given the simplicity of the picture of the ground states, one might expect that the theorem can be proved (with some effort) for finite but sufficiently large u_2 and U, as we have done for the insulating model in Sect. 11.4.3. But, as far as we

understand, there is no hope of extending the proof to finite u_2 or U.[55] The treatment of models with a partially filled band seems to be essentially different from models with filled bands.[56] The proof of Theorem 11.27 in [63] is not long and does not use any advanced techniques than the variational principle. We nevertheless warn the reader that the proof is quite technical and difficult; we had to solve extremely complicated mathematical puzzles in order to justify some "physically plausible" facts. It seems that we still lack proper mathematical techniques as well as physical ideas for treating metallic systems.

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[55] Of course, by continuity, one can show that the ground states are ferromagnetic for sufficiently large u_2 and U for each L. But we do not have any estimates that are independent of L.

[56] The biggest difference is that, in insulating systems, ferromagnetic ground states may be expressed in the k-space basis as in (11.5.5) or in the real space basis as in, e.g., (11.3.9). In a metallic system, one only has the former expression.

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Appendix A
Mathematical Appendices

A.1 Dirac Notation

Let us summarize the Dirac notation for quantum mechanics, which is standard in the physics literature, and used throughout the present book. Note that we do not intend here to provide a self-contained introduction to the formalism of quantum mechanics.

States We consider a finite dimensional Hilbert space $\mathscr{H}$, whose elements, i.e., quantum mechanical states, are denoted as $|\Phi\rangle, |\Psi\rangle, \ldots$ (and pronounced as "Phi-ket", "ket-Phi" etc.). For any $|\Phi\rangle, |\Psi\rangle \in \mathscr{H}$ and $\alpha, \beta \in \mathbb{C}$, one has $\alpha|\Phi\rangle + \beta|\Psi\rangle \in \mathscr{H}$. It is convenient to (fix an orthonormal basis and) identify $\mathscr{H}$ with $\mathbb{C}^D$, and its element with a column vector

$$|\Phi\rangle = \begin{pmatrix} \varphi_1 \\ \varphi_2 \\ \vdots \\ \varphi_D \end{pmatrix}, \tag{A.1.1}$$

where $\varphi_j \in \mathbb{C}$.

For any $|\Phi\rangle, |\Psi\rangle \in \mathscr{H}$, we denote the inner product of $|\Phi\rangle$ and $|\Psi\rangle$ as

$$\langle\Phi|\Psi\rangle := \sum_{j=1}^{D} (\varphi_j)^* \psi_j, \tag{A.1.2}$$

where we wrote $|\Psi\rangle = (\psi_1, \ldots, \psi_D)^{\mathrm{t}}$. The inner product satisfies

$$\langle\Phi|\Psi\rangle = \langle\Psi|\Phi\rangle^*, \tag{A.1.3}$$

and the linearity

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$$\langle \Phi | \big(\alpha |\Psi\rangle + \beta |\Xi\rangle \big) = \alpha \langle \Phi|\Psi\rangle + \beta \langle \Phi|\Xi\rangle, \tag{A.1.4}$$

for any $|\Phi\rangle$, $|\Psi\rangle$, $|\Xi\rangle \in \mathscr{H}$ and $\alpha, \beta \in \mathbb{C}$. The norm of a state $|\Phi\rangle \in \mathscr{H}$, which we write as $\|\Phi\|$ or $\||\Phi\rangle\|$, is defined by

$$\|\Phi\| := \sqrt{\langle \Phi|\Phi\rangle}. \tag{A.1.5}$$

We say that a state $|\Phi\rangle$ is normalized when $\|\Phi\| = 1$.

An orthonormal basis is a set of D states $\{|\Psi_j\rangle\}_{j=1,\ldots,D}$ with the property $\langle \Psi_j|\Psi_k\rangle = \delta_{k,j}$ for any $k, j = 1, \ldots, D$. An arbitrary state $|\Phi\rangle$ is expanded by using an orthonormal basis as $|\Phi\rangle = \sum_{j=1}^{D} \alpha_j |\Psi_j\rangle$, where the coefficients are given by $\alpha_j = \langle \Psi_j|\Phi\rangle$.

The symbol $\langle \Phi|\Psi\rangle$ may be simply understood as expressing the inner product of $|\Phi\rangle$ and $|\Psi\rangle$, but may also be interpreted as the product of the bra-state $\langle \Phi|$ and the ket-state $|\Psi\rangle$. A bra-state is an element of the dual space of $\mathscr{H}$, and is in one-to-one correspondence with a ket-state, an element of $\mathscr{H}$. More precisely the bra-state corresponding to the ket-state (A.1.1) is identified with a row vector

$$\langle \Phi| = (|\Phi\rangle)^\dagger = (\varphi_1^*, \varphi_2^*, \ldots, \varphi_D^*). \tag{A.1.6}$$

Here the conjugation † denotes the one-to-one mapping between the elements of $\mathscr{H}$ and its dual. Then (A.1.2) is consistent with the standard product of a row vector and a column vector. Note that the conjugate of a linear combination of ket-states are given by

$$\big(\alpha|\Phi\rangle + \beta|\Psi\rangle\big)^\dagger = \alpha^* \langle \Phi| + \beta^* \langle \Psi|. \tag{A.1.7}$$

Operators Operators are linear maps from $\mathscr{H}$ to itself. If we make the identification (A.1.1), the operators are nothing but $D \times D$ matrices with complex elements. We denote by $\hat{1}$ the identity operator. For any operators $\hat{A}$ and $\hat{B}$ and $\alpha, \beta \in \mathbb{C}$, the linear combination $\alpha\hat{A} + \beta\hat{B}$ is also an operator, and satisfies

$$(\alpha\hat{A} + \beta\hat{B})|\Phi\rangle = \alpha\hat{A}|\Phi\rangle + \beta\hat{B}|\Phi\rangle, \tag{A.1.8}$$

for any $|\Phi\rangle \in \mathscr{H}$. For any operator $\hat{A}$, its adjoint (or Hermitian conjugate) $\hat{A}^\dagger$ is the unique operator that satisfies

$$\langle \Phi|\hat{A}|\Psi\rangle = \langle \Psi|\hat{A}^\dagger|\Phi\rangle^*, \tag{A.1.9}$$

for any $|\Phi\rangle$, $|\Psi\rangle \in \mathscr{H}$. Let $|\Xi\rangle = \hat{A}|\Psi\rangle$. Then (A.1.3) implies $\langle \Phi|\hat{A}|\Psi\rangle = \langle \Phi|\Xi\rangle = \langle \Xi|\Phi\rangle^*$. Since this should be identical to the right-hand side of (A.1.9) for any $|\Phi\rangle$, we may make an identification $\langle \Xi| = \langle \Psi|\hat{A}^\dagger$, which means

$$(\hat{A}|\Psi\rangle)^\dagger = \langle \Psi|\hat{A}^\dagger, \tag{A.1.10}$$

for any operator $\hat{A}$ and state $|\Psi\rangle \in \mathscr{H}$. It can be then shown that

$$(\hat{A}^\dagger)^\dagger = \hat{A}, \quad (\alpha\hat{A} + \beta\hat{B})^\dagger = \alpha^* \hat{A}^\dagger + \beta^* \hat{B}^\dagger, \quad (\hat{A}\hat{B})^\dagger = \hat{B}^\dagger \hat{A}^\dagger. \tag{A.1.11}$$

By using (A.1.10), one also finds that

$$\|\hat{A}|\Phi\rangle\|^2 = \langle\Phi|\hat{A}^\dagger\hat{A}|\Phi\rangle, \tag{A.1.12}$$

for any operator $\hat{A}$ and $|\Phi\rangle \in \mathscr{H}$.

For any $|\Phi\rangle, |\Psi\rangle \in \mathscr{H}$, we denote by $|\Phi\rangle\langle\Psi|$ the operator which maps an arbitrary state $|\Xi\rangle$ to $\langle\Psi|\Xi\rangle\,|\Phi\rangle$, which means the state $|\Phi\rangle$ multiplied by a complex number $\langle\Psi|\Xi\rangle$. This is quite natural from the interpretation (A.1.1) and (A.1.6) since the Kronecker product of a column vector and a row vector gives a matrix. The action of such an operator is (very conveniently) expressed as

$$\big(|\Phi\rangle\langle\Psi|\big)|\Xi\rangle = |\Phi\rangle\langle\Psi|\Xi\rangle. \tag{A.1.13}$$

In particular if $|\Phi\rangle$ is a normalized state then $|\Phi\rangle\langle\Phi|$ is the projection operator onto $|\Phi\rangle$. A necessary and sufficient condition that D states $|\Psi_1\rangle, \ldots, |\Psi_D\rangle$ form an orthonormal basis is written as

$$\sum_{j=1}^{D} |\Psi_j\rangle\langle\Psi_j| = \hat{1}. \tag{A.1.14}$$

An operator $\hat{A}$ that satisfies $\hat{A} = \hat{A}^\dagger$ is said to be self-adjoint (or Hermitian), and an operator $\hat{U}$ that satisfies $\hat{U}^\dagger\hat{U} = \hat{U}\hat{U}^\dagger = \hat{1}$ is said to be unitary. For any self-adjoint operator $\hat{A}$, there exists an orthonormal basis $\{|\Psi_j\rangle\}_{j=1,\ldots,D}$ such that $\hat{A}|\Psi_j\rangle = a_j|\Psi_j\rangle$ for all $j = 1, \ldots, D$, where $a_j \in \mathbb{R}$ is an eigenvalue of $\hat{A}$. Then the operator $\hat{A}$ admits the spectral decomposition $\hat{A} = \sum_{j=1}^{D} a_j|\Psi_j\rangle\langle\Psi_j|$. Likewise, for any unitary operator $\hat{U}$, there exists an orthonormal basis $\{|\Psi_j\rangle\}_{j=1,\ldots,D}$ such that $\hat{U}|\Psi_j\rangle = u_j|\Psi_j\rangle$ for all $j = 1, \ldots, D$, where $u_j \in \mathbb{C}$ with $|u_j| = 1$ is an eigenvalue of $\hat{U}$. We again have the spectral decomposition $\hat{U} = \sum_{j=1}^{D} u_j|\Psi_j\rangle\langle\Psi_j|$.

Let $\{|\Psi_j\rangle\}_{j=1,\ldots,D}$ be an arbitrary orthonormal basis. Then the trace of any operator $\hat{A}$ is defined by

$$\mathrm{Tr}[\hat{A}] = \sum_{j=1}^{D} \langle\Psi_j|\hat{A}|\Psi_j\rangle. \tag{A.1.15}$$

Recall that the trace has an important property $\mathrm{Tr}[\hat{A}\hat{B}] = \mathrm{Tr}[\hat{B}\hat{A}]$ for any operators $\hat{A}$ and $\hat{B}$.

Transformation of operators Let us make a brief comment on the conventions of unitary transformations of operators.

Let $\hat{U}$ be a unitary operator, and suppose that every state $|\Phi\rangle \in \mathscr{H}$ is transformed to $\hat{U}|\Phi\rangle$. Then the matrix element $\langle\Psi|\hat{A}|\Phi\rangle$ of an operator $\hat{A}$ is transformed to $\langle\Psi|\hat{U}^\dagger\hat{A}\hat{U}|\Phi\rangle$. One gets the same result if the states are unchanged, and every operator $\hat{A}$ is transformed as

$$\hat{A} \;\to\; \hat{U}^\dagger\hat{A}\hat{U}. \tag{A.1.16}$$

This is the most standard convention for the transformation of operators.

To see another convention, suppose that a self-adjoint operator $\hat{A}$ (such as a Hamiltonian) and a state $|\Phi\rangle$ satisfy the eigenvalue equation $\hat{A}|\Phi\rangle = a|\Phi\rangle$. Acted by an arbitrary unitary operator $\hat{U}$, this becomes $\hat{U}\hat{A}\hat{U}^\dagger\hat{U}|\Phi\rangle = a\hat{U}|\Phi\rangle$. Thus we have the same eigenvalue equation $\hat{A}'|\Phi'\rangle = a|\Phi'\rangle$ with $|\Phi'\rangle = \hat{U}|\Phi\rangle$ and $\hat{A}' = \hat{U}\hat{A}\hat{U}^\dagger$. We thus have the second convention

$$\hat{A} \;\to\; \hat{U}\hat{A}\hat{U}^\dagger. \tag{A.1.17}$$

Multiple systems Suppose that there are two quantum mechanical systems with Hilbert spaces $\mathscr{H}_1$ and $\mathscr{H}_2$, whose dimensions are D_1 and D_2, respectively. The Hilbert space of the joint system is given by the tensor product $\mathscr{H}_1 \otimes \mathscr{H}_2$.

The tensor product space $\mathscr{H}_1 \otimes \mathscr{H}_2$ consists of all the states of the form $|\Phi\rangle_1 \otimes |\Psi\rangle_2$ with $|\Phi\rangle_1 \in \mathscr{H}_1$ and $|\Psi\rangle_2 \in \mathscr{H}_2$ and their linear combinations, where we identify states according to linearity $(\alpha|\Phi\rangle_1 + \alpha'|\Phi'\rangle_1) \otimes (\beta|\Psi\rangle_2 + \beta'|\Psi'\rangle_2) = \alpha\beta|\Phi\rangle_1 \otimes |\Psi\rangle_2 + \alpha\beta'|\Phi\rangle_1 \otimes |\Psi'\rangle_2 + \alpha'\beta|\Phi'\rangle_1 \otimes |\Psi\rangle_2 + \alpha'\beta'|\Phi'\rangle_1 \otimes |\Psi'\rangle_2$ for any $|\Phi\rangle_1, |\Phi'\rangle_1 \in \mathscr{H}_1$, $|\Psi\rangle_2, |\Psi'\rangle_2 \in \mathscr{H}_2$ and $\alpha, \alpha', \beta, \beta' \in \mathbb{C}$.

The inner product of $|\Phi\rangle_1 \otimes |\Psi\rangle_2$ and $|\Phi'\rangle_1 \otimes |\Psi'\rangle_2$ is defined to be $\langle\Phi|\Phi'\rangle_1 \langle\Psi|\Psi'\rangle_2$. Then one can define inner products of any pair of states by linearity. Therefore, if $\{|\Phi_j\rangle_1\}_{j=1,\ldots,D_1}$ and $\{|\Psi_k\rangle_2\}_{k=1,\ldots,D_2}$ are orthonormal bases for $\mathscr{H}_1$ and $\mathscr{H}_2$, respectively, then an orthonormal basis of $\mathscr{H}_1 \otimes \mathscr{H}_2$ is given by $\{|\Phi_j\rangle_1 \otimes |\Psi_k\rangle_2\}_{j=1,\ldots,D_1,\, k=1,\ldots,D_2}$. Thus the dimension of $\mathscr{H}_1 \otimes \mathscr{H}_2$ is $D_1 D_2$.

Let $\hat{A}$ and $\hat{B}$ be arbitrary operators on $\mathscr{H}_1$ and $\mathscr{H}_2$, respectively. Their tensor product $\hat{A} \otimes \hat{B}$ is an operator on $\mathscr{H}_1 \otimes \mathscr{H}_2$ whose action is determined by

$$(\hat{A} \otimes \hat{B})|\Phi\rangle_1 \otimes |\Psi\rangle_2 = (\hat{A}|\Phi\rangle_1) \otimes (\hat{B}|\Psi\rangle_2), \tag{A.1.18}$$

and linearity.

We shall freely change the order of tensor products, keeping track of the space to which each state belongs. We can thus write either $|\Phi\rangle_1 \otimes |\Psi\rangle_2$ or $|\Psi\rangle_2 \otimes |\Phi\rangle_1$ to indicate the same state. We sometimes (following physicists' convention) omit the tensor product symbols in states, and simply write $|\Phi\rangle_1|\Psi\rangle_2$ instead of $|\Phi\rangle_1 \otimes |\Psi\rangle_2$.

It should be clear that the above discussion automatically extends to a joint system of more than two systems.

Entanglement and Schmidt decomposition Consider, as above, a quantum system that consists of two parts, and denote its Hilbert space as $\mathscr{H} = \mathscr{H}_1 \otimes \mathscr{H}_2$. A state $|\Xi\rangle \in \mathscr{H}$ is said to be separable if it can be written in a tensor product form as

$|\Xi\rangle = |\Phi\rangle_1 \otimes |\Psi\rangle_2$ with some states $|\Phi\rangle_1 \in \mathscr{H}_1$ and $|\Psi\rangle_2 \in \mathscr{H}_2$. A state $|\Xi\rangle \in \mathscr{H}$ that is not separable is said to be entangled.

A quantitative measure of entanglement is given by entanglement entropy S_{12}. Let $|\Xi\rangle \in \mathscr{H}$ be a normalized state, and define the corresponding reduced density matrices as

$$\hat{\rho}_1 := \mathrm{Tr}_2\big[|\Xi\rangle\langle\Xi|\big], \quad \hat{\rho}_2 := \mathrm{Tr}_1\big[|\Xi\rangle\langle\Xi|\big], \tag{A.1.19}$$

where $\mathrm{Tr}_\nu[\cdots]$ denote trace over $\mathscr{H}_\nu$. Then the entanglement entropy is defined as

$$S_{12} := -\mathrm{Tr}_1[\hat{\rho}_1 \log \hat{\rho}_1] = -\mathrm{Tr}_2[\hat{\rho}_2 \log \hat{\rho}_2]. \tag{A.1.20}$$

One easily finds that $S_{12} = 0$ if $|\Xi\rangle$ is separable.

It is known that an arbitrary normalized state $|\Xi\rangle \in \mathscr{H}$ is written in the Schmidt decomposition form

$$|\Xi\rangle = \sum_{j=1}^{d} q_j |\widetilde{\Phi}_j\rangle_1 \otimes |\widetilde{\Psi}_j\rangle_2, \tag{A.1.21}$$

with d not exceeding $\min\{D_1, D_2\}$, where D_1 and D_2 are the dimensions of $\mathscr{H}_1$ and $\mathscr{H}_2$. Here $\{|\widetilde{\Phi}_1\rangle_1, \ldots, |\widetilde{\Phi}_d\rangle_1\}$ and $\{|\widetilde{\Psi}_1\rangle_2, \ldots, |\widetilde{\Psi}_d\rangle_2\}$ are orthonormal sets of states in $\mathscr{H}_1$ and $\mathscr{H}_2$, respectively, and q_j are constants such that $q_j > 0$ and $\sum_{j=1}^{d} (q_j)^2 = 1$.[1]

Schmidt decomposition is useful for examining entanglement properties of a given state. In particular, we have

$$\hat{\rho}_1 = \sum_{j=1}^{d} (q_j)^2 |\widetilde{\Phi}_j\rangle_{1\,1}\langle\widetilde{\Phi}_j|, \quad \hat{\rho}_2 = \sum_{j=1}^{d} (q_j)^2 |\widetilde{\Psi}_j\rangle_{2\,2}\langle\widetilde{\Psi}_j|, \tag{A.1.22}$$

and hence

$$S_{12} = -\sum_{j=1}^{d} (q_j)^2 \log (q_j)^2. \tag{A.1.23}$$

Note that (A.1.23) is nothing but the Shannon entropy of a classical probability distribution $(p_1, \ldots, p_d)$ with $p_j = (q_j)^2$.

Suppose that $D_1 = D_2$. Then the entanglement entropy (A.1.23) takes the maximum possible value $\log D_1$ when $d = D_1$ and $q_j = 1/\sqrt{D_1}$ for all $j = 1, \ldots, D_1$. A state which has $S_{12} = \log D_1$ is said to be maximally entangled.

Proof of the Decomposition (A.1.21) Take arbitrary orthonormal bases $\{|\Phi_j\rangle_1\}_{j=1,\ldots,D_1}$ and $\{|\Psi_k\rangle_2\}_{k=1,\ldots,D_2}$ of $\mathscr{H}_1$ and $\mathscr{H}_2$, respectively, and expand $|\Xi\rangle$ as

$$|\Xi\rangle = \sum_{j=1}^{D_1} \sum_{k=1}^{D_2} A_{j,k} |\Phi_j\rangle_1 \otimes |\Psi_k\rangle_2, \tag{A.1.24}$$

[1] Sometimes one includes the terms with $q_j = 0$ in (A.1.21).

with coefficients $A_{j,k} \in \mathbb{C}$. We can assume $D_1 = D_2$ without loosing generality. This is because if $D_1 > D_2$, for example, we can add fictitious states $|\Psi_{D_2+1}\rangle_2, \ldots, |\Psi_{D_1}\rangle_2$ to the basis, and set $A_{j,k} = 0$ if $k > D_2$ to formally rewrite (A.1.24) into the same expression with D_2 replaced by D_1.

We then apply the singular value decomposition theorem (Theorem A.20 in p. 477) to the $D_1 \times D_1$ matrix $\mathsf{A} = (A_{j,k})_{j,k=1,\ldots,D_1}$ to find that there are unitary matrices $\mathsf{U} = (U_{j,\ell})_{j,\ell=1,\ldots,D_1}$ and $\mathsf{U} = (U_{k,\ell})_{k,\ell=1,\ldots,D_1}$ such that

$$\mathsf{A} = \mathsf{U} \begin{pmatrix} q_1 & 0 & \cdots & 0 \\ 0 & q_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & q_{D_1} \end{pmatrix} \mathsf{V}^\dagger, \tag{A.1.25}$$

with $q_\ell \geq 0$ for $\ell = 1, \ldots, D_1$, or, equivalently,

$$A_{j,k} = \sum_{\ell=1}^{D_1} U_{j,\ell}\, q_\ell\, (V_{k,\ell})^*. \tag{A.1.26}$$

Substituting this into (A.1.24), we find

$$|\Xi\rangle = \sum_{\ell=1}^{D_1} q_\ell \Big(\sum_{j=1}^{D_1} U_{j,\ell} |\Phi_j\rangle_1 \Big) \otimes \Big(\sum_{k=1}^{D_1} (V_{k,\ell})^* |\Psi_k\rangle_2 \Big) = \sum_{\ell=1}^{D_1} q_\ell |\widetilde{\Phi}_\ell\rangle_1 \otimes |\widetilde{\Psi}_\ell\rangle_2, \tag{A.1.27}$$

with $|\widetilde{\Phi}_\ell\rangle_1 = \sum_{j=1}^{D_1} U_{j,\ell} |\Phi_j\rangle_1$ and $|\widetilde{\Psi}_\ell\rangle_2 = \sum_{k=1}^{D_1} (V_{k,\ell})^* |\Psi_k\rangle_2$. The orthonormality of $\{|\widetilde{\Phi}_\ell\rangle_1\}_{\ell=1,\ldots,D_1}$ and $\{|\widetilde{\Psi}_\ell\rangle_2\}_{\ell=1,\ldots,D_1}$ obviously follows from the unitarity. If necessary we throw away ℓ with $q_\ell = 0$ and relabel the basis states to get (A.1.21). (Then the added states $|\Psi_{D_2+1}\rangle_2, \ldots, |\Psi_{D_1}\rangle_2$ automatically disappear from the final expression.) ∎

A.2 Useful Properties of Operators

We discuss properties of operators used in the book. Some are quite standard and elementary, and some are slightly more advanced. As in Sect. A.1, $\hat{A}$, $\hat{B}$, ... denote operators on the D dimensional Hilbert space $\mathscr{H}$ whose elements are denoted as $|\Phi\rangle$, $|\Psi\rangle$, ...

A.2.1 Commutator and Operator Norm

The commutator of two operators $\hat{A}$ and $\hat{B}$ is defined as

$$[\hat{A}, \hat{B}] := \hat{A}\hat{B} - \hat{B}\hat{A}. \tag{A.2.1}$$

The commutator is clearly linear both in $\hat{A}$ and $\hat{B}$, i.e., $[\hat{A}, \beta\hat{B} + \gamma\hat{C}] = \beta[\hat{A}, \hat{B}] + \gamma[\hat{A}, \hat{C}]$, etc. Easily verifiable relation $[\hat{A}, \hat{B}\hat{C}] = [\hat{A}, \hat{B}]\hat{C} + \hat{B}[\hat{A}, \hat{C}]$, and its generalization

$$[\hat{A}, \hat{B}_1 \cdots \hat{B}_n] = \sum_{j=1}^{n} \hat{B}_1 \cdots \hat{B}_{j-1}[\hat{A}, \hat{B}_j]\hat{B}_{j+1} \cdots \hat{B}_n \tag{A.2.2}$$

are useful.

We define the norm (or the operator norm) of any operator $\hat{A}$ as[2]

$$\|\hat{A}\| := \max_{\substack{|\Phi\rangle \in \mathscr{H} \\ (|\Phi\rangle \neq 0)}} \frac{\|\hat{A}|\Phi\rangle\|}{\|\Phi\|} = \max_{\substack{|\Phi\rangle \in \mathscr{H} \\ (\|\Phi\|=1)}} \|\hat{A}|\Phi\rangle\|. \tag{A.2.3}$$

It readily follows from the definition that, for any $\hat{A}$ and for any unitary operators $\hat{U}$ and $\hat{V}$,

$$\|\hat{U}\hat{A}\hat{V}\| = \|\hat{A}\|. \tag{A.2.4}$$

It holds, for any operators $\hat{A}$ and $\hat{B}$, that

$$\|\hat{A} + \hat{B}\| \leq \|\hat{A}\| + \|\hat{B}\|, \tag{A.2.5}$$

and

$$\|\hat{A}\hat{B}\| \leq \|\hat{A}\|\|\hat{B}\|. \tag{A.2.6}$$

Proof By using the triangle inequality for state norm $\||\Phi\rangle + |\Psi\rangle\| \leq \|\Phi\| + \|\Psi\|$, we see

$$\begin{aligned} \|\hat{A} + \hat{B}\| &= \max_{\substack{|\Phi\rangle \in \mathscr{H} \\ (\|\Phi\|=1)}} \|(\hat{A} + \hat{B})|\Phi\rangle\| \leq \max_{\substack{|\Phi\rangle \in \mathscr{H} \\ (\|\Phi\|=1)}} \left\{\|\hat{A}|\Phi\rangle\| + \|\hat{B}|\Phi\rangle\|\right\} \\ &\leq \max_{\substack{|\Phi\rangle \in \mathscr{H} \\ (\|\Phi\|=1)}} \|\hat{A}|\Phi\rangle\| + \max_{\substack{|\Phi\rangle \in \mathscr{H} \\ (\|\Phi\|=1)}} \|\hat{B}|\Phi\rangle\| = \|\hat{A}\| + \|\hat{B}\|, \end{aligned} \tag{A.2.7}$$

which is (A.2.5). From the definition, we find

$$\frac{\|\hat{A}\hat{B}|\Phi\rangle\|}{\||\Phi\rangle\|} = \frac{\|\hat{A}\hat{B}|\Phi\rangle\|}{\|\hat{B}|\Phi\rangle\|} \frac{\|\hat{B}|\Phi\rangle\|}{\||\Phi\rangle\|} \leq \|\hat{A}\|\|\hat{B}\|. \tag{A.2.8}$$

We then get (A.2.6) by taking maximum over $|\Phi\rangle$. ∎

[2]It is standard to use sup (supremum) in the definition, but we can safely use max here since the maximum always exists in a finite dimensional Hilbert space (whose unit sphere is compact).

It is also useful to characterize the operator norm (A.2.3) as

$$\|\hat{A}\| = \max_{\substack{|\Phi\rangle, |\Psi\rangle \in \mathscr{H} \\ (\||\Phi\rangle\| = \||\Psi\rangle\| = 1)}} \left|\langle \Psi | \hat{A} | \Phi \rangle\right|. \tag{A.2.9}$$

Proof Note for any state $|\Xi\rangle$ that $\|\Xi\| = \max_{(\||\Psi\rangle\|=1)} \left|\langle \Psi | \Xi \rangle\right|$. Thus for any $|\Phi\rangle \in \mathscr{H}$ such that $\|\Phi\| = 1$, we have

$$\|\hat{A}|\Phi\rangle\| = \max_{\substack{|\Psi\rangle \in \mathscr{H} \\ (\||\Psi\rangle\| = 1)}} \left|\langle \Psi | \hat{A} | \Phi \rangle\right|. \tag{A.2.10}$$

Then we get (A.2.9) from (A.2.3). ∎

Since $\langle \Psi | \hat{A}^\dagger | \Phi \rangle = \langle \Phi | \hat{A} | \Psi \rangle^*$, (A.2.9) implies

$$\|\hat{A}^\dagger\| = \|\hat{A}\|. \tag{A.2.11}$$

It also follows from (A.2.9) that[3]

$$\left|\langle \Phi | \hat{A} | \Phi \rangle\right| \le \|\hat{A}\| \, \langle \Phi | \Phi \rangle, \tag{A.2.12}$$

for any $|\Phi\rangle \in \mathscr{H}$. For any operators $\hat{A}$ and $\hat{X}$, it holds that

$$\left|\mathrm{Tr}[\hat{X}^\dagger \hat{A} \hat{X}]\right| \le \|\hat{A}\| \, \mathrm{Tr}[\hat{X}^\dagger \hat{X}]. \tag{A.2.13}$$

Proof We choose an arbitrary orthonormal basis $\{|\Psi_j\rangle\}_{j=1,\dots,D}$, and observe that

$$\left|\mathrm{Tr}[\hat{X}^\dagger \hat{A} \hat{X}]\right| \le \sum_{j=1}^{D} \left|\langle \Psi_j | \hat{X}^\dagger \hat{A} \hat{X} | \Psi_j \rangle\right| \le \sum_{j=1}^{D} \|\hat{A}\| \langle \Psi_j | \hat{X}^\dagger \hat{X} | \Psi_j \rangle = \|\hat{A}\| \, \mathrm{Tr}[\hat{X}^\dagger \hat{X}], \tag{A.2.14}$$

where we used (A.2.12), and noted that $\langle \Psi_j | \hat{X}^\dagger \hat{X} | \Psi_j \rangle = \|\hat{X}|\Psi_j\rangle\|^2 \ge 0$. ∎

It is useful to note that for any self-adjoint operator $\hat{A}$ with eigenvalues $\lambda_1, \dots, \lambda_D$, the definition (A.2.3) readily implies

$$\|\hat{A}\| = \max\{|\lambda_1|, \dots, |\lambda_D|\}. \tag{A.2.15}$$

A.2.2 Exponential of an Operator

The exponential of any operator $\hat{A}$ is defined by the power series expansion as

[3] ***Proof*** Equation (A.2.9) implies $|\langle \Psi | \hat{A} | \Psi \rangle| \le \|\hat{A}\|$ for any normalized $|\Psi\rangle$. By setting $|\Psi\rangle = |\Phi\rangle / \|\Phi\|$, we get (A.2.12).

$$e^{\hat{A}} := \sum_{n=0}^{\infty} \frac{1}{n!} \hat{A}^n, \tag{A.2.16}$$

where the convergence is always guaranteed in a finite dimensional Hilbert space. Note that one has $[e^{\hat{A}}, \hat{B}] = 0$ if $[\hat{A}, \hat{B}] = 0$. If P is an invertible matrix, we have

$$\mathsf{P}\, e^{\hat{A}}\, \mathsf{P}^{-1} = \sum_{n=0}^{\infty} \frac{1}{n!} \mathsf{P} \hat{A}^n \mathsf{P}^{-1} = \sum_{n=0}^{\infty} \frac{1}{n!} (\mathsf{P} \hat{A} \mathsf{P}^{-1})^n = e^{\mathsf{P} \hat{A} \mathsf{P}^{-1}}, \tag{A.2.17}$$

which is used frequently. For a real variable t, it is readily verified that

$$\frac{d}{dt} e^{t\hat{A}} = \hat{A}\, e^{t\hat{A}} = e^{t\hat{A}} \hat{A}. \tag{A.2.18}$$

The relation

$$\frac{d}{dt} \left(e^{t\hat{A}} \hat{B} e^{-t\hat{A}} \right) = \hat{A}\, e^{t\hat{A}} \hat{B} e^{-t\hat{A}} - e^{t\hat{A}} \hat{B} e^{-t\hat{A}} \hat{A} = [\hat{A}, e^{t\hat{A}} \hat{B} e^{-t\hat{A}}] \tag{A.2.19}$$

is also useful.

Unlike the exponential function for numbers the identity $e^{\hat{A}+\hat{B}} = e^{\hat{A}} e^{\hat{B}}$ is not valid in general, but can be shown when $[\hat{A}, \hat{B}] = 0$.[4] The proof is essentially the same as that for the standard exponential function, and hence omitted. This in particular means

$$e^{(x+y)\hat{A}} = e^{x\hat{A}} e^{y\hat{A}}, \tag{A.2.20}$$

for any $x, y \in \mathbb{C}$. From this identity we find that $e^{i\hat{A}}$ is unitary if $\hat{A}$ is self-adjoint.

The following Lie product formula is useful in quantum physics.[5]

Theorem A.1 (Lie product formula) *For any operators $\hat{A}$ and $\hat{B}$, one has*

$$e^{\hat{A}+\hat{B}} = \lim_{N \uparrow \infty} \left(e^{\hat{A}/N} e^{\hat{B}/N} \right)^N. \tag{A.2.21}$$

[4] In general the Baker–Campbell–Hausdorff formula $e^{\hat{A}} e^{\hat{B}} = \exp[\hat{A} + \hat{B} + [\hat{A}, \hat{B}]/2 + [\hat{A}, [\hat{A}, \hat{B}]]/12 - [\hat{B}, [\hat{A}, \hat{B}]]/12 + \cdots]$ is valid.

[5] The relation (A.2.21) is sometimes referred to as the Trotter formula, but this is incorrect. The Trotter formula stands for the same relation for certain unbounded operators. See, e.g., Sect. VIII.8 of [8]. The relation for bounded operators (which we are dealing with) belongs to nineteenth century mathematics.

More generally for any operators $\hat{A}_1, \dots, \hat{A}_n$, one has

$$e^{\hat{A}_1+\cdots+\hat{A}_n} = \lim_{N\uparrow\infty} \left(e^{\hat{A}_1/N} \dots e^{\hat{A}_n/N}\right)^N. \tag{A.2.22}$$

Proof From (A.2.20), we find $e^{\hat{A}+\hat{B}} = (e^{(\hat{A}+\hat{B})/N})^N$, and from the definition (A.2.16), we observe

$$\begin{aligned} e^{(\hat{A}+\hat{B})/N} &= 1 + \frac{\hat{A}+\hat{B}}{N} + O\Big(\frac{1}{N^2}\Big) = \Big(1+\frac{\hat{A}}{N}\Big)\Big(1+\frac{\hat{B}}{N}\Big) + O\Big(\frac{1}{N^2}\Big) \\ &= e^{\hat{A}/N} e^{\hat{B}/N} + O\Big(\frac{1}{N^2}\Big). \end{aligned} \tag{A.2.23}$$

This means $e^{\hat{A}+\hat{B}} = (e^{\hat{A}/N} e^{\hat{B}/N})^N + O(1/N)$, which implies (A.2.21).[6] The proof of (A.2.22) is essentially the same. ∎

The following inequality, which was used in Sect. 4.4 (see (4.4.35)), is sometimes useful in quantum statistical mechanics. As far as we know the inequality was first proved in [7]. The following proof is due to [9]. See [3, 6] for another proof.

Lemma A.2 *For an arbitrary operator $\hat{A}$ and self-adjoint operators $\hat{V}$ and $\hat{W}$, one has*

$$\left|\mathrm{Tr}[\hat{A}\, e^{\hat{V}+i\hat{W}}]\right| \le \|\hat{A}\|\ \mathrm{Tr}[e^{\hat{V}}]. \tag{A.2.24}$$

Proof From the Schwarz inequality for trace,[7] one finds

$$\begin{aligned} \left|\mathrm{Tr}[\hat{A}\, e^{\hat{V}+i\hat{W}}]\right| &= \left|\mathrm{Tr}[\hat{A}\, e^{(\hat{V}+i\hat{W})/2}\, e^{(\hat{V}+i\hat{W})/2}]\right| \\ &\le \sqrt{\mathrm{Tr}[e^{(\hat{V}-i\hat{W})/2}\, \hat{A}^\dagger \hat{A}\, e^{(\hat{V}+i\hat{W})/2}]\ \mathrm{Tr}[e^{(\hat{V}-i\hat{W})/2}\, e^{(\hat{V}+i\hat{W})/2}]} \\ &\le \|\hat{A}\|\ \mathrm{Tr}[e^{(\hat{V}-i\hat{W})/2}\, e^{(\hat{V}+i\hat{W})/2}], \end{aligned} \tag{A.2.25}$$

where we used (A.2.13), (A.2.6), and (A.2.11). By using the Lie product formula (A.2.21), we can write

$$\mathrm{Tr}[e^{(\hat{V}-i\hat{W})/2}\, e^{(\hat{V}+i\hat{W})/2}] = \lim_{n\uparrow\infty} \mathrm{Tr}[(\hat{X}_n)^n (\hat{X}_n^\dagger)^n], \tag{A.2.26}$$

with $\hat{X}_n = e^{\hat{V}/(2n)} e^{-i\hat{W}/(2n)}$. Then from the bound (A.2.28) below, we see that

$$\mathrm{Tr}[(\hat{X}_n)^n (\hat{X}_n^\dagger)^n] \le \mathrm{Tr}[(\hat{X}_n \hat{X}_n^\dagger)^n] = \mathrm{Tr}[e^{\hat{V}}], \tag{A.2.27}$$

which proves the desired bound (A.2.24).

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[6] The reader uncomfortable with the $O(1/N)$ notation may readily prove more formal estimates like $\|e^{\hat{A}+\hat{B}} - (e^{\hat{A}/N} e^{\hat{B}/N})^N\| \le (\text{constant})/N$.

[7] It is easily proved that $|\mathrm{Tr}[\hat{X}^\dagger \hat{Y}]|^2 \le \mathrm{Tr}[\hat{X}^\dagger \hat{X}]\, \mathrm{Tr}[\hat{Y}^\dagger \hat{Y}]$.

We finally prove

$$\mathrm{Tr}[\hat{X}^n(\hat{X}^\dagger)^n] \le \mathrm{Tr}[(\hat{X}\hat{X}^\dagger)^n], \tag{A.2.28}$$

for any operator $\hat{X}$.[8] Fix $\hat{X}$, and denote $\hat{X}$ and $\hat{X}^\dagger$ as $\hat{X}^+$ and $\hat{X}^-$, respectively. For a sequence $\boldsymbol{\sigma} = (\sigma_1, \sigma_2, \ldots, \sigma_{2n})$ such that $\sigma_j = \pm$ and $\sum_{j=1}^{2n} \sigma_j = 0$, let $f(\boldsymbol{\sigma}) = |\mathrm{Tr}[\hat{X}^{\sigma_1}\hat{X}^{\sigma_2}\cdots\hat{X}^{\sigma_{2n}}]|$ and $f_{\max} = \max_{\boldsymbol{\sigma}} f(\boldsymbol{\sigma})$. We also denote by $m(\boldsymbol{\sigma})$ the number of j such that $\sigma_j = \sigma_{j+1}$ in the sequence $\boldsymbol{\sigma}$, where we identify σ_{2n+1} with σ_1. Note that $m(\boldsymbol{\sigma}) = 0$ means $\boldsymbol{\sigma} = (+,-,+,-,\ldots,+,-)$ or $(-,+,-,+,\ldots,-,+)$. Our goal is to show that $f(\boldsymbol{\sigma}) = f_{\max}$ if $m(\boldsymbol{\sigma}) = 0$. This fact and $\mathrm{Tr}[(\hat{X}\hat{X}^\dagger)^n] \ge 0$[9] proves the desired (A.2.28).

Suppose that $f(\boldsymbol{\sigma}) = f_{\max}$ for some $\boldsymbol{\sigma}$ with $m(\boldsymbol{\sigma}) > 0$, i.e., there is a j such that $\sigma_j = \sigma_{j+1}$. By using the cyclicity of the trace, we can assume that $\sigma_1 = \sigma_{2n}$. From the Schwarz inequality for trace, we have $f(\boldsymbol{\sigma}) \le \sqrt{f(\boldsymbol{\sigma}')\, f(\boldsymbol{\sigma}'')}$, where $\boldsymbol{\sigma}' = (\sigma_1, \sigma_2, \ldots, \sigma_n, -\sigma_n, \ldots, -\sigma_2, -\sigma_1)$ and $\boldsymbol{\sigma}'' = (-\sigma_{2n}, -\sigma_{2n-1}, \ldots, -\sigma_{n+1}, \sigma_{n+1}, \ldots, \sigma_{2n-1}, \sigma_{2n})$. The assumption $f(\boldsymbol{\sigma}) = f_{\max}$ implies $f(\boldsymbol{\sigma}') = f(\boldsymbol{\sigma}'') = f_{\max}$. An inspection shows that either $m(\sigma')$ or $m(\sigma'')$ is strictly less than $m(\boldsymbol{\sigma})$. We then repeat the above consideration for the new sequence σ' or σ'' with smaller m. By repeating the procedure, we finally see that $f(\boldsymbol{\sigma}) = f_{\max}$ if $m(\boldsymbol{\sigma}) = 0$. ∎

A.2.3 *Inequality Between Self-adjoint Operators and Nonnegative Operators*

We define the notion of inequality between self-adjoint operators (Hermitian matrices), and summarize basic facts.

Definition A.3 We say that an operator $\hat{A}$ is nonnegative (or positive semidefinite) and write $\hat{A} \ge 0$ if it is self-adjoint (Hermitian) and satisfies $\langle\Phi|\hat{A}|\Phi\rangle \ge 0$ for any $|\Phi\rangle \in \mathscr{H}$. For two self-adjoint operators $\hat{A}$ and $\hat{B}$, we write $\hat{A} \le \hat{B}$ if $\hat{B} - \hat{A} \ge 0$.

We write $\hat{A} \le b$ when we have $\hat{A} \le b\hat{1}$ for a self-adjoint operator $\hat{A}$ and $b \in \mathbb{R}$. Note that (A.2.12) implies that $\hat{A} \le \|\hat{A}\|$ for any self-adjoint $\hat{A}$.

Let us list some elementary properties of nonnegative operators which are used throughout the main body of the book.

Lemma A.4 *A self-adjoint operator $\hat{A}$ is nonnegative if and only if all the eigenvalues of $\hat{A}$ are nonnegative.*

Proof The proof is straightforward if one diagonalizes $\hat{A}$. ∎

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[8] One might notice that the following proof is very similar to the proof of the chessboard estimate (Lemma 4.5 in p. 87).

[9] Note that $(\hat{X}\hat{X}^\dagger)^n = \hat{B}^\dagger\hat{B}$ with $\hat{B} = (\hat{X}\hat{X}^\dagger)^{n/2}$ if n is even, and $\hat{B} = \hat{X}^\dagger(\hat{X}\hat{X}^\dagger)^{(n-1)/2}$ if n is odd. Then the desired $\mathrm{Tr}[\hat{B}^\dagger\hat{B}] \ge 0$ follows from Lemma A.6 below.

Lemma A.5 *If $\hat{A} \geq 0$ and $\hat{B} \geq 0$, we have $\hat{A} + \hat{B} \geq 0$.*

Proof $\langle \Phi | (\hat{A} + \hat{B}) | \Phi \rangle = \langle \Phi | \hat{A} | \Phi \rangle + \langle \Phi | \hat{B} | \Phi \rangle \geq 0$ for any $|\Phi\rangle$. ∎

Lemma A.6 *For an arbitrary operator $\hat{B}$, we have $\hat{B}^\dagger \hat{B} \geq 0$. Conversely, for any $\hat{A} \geq 0$, there is a unique $\hat{C} \geq 0$ such that $\hat{A} = \hat{C}^2$. One often writes $\hat{C} = \sqrt{\hat{A}}$.*

Proof It suffices to note that $0 \leq \|\hat{B}|\Phi\rangle\|^2 = \langle \Phi | \hat{B}^\dagger \hat{B} | \Phi \rangle$ for any $|\Phi\rangle$. To show the second part, we use the spectral decomposition $\hat{A} = \sum_{j=1}^{D} |\Psi_j\rangle a_j \langle \Psi_j|$ (where $\{|\Psi_j\rangle\}_{j=1,\ldots,D}$ is an orthonormal basis), and set $\hat{C} = \sum_{j=1}^{D} |\Psi_j\rangle \sqrt{a_j} \langle \Psi_j|$. The uniqueness is obvious if we diagonalize C. ∎

The following theorem is relatively unknown to physicists, but we believe it important and worth knowing.

Theorem A.7 *Let $\hat{A}$ and $\hat{B}$ be self-adjoint operators such that $\hat{A} \leq \hat{B}$. We denote by $a_1, \ldots, a_D$ and $b_1, \ldots, b_D$ the eigenvalues of $\hat{A}$ and $\hat{B}$, respectively, ordered so that $a_j \leq a_{j+1}$ and $b_j \leq b_{j+1}$. Then it holds that $a_j \leq b_j$ for any $j = 1, \ldots, D$.*

Proof For an arbitrary j-dimensional subspace $\mathscr{M}$ of $\mathscr{H}$, where $j \in \{1, \ldots, D\}$, let

$$\lambda_{\mathscr{M}}(\hat{A}) = \max_{\substack{|\Phi\rangle \in \mathscr{M} \\ (\|\Phi\|=1)}} \langle \Phi | \hat{A} | \Phi \rangle. \tag{A.2.29}$$

Let us minimize $\lambda_{\mathscr{M}}(\hat{A})$ by varying the j-dimensional subspace $\mathscr{M}$. Clearly the minimum is attainable and realized when $\mathscr{M}$ is the subspace spanned by the j eigenstates of $\hat{A}$ corresponding to the eigenvalues $a_1, \ldots, a_j$. We thus find an interesting expression

$$a_j = \min_{\substack{\mathscr{M} \\ (\dim \mathscr{M} = j)}} \lambda_{\mathscr{M}}(\hat{A}) = \min_{\substack{\mathscr{M} \\ (\dim \mathscr{M} = j)}} \max_{\substack{|\Phi\rangle \in \mathscr{M} \\ (\|\Phi\|=1)}} \langle \Phi | \hat{A} | \Phi \rangle, \tag{A.2.30}$$

which is known as the mini-max principle. Note that, when $j = 1$, it reduces to the familiar variational principle $a_1 = \min_{|\Phi\rangle\,(\|\Phi\|=1)} \langle \Phi | \hat{A} | \Phi \rangle$. Since $\langle \Phi | \hat{A} | \Phi \rangle \leq \langle \Phi | \hat{B} | \Phi \rangle$ for any $|\Phi\rangle$ by assumption, (A.2.30) implies $a_j \leq b_j$. ∎

The following corollary is useful in quantum statistical mechanics.

Corollary A.8 *For self-adjoint operators $\hat{A}$ and $\hat{B}$ such that $\hat{A} \leq \hat{B}$, we have*

$$\mathrm{Tr}[e^{\hat{A}}] \leq \mathrm{Tr}[e^{\hat{B}}], \tag{A.2.31}$$

or, more generally,

$$\mathrm{Tr}[f(\hat{A})] \leq \mathrm{Tr}[f(\hat{B})], \tag{A.2.32}$$

for any non-decreasing function[10] $f : \mathbb{R} \to \mathbb{R}$.

[10] On may define $f(\hat{A})$ from the series expansion of $f(x)$ as in (A.2.16). For a self-adjoint $\hat{A}$, let us use the spectral decomposition $\hat{A} = \sum_{j=1}^{D} |\Psi_j\rangle a_j \langle \Psi_j|$ and define $f(\hat{A}) := \sum_{j=1}^{D} |\Psi_j\rangle f(a_j) \langle \Psi_j|$.

Proof $a_j \le b_j$ implies $\sum_{j=1}^{D} f(a_j) \le \sum_{j=1}^{D} f(b_j)$, which is (A.2.32). ∎

The following lemma is used several times in the present book (and frequently in modern research of quantum many-body systems).

Lemma A.9 (Frustration-free Hamiltonian 1) *Consider an arbitrary Hamiltonian written as* $\hat{H} = \sum_{j=1}^{N} \hat{h}_j$ *with* $\hat{h}_j \ge \varepsilon_j$ *for all* $j = 1, \ldots, N$. *If there is a state* $|\Phi\rangle$ *such that* $\hat{h}_j|\Phi\rangle = \varepsilon_j|\Phi\rangle$ *for any* $j = 1, \ldots, N$, *then* $|\Phi\rangle$ *is a ground state of* $\hat{H}$, *and the ground state energy is* $E_{\mathrm{GS}} = \sum_{j=1}^{N} \varepsilon_j$.

We say that a Hamiltonian $\hat{H}$ is frustration free when it allows the decomposition as above and has a ground state with the above property. One should note that this notion is different from frustration in the context of antiferromagnetic spin systems.[11]

Proof By using Lemma A.5 repeatedly, one finds $\hat{H} \ge \sum_{j=1}^{N} \varepsilon_j$. Then $\hat{H}|\Phi\rangle = (\sum_{j=1}^{N} \varepsilon_j)|\Phi\rangle$ implies the $|\Phi\rangle$ is a ground state. ∎

The following lemma, although being almost trivial, also characterizes a frustration free system.

Lemma A.10 (Frustration-free Hamiltonian 2) *Consider an arbitrary Hamiltonian written as* $\hat{H} = \sum_{j=1}^{N} \hat{h}_j$ *with* $\hat{h}_j \ge \varepsilon_j$ *for all* $j = 1, \ldots, N$. *Suppose that the ground state energy is* $\sum_{j=1}^{N} \varepsilon_j$, *i.e., there is a state* $|\Phi\rangle$ *such that* $\hat{H}|\Phi\rangle = (\sum_{j=1}^{N} \varepsilon_j)|\Phi\rangle$. *Then the ground state* $|\Phi\rangle$ *satisfies* $\hat{h}_j|\Phi\rangle = \varepsilon_j|\Phi\rangle$ *for each* $j = 1, \ldots, N$.

Proof We can assume that $|\Phi\rangle$ is normalized. Then $\langle\Phi|\hat{H}|\Phi\rangle = \sum_{j=1}^{N} \langle\Phi|\hat{h}_j|\Phi\rangle = \sum_{j=1}^{N} \varepsilon_j$, along with $\langle\Phi|\hat{h}_j|\Phi\rangle \ge \varepsilon_j$, implies $\langle\Phi|\hat{h}_j|\Phi\rangle = \varepsilon_j$ for $j = 1, \ldots, N$. Since ε_j is the lowest eigenvalue, the variational principle implies $\hat{h}_j|\Phi\rangle = \varepsilon_j|\Phi\rangle$. ∎

The following lemma is sometimes powerful and useful.

Lemma A.11 *If* $\hat{A} \ge 0$, *the condition* $\langle\Phi|\hat{A}|\Phi\rangle = 0$ *implies* $\hat{A}|\Phi\rangle = 0$. *If* $\hat{A} = \hat{B}^\dagger\hat{B}$ *with any* $\hat{B}$, *the condition* $\langle\Phi|\hat{A}|\Phi\rangle = 0$ *(or* $\hat{A}|\Phi\rangle = 0$*) implies* $\hat{B}|\Phi\rangle = 0$.

Proof Because of Lemma A.6, we can always assume that $\hat{A} = \hat{B}^\dagger\hat{B}$ (because one can take $B = \sqrt{A}$). Then $\|\hat{B}|\Phi\rangle\|^2 = \langle\Phi|\hat{B}^\dagger\hat{B}|\Phi\rangle = \langle\Phi|\hat{A}|\Phi\rangle = 0$ implies $\hat{B}|\Phi\rangle = 0$. By operating $\hat{B}^\dagger$, we get $\hat{A}|\Phi\rangle = 0$. ∎

Here is a simple application to angular momentum operators (see Appendix A.3). Let $\hat{\boldsymbol{J}}^2 = (\hat{J}^{(1)})^2 + (\hat{J}^{(2)})^2 + (\hat{J}^{(3)})^2$ with self-adjoint $\hat{J}^{(1)}$, $\hat{J}^{(2)}$, and $\hat{J}^{(3)}$, and assume that $\hat{\boldsymbol{J}}^2|\Phi\rangle = 0$. Then $\langle\Phi|\{(\hat{J}^{(1)})^2 + (\hat{J}^{(2)})^2 + (\hat{J}^{(3)})^2\}|\Phi\rangle = 0$ obviously implies $\langle\Phi|(\hat{J}^{(\alpha)})^2|\Phi\rangle = 0$ and hence $\hat{J}^{(\alpha)}|\Phi\rangle = 0$ for $\alpha = 1, 2, 3$.

We finally present a useful theorem which allows us to construct low energy effective theory by making a parameter in a Hamiltonian infinitely large. The theorem

[11] See footnote 30 in p. 37.

is widely used in the physics literature. We also used it in Sects. 5.1 and 11.2. See (5.1.4) and (11.2.2).

Consider a general Hamiltonian written as $\hat{H}_v = \hat{H}_0 + v\hat{V}$, where $\hat{H}_0$ is an arbitrary self-adjoint operator, $\hat{V}$ is an arbitrary nonnegative operator, and $v \geq 0$ is a parameter. Let $\mathscr{H}_0$ be the subspace that consists of $|\Phi\rangle$ such that $\hat{V}|\Phi\rangle = 0$. We assume that $\mathscr{H}_0$ is not empty. Let us denote by $\hat{P}_0$ the orthogonal projection onto $\mathscr{H}_0$, and by D_0 the dimension of $\mathscr{H}_0$. Note that all the energy eigenvalues and eigenstates of $\hat{H}_v$ depend continuously on v.

Eigenstates of $\hat{H}_v$ are classified into two classes, those with eigenvalues diverging as $v \uparrow \infty$ and those with eigenvalues converging to finite values as $v \uparrow \infty$. By continuity we see that the number of the latter is exactly D_0.

Theorem A.12 *The eigenstates and the eigenvalues in the second class (in the limit $v \uparrow \infty$) can be obtained from the effective Schrödinger equation $\hat{P}_0\hat{H}_0|\Phi\rangle = E|\Phi\rangle$ with $|\Phi\rangle \in \mathscr{H}_0$.*

Proof Take $|\Phi_v\rangle$ and E_v that depend continuously on $v \geq 0$ and satisfy $\hat{H}_v|\Phi_v\rangle = E_v|\Phi_v\rangle$ and $\|\Phi_v\| = 1$ for all v. We assume that they belong to the second class, i.e., $\lim_{v\uparrow\infty} E_v < \infty$. This means that $\lim_{v\uparrow\infty}\langle\Phi_v|\hat{V}|\Phi_v\rangle = 0$, and hence the limiting state[12] $|\Phi_\infty\rangle = \lim_{v\uparrow\infty}|\Phi_v\rangle$ satisfies $\langle\Phi_\infty|\hat{V}|\Phi_\infty\rangle = 0$. We then see from Lemma A.11 that $\hat{V}|\Phi_\infty\rangle = 0$, and hence $|\Phi_\infty\rangle \in \mathscr{H}_0$.

Since $\hat{P}_0\hat{V} = 0$, the Schrödinger equation $\hat{H}_v|\Phi_v\rangle = E_v|\Phi_v\rangle$ implies $\hat{P}_0\hat{H}_0|\Phi_v\rangle = E_v\hat{P}_0|\Phi_v\rangle$ for any $v \geq 0$. By letting $v \uparrow \infty$, one gets $\hat{P}_0\hat{H}_0|\Phi_\infty\rangle = E_\infty|\Phi_\infty\rangle$, which is the desired effective equation. Note that the effective Schrödinger equation has D_0 distinct eigenstates. They must coincide with the eigenstates in question. ∎

A.3 Quantum Mechanical Angular Momentum

Let us give a very brief (but hopefully self-contained) review of the theory of quantum mechanical angular momentum.

A.3.1 Definition and Basic Properties

Mathematically the theory of quantum mechanical angular momentum is equivalent to the representation theory of the Lie algebra $\mathfrak{su}(2)$. (See Appendix A.5.) Let $\hat{J}^{(1)}$, $\hat{J}^{(2)}$, $\hat{J}^{(3)}$ be self-adjoint operators (equivalently, Hermitian matrices) on a finite dimensional Hilbert space $\mathscr{H}$. They are assumed to satisfy the commutation relations

[12] The limit exists because the unit sphere of $\mathscr{H}$ is compact. Thus the proof relies essentially on the fact that the dimension of the Hilbert space is finite.

$$[\hat{J}^{(\alpha)}, \hat{J}^{(\beta)}] = i \sum_{\gamma=1}^{3} \varepsilon_{\alpha\beta\gamma}\, \hat{J}^{(\gamma)}, \tag{A.3.1}$$

for $\alpha, \beta = 1, 2, 3$. The Levi-Civita symbol $\varepsilon_{\alpha\beta\gamma}$ is defined as $\varepsilon_{123} = \varepsilon_{231} = \varepsilon_{312} = 1$, $\varepsilon_{321} = \varepsilon_{213} = \varepsilon_{132} = -1$, and $\varepsilon_{\alpha\beta\gamma} = 0$ for other components. We combine the three operators in a vector form as $\hat{\boldsymbol{J}} = (\hat{J}^{(1)}, \hat{J}^{(2)}, \hat{J}^{(3)})$, and write

$$\hat{\boldsymbol{J}}^2 = (\hat{J}^{(1)})^2 + (\hat{J}^{(2)})^2 + (\hat{J}^{(3)})^2. \tag{A.3.2}$$

Note that $\hat{\boldsymbol{J}}^2 \geq 0$. We also define

$$\hat{J}^{\pm} := \hat{J}^{(1)} \pm i\, \hat{J}^{(2)}, \tag{A.3.3}$$

which satisfy $(\hat{J}^{\pm})^{\dagger} = \hat{J}^{\mp}$. From the basic commutation relations (A.3.1), one can verify the following relations:

$$[\hat{\boldsymbol{J}}^2, \hat{J}^{(\alpha)}] = 0 \text{ for } \alpha = 1, 2, 3 \tag{A.3.4}$$

$$[\hat{\boldsymbol{J}}^2, \hat{J}^{\pm}] = 0 \tag{A.3.5}$$

$$[\hat{J}^{(3)}, \hat{J}^{\pm}] = \pm \hat{J}^{\pm} \tag{A.3.6}$$

$$\hat{J}^{-}\hat{J}^{+} = \hat{\boldsymbol{J}}^2 - \hat{J}^{(3)}(\hat{J}^{(3)} + 1) \tag{A.3.7}$$

$$\hat{J}^{+}\hat{J}^{-} = \hat{\boldsymbol{J}}^2 - \hat{J}^{(3)}(\hat{J}^{(3)} - 1) \tag{A.3.8}$$

Denote the eigenvalues of $\hat{\boldsymbol{J}}^2$ and $\hat{J}^{(3)}$ as $J(J+1)$ and M, respectively, where $J \geq 0$ and $M \in \mathbb{R}$. Since $\hat{\boldsymbol{J}}^2$ and $\hat{J}^{(3)}$ commute, one can decompose the whole Hilbert space according to the eigenvalues as $\mathscr{H} = \bigoplus_{J,M} \mathscr{H}_{J,M}$, where one has $\hat{\boldsymbol{J}}^2|\Phi\rangle = J(J+1)|\Phi\rangle$ and $\hat{J}^{(3)}|\Phi\rangle = M|\Phi\rangle$ for any $|\Phi\rangle \in \mathscr{H}_{J,M}$. The most basic result for quantum mechanical angular momentum is the following.

Theorem A.13 *The value of J is restricted to $n/2$, where n is a nonnegative integer. For a given J, the other eigenvalue M takes $2J+1$ values $-J, -J+1, \ldots, J-1, J$.*

We shall prove the theorem below. For the moment we only assume that J and M may take any values with $J \geq 0$ and $M \in \mathbb{R}$.

Lemma A.14 *If there is a nonzero state $|\Phi\rangle \in \mathscr{H}_{J,M}$ with J and M such that $M < J$, then one has $\hat{J}^{+}|\Phi\rangle \neq 0$ and $\hat{J}^{+}|\Phi\rangle \in \mathscr{H}_{J,M+1}$. Similarly, if there is a nonzero state $|\Phi\rangle \in \mathscr{H}_{J,M}$ with J and M such that $M > -J$, then one has $\hat{J}^{-}|\Phi\rangle \neq 0$ and $\hat{J}^{-}|\Phi\rangle \in \mathscr{H}_{J,M-1}$.*

Proof Note that the conditions $M < J$ and $M > -J$ imply $M(M+1) < J(J+1)$ and $M(M-1) < J(J+1)$, respectively. From (A.3.7) and (A.3.8), one finds

$$\begin{aligned}\|\hat{J}^{\pm}|\Phi\rangle\|^2 &= \langle\Phi|\hat{J}^{\mp}\hat{J}^{\pm}|\Phi\rangle = \langle\Phi|\left\{\hat{\boldsymbol{J}}^2 - \hat{J}^{(3)}(\hat{J}^{(3)} \pm 1)\right\}|\Phi\rangle \\ &= \{J(J+1) - M(M \pm 1)\}\,\|\Phi\|^2, \end{aligned} \tag{A.3.9}$$

which shows that $\hat{J}^{\pm}|\Phi\rangle \neq 0$ under assumed conditions. Then by using (A.3.5) and (A.3.6), one sees that

$$\hat{\boldsymbol{J}}^2\hat{J}^{\pm}|\Phi\rangle = \hat{J}^{\pm}\hat{\boldsymbol{J}}^2|\Phi\rangle = J(J+1)\,\hat{J}^{\pm}|\Phi\rangle, \tag{A.3.10}$$

$$\hat{J}^{(3)}\hat{J}^{\pm}|\Phi\rangle = \hat{J}^{\pm}\hat{J}^{(3)}|\Phi\rangle \pm \hat{J}^{\pm}|\Phi\rangle = (M \pm 1)\hat{J}^{\pm}|\Phi\rangle, \tag{A.3.11}$$

i.e., $\hat{J}^{\pm}|\Phi\rangle \in \mathscr{H}_{J,M\pm1}$. ∎

Lemma A.15 *Both $J - M$ and $J + M$ must be nonnegative integers.*

Proof Let $M > J$, and suppose that there is a nonzero state $|\Phi\rangle \in \mathscr{H}_{J,M}$. Then (A.3.9) implies that $\|\hat{J}^{+}|\Phi\rangle\|^2 = \{J(J+1) - M(M+1)\}\,\|\Phi\|^2 < 0$, which is a contradiction. We thus see $M \leq J$. Take J, M such that $J - M$ is not an integer, and suppose that there is nonzero $|\Phi\rangle \in \mathscr{H}_{J,M}$. We let n be a unique positive integer such that $M + n - 1 < J < M + n$. Then Lemma A.14 implies that $(\hat{J}^{+})^n|\Phi\rangle \neq 0$ and $(\hat{J}^{+})^n \in \mathscr{H}_{J,M+n}$, which is a contradiction. We have thus shown that $J - M$ is a nonnegative integer. The proof for $J + M$ is the same. ∎

Proof of the Theorem A.13 From Lemma A.15, we find that $2J$ is a nonnegative integer. The range of M then follows again from Lemma A.15. ∎

Let $J = n/2$ with a nonnegative integer n. A $2J + 1 = n + 1$ dimensional representation of the angular momentum operators is constructed by taking a Hilbert space spanned by normalized basis states $|\Psi_M\rangle$ with $M = -J, -J+1, \ldots, J$, and defining the action of $\hat{\boldsymbol{J}}$ as

$$\hat{J}^{(3)}|\Psi_M\rangle = M|\Psi_M\rangle, \tag{A.3.12}$$

$$\hat{J}^{\pm}|\Psi_M\rangle = \sqrt{J(J+1) - M(M \pm 1)}\,|\Psi_{M\pm1}\rangle. \tag{A.3.13}$$

It is easily verified that (A.3.9) guarantees that (A.3.13) is consistent with normalization of $|\Psi_M\rangle$. Note that (A.3.12) and (A.3.13) are the same as (2.1.2) and (2.1.3).

A.3.2 SU(2) Invariant Hamiltonian

We shall prove useful theorems about the eigenvalues and eigenstates of an SU(2) invariant Hamiltonian. Let $\hat{\boldsymbol{J}} = (\hat{J}^{(1)}, \hat{J}^{(2)}, \hat{J}^{(3)})$ be a quantum mechanical angular momentum, and $\hat{H}$ be a Hamiltonian (i.e., a certain self-adjoint operator), acting

on the same Hilbert space $\mathscr{H}$. We assume that they satisfy $[\hat{H}, \hat{J}^{(\alpha)}] = 0$ for any $\alpha = 1, 2, 3$. We again decompose the Hilbert space as $\mathscr{H} = \bigoplus_{J,M} \mathscr{H}_{J,M}$, according to the eigenvalues of $\hat{\boldsymbol{J}}^2$ and $\hat{J}^{(3)}$.

Theorem A.16 *Suppose that there is a nonzero state $|\Phi\rangle \in \mathscr{H}_{J,M_0}$ such that $\hat{H}|\Phi\rangle = E|\Phi\rangle$. Then for each $M = -J, -J+1, \ldots, J-1, J$, there is a nonzero state $|\Phi_M\rangle \in \mathscr{H}_{J,M}$ such that $\hat{H}|\Phi_M\rangle = E|\Phi_M\rangle$. Thus the energy eigenvalue E is at least $(2J+1)$-fold degenerate. Moreover theses eigenstates are "copy" of each other in the sense that*

$$|\Phi_M\rangle = c_M(\hat{J}^-)^{J-M}|\Phi_J\rangle, \tag{A.3.14}$$

for $M = -J, \ldots, J$, with $c_M \in \mathbb{C}$.

Proof By using Lemma A.14 repeatedly, we see that $|\Phi_J\rangle = (\hat{J}^+)^{J-M_0}|\Phi\rangle \in \mathscr{H}_{J,J}$ is nonzero. Because $[\hat{H}, \hat{J}^+] = 0$, we have $\hat{H}|\Phi_J\rangle = E|\Phi_J\rangle$. Again by Lemma A.14, the states (A.3.14) are all nonvanishing. That $\hat{H}|\Phi_M\rangle = E|\Phi_M\rangle$ again follows from $[\hat{H}, \hat{J}^-] = 0$. ∎

The following theorem is used repeatedly in the present book. It shows that one only needs to look at the sector with $J^{(3)} = 0$ or $1/2$ to find all the energy eigenvalues.

Theorem A.17 *Let E be an eigenvalue of $\hat{H}$. Then there exists a corresponding eigenstate $|\Phi\rangle$ that satisfies either $\hat{J}^{(3)}|\Phi\rangle = 0$ or $\hat{J}^{(3)}|\Phi\rangle = (1/2)|\Phi\rangle$.*

Proof Recall that 0 or 1/2 is the minimum possible value of J. Then the theorem is a straightforward consequence of Theorem A.16. ∎

A.3.3 Addition of Angular Momenta

We discuss the addition of angular momenta, which plays important roles throughout the book.

Addition of two spins with $S = 1/2$ Let us start by carefully discussing the simplest but an extremely important example of the addition of two spins with $S = 1/2$. The reader who is not familiar with the theory of quantum mechanical angular momentum is strongly encouraged to work out this example.

We consider a system of two spins with spin quantum number $S = 1/2$, which we call the spin 1 and spin 2. For $x = 1, 2$, we denote by $\mathfrak{h}_x \cong \mathbb{C}^2$ the Hilbert space and by $\{|\uparrow\rangle_x, |\downarrow\rangle_x\}$ the corresponding standard basis of the spin x. The Hilbert space of the whole system is $\mathscr{H} = \mathfrak{h}_1 \otimes \mathfrak{h}_2$, whose basis states are $|\sigma\rangle_1|\sigma'\rangle_2$ with $\sigma, \sigma' = \uparrow, \downarrow$. See (2.2.3). Let $\hat{\boldsymbol{S}}_x$ be the spin operator for the spin x as in (2.2.4) or (2.2.5), and define the total spin operator by $\hat{\boldsymbol{S}}_{\mathrm{tot}} = \hat{\boldsymbol{S}}_1 + \hat{\boldsymbol{S}}_2$. Then from the commutation relations (2.2.6), we see that $[\hat{S}^\alpha_{\mathrm{tot}}, \hat{S}^\beta_{\mathrm{tot}}] = i\sum_{\gamma=1,2,3} \varepsilon_{\alpha,\beta,\gamma}\, \hat{S}^\gamma_{\mathrm{tot}}$, and hence $\hat{\boldsymbol{S}}_{\mathrm{tot}}$ is also a quantum mechanical angular momentum. We denote the eigenvalues of $(\hat{\boldsymbol{S}}_{\mathrm{tot}})^2$ and $\hat{S}^{(3)}_{\mathrm{tot}}$ as $S_{\mathrm{tot}}(S_{\mathrm{tot}}+1)$ and $S^{(3)}_{\mathrm{tot}}$, respectively. Our goal is to find corresponding simultaneous eigenstates, i.e., $|\Phi_{S_{\mathrm{tot}}, S^{(3)}_{\mathrm{tot}}}\rangle \in \mathscr{H}$ such that

$$(\hat{\boldsymbol{S}}_{\rm tot})^2|\Phi_{S_{\rm tot},S^{(3)}_{\rm tot}}\rangle = S_{\rm tot}(S_{\rm tot}+1)|\Phi_{S_{\rm tot},S^{(3)}_{\rm tot}}\rangle, \tag{A.3.15}$$

$$\hat{S}^{(3)}_{\rm tot}|\Phi_{S_{\rm tot},S^{(3)}_{\rm tot}}\rangle = S^{(3)}_{\rm tot}|\Phi_{S_{\rm tot},S^{(3)}_{\rm tot}}\rangle. \tag{A.3.16}$$

We first note that

$$(\hat{\boldsymbol{S}}_{\rm tot})^2 = (\hat{\boldsymbol{S}}_1)^2 + (\hat{\boldsymbol{S}}_2)^2 + 2\hat{\boldsymbol{S}}_1\cdot\hat{\boldsymbol{S}}_2 = \hat{S}_1^+\hat{S}_2^- + \hat{S}_1^-\hat{S}_2^+ + 2\hat{S}_1^{(3)}\hat{S}_2^{(3)} + \frac{3}{2}, \tag{A.3.17}$$

where we used $(\hat{\boldsymbol{S}}_x)^2 = \frac{1}{2}(\frac{1}{2}+1) = 3/4$, and used (2.2.16). Then, from the basic actions (2.1.4) and (2.1.5) of spin operators onto the basis states, we find

$$(\hat{\boldsymbol{S}}_{\rm tot})^2|\uparrow\rangle_1|\uparrow\rangle_2 = 2|\uparrow\rangle_1|\uparrow\rangle_2, \quad \hat{S}^{(3)}_{\rm tot}|\uparrow\rangle_1|\uparrow\rangle_2 = |\uparrow\rangle_1|\uparrow\rangle_2, \tag{A.3.18}$$

$$(\hat{\boldsymbol{S}}_{\rm tot})^2|\downarrow\rangle_1|\downarrow\rangle_2 = 2|\downarrow\rangle_1|\downarrow\rangle_2, \quad \hat{S}^{(3)}_{\rm tot}|\downarrow\rangle_1|\downarrow\rangle_2 = -|\downarrow\rangle_1|\downarrow\rangle_2, \tag{A.3.19}$$

which shows these states are indeed the desired simultaneous eigenstates. For the remaining two basis states, we get

$$(\hat{\boldsymbol{S}}_{\rm tot})^2|\uparrow\rangle_1|\downarrow\rangle_2 = |\uparrow\rangle_1|\downarrow\rangle_2 + |\downarrow\rangle_1|\uparrow\rangle_2, \quad \hat{S}^{(3)}_{\rm tot}|\uparrow\rangle_1|\downarrow\rangle_2 = 0, \tag{A.3.20}$$

$$(\hat{\boldsymbol{S}}_{\rm tot})^2|\downarrow\rangle_1|\uparrow\rangle_2 = |\uparrow\rangle_1|\downarrow\rangle_2 + |\downarrow\rangle_1|\uparrow\rangle_2, \quad \hat{S}^{(3)}_{\rm tot}|\downarrow\rangle_1|\uparrow\rangle_2 = 0, \tag{A.3.21}$$

which shows that their linear combinations $(|\uparrow\rangle_1|\downarrow\rangle_2 \pm |\downarrow\rangle_1|\uparrow\rangle_2)/\sqrt{2}$ are the simultaneous eigenstates.

To summarize we have found that there are three simultaneous eigenstates

$$|\Phi_{1,1}\rangle = |\uparrow\rangle_1|\uparrow\rangle_2, \quad |\Phi_{1,0}\rangle = \frac{1}{\sqrt{2}}\big(|\uparrow\rangle_1|\downarrow\rangle_2 + |\downarrow\rangle_1|\uparrow\rangle_2\big), \quad |\Phi_{1,-1}\rangle = |\downarrow\rangle_1|\downarrow\rangle_2, \tag{A.3.22}$$

with $S_{\rm tot} = 1$, which are called the triplet states (or the spin-triplet states), and one simultaneous eigenstate

$$|\Phi_{0,0}\rangle = \frac{1}{\sqrt{2}}\big(|\uparrow\rangle_1|\downarrow\rangle_2 - |\downarrow\rangle_1|\uparrow\rangle_2\big), \tag{A.3.23}$$

with $S_{\rm tot} = 0$, which is called the singlet state (or the spin-singlet state). The spin-singlet is sometimes called the valence-bond. See p. 182. As we noted in p. 469 after Lemma A.11, the singlet state satisfies

$$\hat{S}^{(\alpha)}_{\rm tot}|\Phi_{0,0}\rangle = 0, \tag{A.3.24}$$

for any $\alpha = 1, 2, 3$, which represents the SU(2) invariance of the singlet.

Addition of two general angular momenta The above example can be generalized. Let us briefly discuss the setting and the most important result.

Consider two quantum mechanical systems with Hilbert spaces $\mathscr{H}_1$ and $\mathscr{H}_2$. Suppose that there are angular momenta for these systems, which we denote as $\hat{\boldsymbol{J}}_1$ and $\hat{\boldsymbol{J}}_2$. For simplicity we assume that $\hat{\boldsymbol{J}}_1$ and $\hat{\boldsymbol{J}}_2$ have constant magnitudes, i.e., there are constants J_1 and J_2 such that $(\hat{\boldsymbol{J}}_1)^2|\Phi\rangle = J_1(J_1+1)|\Phi\rangle$ for any $|\Phi\rangle \in \mathscr{H}_1$, and $(\hat{\boldsymbol{J}}_2)^2|\Psi\rangle = J_2(J_2+1)|\Psi\rangle$ for any $|\Psi\rangle \in \mathscr{H}_2$. We then define the total angular momentum by $\hat{\boldsymbol{J}} = \hat{\boldsymbol{J}}_1 \otimes \hat{1}_2 + \hat{1}_1 \otimes \hat{\boldsymbol{J}}_2$, which of course satisfies the commutation relations (A.3.1). We denote the eigenvalue of $\hat{\boldsymbol{J}}^2$ as $J(J+1)$.

The problem of addition of angular momenta is to determine the range of the eigenvalues J, and to represent the corresponding simultaneous eigenstates of $\hat{\boldsymbol{J}}^2$ and $\hat{J}^{(3)}$ in terms of simultaneous eigenstates of $(\hat{\boldsymbol{J}}_j)^2$ and $\hat{J}_j^{(3)}$ for $j = 1, 2$. The solution and the derivation can be found in almost any advanced textbook in quantum mechanics. One fact that the reader must know (in order to read the present book) is that J takes the values $J_1 + J_2, J_1 + J_2 - 1, \ldots, |J_1 - J_2|$.

A.4 Some Linear Algebra

We discuss important results about matrices in Appendices A.4.1 and A.4.2, and summarize basic treatment of antilinear operators in Appendix A.4.3. Each subsection can be read independently.

A.4.1 Perron–Frobenius Theorem

The Perron–Frobenius theorem is an important and useful theorem for a class of matrices with real elements. In physics the theorem plays a fundamental role in the theory of Markov processes. Here, with applications to quantum physics in mind, we present and prove a simpler version of the theorem for a real symmetric matrix.

Theorem A.18 (Perron–Frobenius theorem for a real symmetric matrix) *Let* $\mathsf{M} = (m_{i,j})_{i,j=1,\ldots,N}$ *be an* $N \times N$ *real symmetric matrix (i.e.,* $m_{i,j} = m_{j,i} \in \mathbb{R}$ *) with the properties that (i)* $m_{i,j} \leq 0$ *for any* $i \neq j$*, and (ii) All* $i \neq j$ *are connected via nonvanishing matrix elements of* M*, or, more precisely, for any* $i \neq j$*, we can take a sequence* $(i_1, \ldots, i_K)$ *such that* $i_1 = i$*,* $i_K = j$*, and* $m_{i_k,i_{k+1}} \neq 0$ *for all* $k = 1, 2, \ldots, K-1$*. Then the lowest eigenvalue of* M *is nondegenerate and the corresponding eigenvector* $\boldsymbol{v} = (v_i)_{i=1,\ldots,N}$ *can be taken to satisfy* $v_i > 0$ *for all* i*.*

Proof Let us present a standard elementary proof based on a variational argument. The essence of the argument is that a state without "nodes" has low energy, an idea standard in quantum mechanics. See (A.4.1). In what follows we assume (without loss of generality) that all components of vectors are real.

(1) We first prove that if an eigenvector $\boldsymbol{u} = (u_i)_{i=1,\ldots,N}$ of M satisfies $u_i \geq 0$ for all i, then it inevitably satisfies $u_i > 0$ for all i. For $\alpha > 0$ let $\tilde{\mathsf{M}} = \alpha\mathsf{I} - \mathsf{M}$, where

I denotes the identity matrix. By taking α large enough, we can assume that all the eigenvalues of $\tilde{\mathsf{M}}$ are positive, and $(\tilde{\mathsf{M}})_{i,i} > 0$ for any i. We also have $(\tilde{\mathsf{M}})_{i,j} \geq 0$ for any i, j from (i). By also using (ii) above, we see that there is n such that $(\tilde{\mathsf{M}}^n)_{i,j} > 0$ for any i, j. Note that $\boldsymbol{u}$ is an eigenvector of $\tilde{\mathsf{M}}^n$ with a positive eigenvalue, say, β. Then we have $\beta u_i = \sum_j (\tilde{\mathsf{M}}^n)_{i,j} u_j$, which implies $u_i > 0$ under the assumption that $u_j \geq 0$ and $\boldsymbol{u} \neq 0$.

(2) Let $\boldsymbol{v} = (v_i)_{i=1,\ldots,N}$ be a normalized eigenvector corresponding to the lowest eigenvalue μ_0. We shall prove that $\boldsymbol{v}$ satisfies either $v_i > 0$ for all i or $v_i < 0$ for all i. Define a vector $\boldsymbol{u}$ by $u_i = |v_i|$ for $i = 1, \ldots, N$. Because $\boldsymbol{v}$ is a normalized eigenvector, we have

$$\mu_0 = \boldsymbol{v}^{\mathrm{t}} \mathsf{M} \boldsymbol{v} = \sum_{i,j=1}^{N} v_i m_{i,j} v_j \geq \sum_{i,j=1}^{N} u_i m_{i,j} u_j = \boldsymbol{u}^{\mathrm{t}} \mathsf{M} \boldsymbol{u}, \tag{A.4.1}$$

where we used (i). Since $\boldsymbol{u}$ is normalized and μ_0 is the lowest eigenvalue, the variational principle implies that $\boldsymbol{u}$ is also an eigenvector with eigenvalue μ_0. Then (1) implies $u_i > 0$ (and hence $v_i \neq 0$) for all i. Since $\boldsymbol{u}^{\mathrm{t}} \mathsf{M} \boldsymbol{u} = \mu_0$, we have $\sum_{i,j} v_i m_{i,j} v_j = \sum_{i,j} u_i m_{i,j} u_j$. Since $(v_i)^2 = (u_i)^2$, this means $\sum_{i \neq j} v_i m_{i,j} v_j = \sum_{i \neq j} u_i m_{i,j} u_j$ (where the sum is over all i and j such that $i \neq j$). Since $u_i m_{i,j} u_j \leq 0$ for any $i \neq j$, we conclude that $v_i m_{i,j} v_j = u_i m_{i,j} u_j$ for any $i \neq j$. This means that $v_i v_j = u_i u_j > 0$ whenever $m_{i,j} \neq 0$. From (ii), we see that all v_i have the same sign.

(3) Finally suppose that the lowest eigenvalue of M is degenerate. Then we can find two mutually orthogonal eigenvectors $\boldsymbol{v}$ and $\boldsymbol{v}'$. But (2) implies that both have components with a fixed sign, which means $\boldsymbol{v} \cdot \boldsymbol{v}' \neq 0$. But this is a contradiction. ∎

A.4.2 Decomposition of Matrices

Here we state and prove two important decomposition theorems for general square matrices. Like any complex number z can be written in the polar form $z = r\, e^{i\theta}$ with $r \geq 0$ and $|e^{i\theta}| = 1$, any matrix A admits the polar decomposition as follows.

Theorem A.19 (Polar decomposition theorem) *Any $N \times N$ matrix A is written as*

$$\mathsf{A} = \mathsf{W}\mathsf{C}, \tag{A.4.2}$$

where W is a unitary matrix and C is a nonnegative (or, equivalently, positive semidefinite) matrix. When A is real (in the sense that all the entries are real) W can be chosen to be an orthogonal matrix.

The following singular value decomposition theorem, which is closely related to the above theorem, shows that any matrix can be written in a "nearly diagonalized" form. The decomposition is the basis of (or equivalent to) the Schmidt decomposition, which is a fundamental tool in many-body quantum physics. (See the end of

Sect. A.1.) Although we only discuss the theorem for square matrices, the extension to non-square matrices is not difficult, and is also useful.

Theorem A.20 (Singular value decomposition theorem) *Any $N \times N$ matrix A is written as*

$$\mathsf{A} = \mathsf{U}\mathsf{D}\mathsf{V}^\dagger, \tag{A.4.3}$$

where U and V are unitary matrices, and D is a diagonal matrix with nonnegative entries. When A is real (in the sense that all the entries are real) U and V can be chosen to be orthogonal matrices.

We see from the proof that the diagonal matrix D is written as

$$\mathsf{D} = \begin{pmatrix} \sqrt{\lambda_1} & 0 & \dots & 0 \\ 0 & \sqrt{\lambda_2} & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \sqrt{\lambda_N} \end{pmatrix}, \tag{A.4.4}$$

where $\lambda_1, \dots, \lambda_N$ (with $\lambda_j \geq 0$ for $j = 1, \dots, N$) are the eigenvalues of the nonnegative matrix $\mathsf{A}^\dagger \mathsf{A}$, or, equivalently, of $\mathsf{A}\mathsf{A}^\dagger$. (We prove that these two matrices have the same eigenvalues.) The two unitary matrices are written as

$$\mathsf{U} = (\boldsymbol{u}_1, \boldsymbol{u}_2, \dots, \boldsymbol{u}_N), \quad \mathsf{V} = (\boldsymbol{v}_1, \boldsymbol{v}_2, \dots, \boldsymbol{v}_N), \tag{A.4.5}$$

where $\{\boldsymbol{u}_j\}_{j=1,\dots,N}$ and $\{\boldsymbol{v}_j\}_{j=1,\dots,N}$ are orthonormal basis such that

$$\mathsf{A}\mathsf{A}^\dagger \boldsymbol{u}_j = \lambda_j \boldsymbol{u}_j, \quad \mathsf{A}^\dagger \mathsf{A} \boldsymbol{v}_j = \lambda_j \boldsymbol{v}_j. \tag{A.4.6}$$

We prove Theorems A.19 and A.20 together. In our notation, $\boldsymbol{u} = (u_1, \dots, u_N)^{\mathrm{t}}$, $\boldsymbol{v} = (v_1, \dots, v_N)^{\mathrm{t}}$ are column vectors, and their Hermitian conjugate $\boldsymbol{u}^\dagger$, $\boldsymbol{v}^\dagger$ are row vectors. $\boldsymbol{u}^\dagger \boldsymbol{v} = \sum_{j=1}^N (u_j)^* v_j$ is a scalar, and $\boldsymbol{u}\boldsymbol{v}^\dagger$ is a matrix whose j, k entry is $u_j (v_k)^*$. We also recall that any orthonormal basis $\{\boldsymbol{w}_j\}_{j=1,\dots,N}$ satisfies the orthonormality $\boldsymbol{w}_j^\dagger \boldsymbol{w}_k = \delta_{j,k}$ and the completeness $\sum_{j=1}^N \boldsymbol{w}_j \boldsymbol{w}_j^\dagger = \mathsf{I}$.

Proof of the Theorem A.13 *A.19 and A.20* Note that the matrix $\mathsf{A}^\dagger \mathsf{A}$ is nonnegative by Lemma A.6. Let $\{\boldsymbol{v}_j\}_{j=1,\dots,N}$ be the orthonormal basis formed by eigenvectors of $\mathsf{A}^\dagger \mathsf{A}$. See (A.4.6). We assume that the corresponding eigenvalues $\lambda_1, \dots, \lambda_N$ are ordered so that $\lambda_j > 0$ for $j = 1, \dots, M$, and $\lambda_j = 0$ for $j = M+1, \dots, N$. (Of course it is possible that $M = N$.)

For $j = 1, \dots, M$, we let $\boldsymbol{u}_j = (\lambda_j)^{-1/2} \mathsf{A} \boldsymbol{v}_j$. Note that $(\boldsymbol{u}_j)^\dagger \boldsymbol{u}_k = (\lambda_j \lambda_k)^{-1/2} (\boldsymbol{v}_j)^\dagger \mathsf{A}^\dagger \mathsf{A} \boldsymbol{v}_k = \delta_{j,k}$. By choosing suitable unit vectors $\boldsymbol{u}_{M+1}, \dots, \boldsymbol{u}_N$, we can make $\{\boldsymbol{u}_j\}_{j=1,\dots,N}$ an orthonormal basis, i.e., $\boldsymbol{u}_j^\dagger \boldsymbol{u}_k = \delta_{j,k}$ for $j, k = 1, \dots, N$.

We define $\mathsf{W} = \sum_{j=1}^N \boldsymbol{u}_j \boldsymbol{v}_j^\dagger$, which is unitary, and $\mathsf{C} = \sum_{k=1}^M \sqrt{\lambda_k} \boldsymbol{v}_k \boldsymbol{v}_k^\dagger$, which is nonnegative. Then one confirms the desired polar decomposition (A.4.2) by observing that

$$\mathsf{WC} = \sum_{k=1}^{M} \boldsymbol{u}_k \sqrt{\lambda_k} \boldsymbol{v}_k^\dagger = \sum_{k=1}^{M} \mathsf{A} \boldsymbol{v}_k \boldsymbol{v}_k^\dagger = \sum_{j=1}^{N} \mathsf{A} \boldsymbol{v}_j \boldsymbol{v}_j^\dagger = \mathsf{A}. \tag{A.4.7}$$

Here we added terms with $j = M+1, \ldots, N$ by noting that $\lambda_j = 0$ implies $\mathsf{A}^\dagger \mathsf{A} \boldsymbol{v}_j = 0$ and hence $\mathsf{A} \boldsymbol{v}_j = 0$ because of Lemma A.11.

Define D by (A.4.4) and V by the second relation in (A.4.5). Then C defined above is written as $\mathsf{C} = \mathsf{V} \mathsf{D} \mathsf{V}^\dagger$. From the polar decomposition (A.4.2) we find

$$\mathsf{A} = \mathsf{WC} = \mathsf{WVDV}^\dagger = \mathsf{UDV}^\dagger, \tag{A.4.8}$$

where we defined $\mathsf{U} = \mathsf{WV}$, which is unitary. This is the desired singular value decomposition (A.4.3). It is also easily verified that U is written as in the first relation in (A.4.5) because $\mathsf{W} \boldsymbol{v}_j = \boldsymbol{u}_j$.

Note that (A.4.3) implies

$$\mathsf{A}\,\mathsf{A}^\dagger \mathsf{U} = \mathsf{UDV}^\dagger\, \mathsf{VDU}^\dagger\, \mathsf{U} = \mathsf{UD}^2 = (\lambda_1 \boldsymbol{u}_1, \ldots, \lambda_N \boldsymbol{u}_N). \tag{A.4.9}$$

This is nothing but the first relation in (A.4.6). We have thus confirmed that $\mathsf{A}^\dagger \mathsf{A}$ and $\mathsf{A}\,\mathsf{A}^\dagger$ have the same eigenvalues.

To show the statements about real matrices, we only need to note that eigenvectors of a real symmetric matrices can be chosen to be real. ∎

A.4.3 Antilinear Operators

We summarize basic conventions of antilinear operators, which appear mainly in discussions involving time-reversal transformation. Let $V \cong \mathbb{C}^D$ be the space of D-dimensional complex vectors. We express a vector as $\boldsymbol{v} = (v_1, \ldots, v_D)^{\mathrm{t}} \in V$, and denote by $\langle \boldsymbol{u}, \boldsymbol{v} \rangle = \sum_{j=1}^{D} (u_j)^* v_j$ the inner product of $\boldsymbol{u}, \boldsymbol{v} \in V$.

A map $\mathsf{X} : V \to V$ is said to be an antilinear operator if

$$\mathsf{X}(\alpha \boldsymbol{u} + \beta \boldsymbol{v}) = \alpha^* \mathsf{X} \boldsymbol{u} + \beta^* \mathsf{X} \boldsymbol{v}, \tag{A.4.10}$$

for any $\boldsymbol{u}, \boldsymbol{v} \in V$ and $\alpha, \beta \in \mathbb{C}$. The complex conjugation map K defined by

$$\mathsf{K} \begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_D \end{pmatrix} = \begin{pmatrix} (v_1)^* \\ (v_2)^* \\ \vdots \\ (v_D)^* \end{pmatrix} \tag{A.4.11}$$

is an important example. If A is a linear operator, and X and Y are antilinear operators, we see that AX and XA are antilinear, and XY is linear.

If X is an antilinear operator, its conjugate (or adjoint) $\mathsf{X}^\dagger$ is the unique antilinear operator such that

$$\langle \boldsymbol{u}, \mathsf{X}\boldsymbol{v}\rangle = \langle \mathsf{X}^\dagger \boldsymbol{u}, \boldsymbol{v}\rangle^*, \tag{A.4.12}$$

for any $\boldsymbol{u}, \boldsymbol{v} \in V$.[13] It is obvious that $(\mathsf{X}^\dagger)^\dagger = \mathsf{X}$. We also find that $\mathsf{K}^\dagger = \mathsf{K}$.

For any antilinear operators X and Y, we have

$$\langle \boldsymbol{u}, \mathsf{XY}\boldsymbol{v}\rangle = \langle \mathsf{X}^\dagger \boldsymbol{u}, \mathsf{Y}\boldsymbol{v}\rangle^* = \langle \mathsf{Y}^\dagger \mathsf{X}^\dagger \boldsymbol{u}, \boldsymbol{v}\rangle, \tag{A.4.13}$$

which implies

$$(\mathsf{XY})^\dagger = \mathsf{Y}^\dagger \mathsf{X}^\dagger. \tag{A.4.14}$$

Similarly for any antilinear X and linear A, we can show that

$$(\mathsf{AX})^\dagger = \mathsf{X}^\dagger \mathsf{A}^\dagger, \quad (\mathsf{XA})^\dagger = \mathsf{A}^\dagger \mathsf{X}^\dagger. \tag{A.4.15}$$

Note in particular that $(\alpha\mathsf{X})^\dagger = \mathsf{X}^\dagger \alpha^* = \alpha \mathsf{X}^\dagger$ for $\alpha \in \mathbb{C}$.

Let $\boldsymbol{u} = \mathsf{X}\boldsymbol{v}$ with some antilinear X. Then, for any linear operator A, we have

$$\langle \boldsymbol{v}, \mathsf{X}^\dagger \mathsf{AX}\boldsymbol{v}\rangle = \langle \boldsymbol{u}, \mathsf{A}\boldsymbol{u}\rangle^* = \langle \boldsymbol{u}, \mathsf{A}^\dagger \boldsymbol{u}\rangle. \tag{A.4.16}$$

An antilinear operator V is said to be antiunitary if

$$\langle \mathsf{V}\boldsymbol{u}, \mathsf{V}\boldsymbol{v}\rangle = \langle \boldsymbol{u}, \boldsymbol{v}\rangle^* \tag{A.4.17}$$

for any $\boldsymbol{u}, \boldsymbol{v} \in V$. Note that, if V is antiunitary, we have

$$\langle \mathsf{KV}\boldsymbol{u}, \mathsf{KV}\boldsymbol{v}\rangle = \langle \mathsf{V}\boldsymbol{u}, \mathsf{V}\boldsymbol{v}\rangle^* = \langle \boldsymbol{u}, \boldsymbol{v}\rangle \tag{A.4.18}$$

and

$$\langle \mathsf{VK}\boldsymbol{u}, \mathsf{VK}\boldsymbol{v}\rangle = \langle \mathsf{K}\boldsymbol{u}, \mathsf{K}\boldsymbol{v}\rangle^* = \langle \boldsymbol{u}, \boldsymbol{v}\rangle. \tag{A.4.19}$$

We thus find that both KV and VK are unitary. In other words, antiunitary operator V can always be written as $\mathsf{V} = \mathsf{KU}$ and $\mathsf{V} = \mathsf{U}'\mathsf{K}$ with some unitary operators U and U'. This in particular implies that $\mathsf{VV}^\dagger = \mathsf{V}^\dagger \mathsf{V} = \mathsf{I}$, which is also evident from (A.4.17).

A.5 Groups and Their Representations

The group theory provides a useful mathematical language for describing symmetry and transformations of physical systems. Although we do not make use of any non-

[13] Needless to say the conjugate of a linear operator satisfies $\langle \boldsymbol{u}, \mathsf{A}\boldsymbol{v}\rangle = \langle \mathsf{A}^\dagger \boldsymbol{u}, \boldsymbol{v}\rangle$.

trivial results from the group theory in the present book, we shall discuss the basics of the group theory for the reader's convenience.

Definition and basic examples Let G be a set, and suppose that there is a multiplication rule which assigns a unique "product" $ab \in G$ to any two elements $a, b \in G$. We say that G (along with the multiplication rule) is a group when (i) the multiplication is associative, i.e., $(ab)c = a(bc)$ for any $a, b, c \in G$, (ii) there is an element $e \in G$, which is called the identity, such that $ae = ea = a$ for any $a \in G$, and (iii) for every $a \in G$ there is an element $a^{-1} \in G$ such that $aa^{-1} = a^{-1}a = e$. It easily follows that a group has a unique identity, and for each $a \in G$ its inverse a^{-1} is unique.

The cyclic group of order 2, denoted as $\mathbb{Z}_2$, is the simplest nontrivial group. It consists of two elements as $\mathbb{Z}_2 = \{e, a\}$, and is specified by the multiplication rule $ea = ae = a$ and $a^2 = e$. We have defined slightly more complicated group $\mathbb{Z}_2 \times \mathbb{Z}_2$ in (2.1.27).

Sets of matrices with the standard matrix multiplication rule provide important and useful class of groups. Let n be a positive integer. The n-dimensional orthogonal group $\mathrm{O}(n)$ is the set of all $n \times n$ orthogonal matrices, and the n-dimensional special orthogonal group $\mathrm{SO}(n)$ is the set of all $n \times n$ orthogonal matrices with determinant 1. The group $\mathrm{SO}(n)$ is also known as the rotation group. SO(2) consists of the rotation matrix

$$\mathsf{O}_\theta = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}, \tag{A.5.1}$$

with $\theta \in [0, 2\pi)$. The three dimensional rotation matrices (2.1.11) are elements of SO(3).

The unitary group of degree n, denoted as $\mathrm{U}(n)$, is the set of all $n \times n$ unitary matrices, and the special unitary group of degree n, denoted as $\mathrm{SU}(n)$, is the set of all $n \times n$ unitary matrices with determinant 1. The group U(1) is simply the set of complex numbers with absolute value 1, and its element is written as $e^{i\theta}$ with $\theta \in [0, 2\pi)$. From (A.5.1), we immediately see that U(1) and SO(2) are isomorphic.[14]

The group SU(2) and its generators Let us concentrate on the group SU(2), which plays a central role throughout this book.

Let U be an element of SU(2), i.e., a unitary matrix of degree 2 with determinant 1, and write it as

$$\mathsf{U} = \exp[-i\mathsf{A}], \tag{A.5.2}$$

where A is a Hermitian matrix. One easily finds by diagonalizing U that the rewriting (A.5.2) is always possible. Recalling that $\det \exp[-i\mathsf{A}] = \exp[-i\,\mathrm{Tr}[\mathsf{A}]]$ (which is verified by diagonalizing A) we see that U written as (A.5.2) is an element of SU(2) if and only if $\hat{A}$ is a traceless Hermitian matrix. Such A is in general written as $\mathsf{A} = \begin{pmatrix} a & b - ic \\ b + ic & -a \end{pmatrix}$ with arbitrary $a, b, c \in \mathbb{R}$. Equivalently, it is written as

[14] Two groups are isomorphic if and only if there is a one-to-one map between them which preserves the multiplication rules.

$$\mathsf{A} = \theta_1 \mathsf{S}^{(1)} + \theta_2 \mathsf{S}^{(2)} + \theta_3 \mathsf{S}^{(3)}, \tag{A.5.3}$$

with arbitrary $\theta_1, \theta_2, \theta_3 \in \mathbb{R}$, where

$$\mathsf{S}^{(1)} = \frac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \mathsf{S}^{(2)} = \frac{1}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \mathsf{S}^{(3)} = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{A.5.4}$$

are nothing but (the matrix representations of) the spin operators (2.1.7) for $S = 1/2$. The matrices $\mathsf{S}^{(1)}$, $\mathsf{S}^{(2)}$, and $\mathsf{S}^{(3)}$ are called the generators of the group SU(2).

The group SU(2) is an example of a Lie group. (This is also true for general O(n), SO(n), U(n), and SU(n).) The set of matrices (A.5.3) is the corresponding Lie algebra, which is written as $\mathfrak{su}(2)$.[15]

Representation of a group A representation,[16] or, more precisely, a linear representation, of a group G is a map ρ from G to the set of square matrices with a fixed degree that satisfies $\rho(e) = \mathsf{I}$ and $\rho(a)\rho(b) = \rho(ab)$ for any $a, b \in G$.

For example a two dimensional representation of $\mathbb{Z}_2 = \{e, a\}$ is given by

$$\rho(e) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \rho(a) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \tag{A.5.5}$$

If $\hat{N}$ is any Hermitian matrix whose eigenvalues are integer, then $\hat{U}_\theta = \exp[-i\theta\hat{N}]$ gives a representation of U(1) or SO(2). This is the reason why we refer to the symmetry with respect to the change of the phase, which is an intrinsic symmetry in quantum theory, as the U(1) symmetry.

A quantum mechanical spin or a quantum spin system provide representations of SU(2). The spin operators $\hat{S}^{(1)}$, $\hat{S}^{(2)}$, and $\hat{S}^{(3)}$ with spin quantum number S (discussed in Sect. 2.1) give a $2S+1$ dimensional representation of the generators $\mathsf{S}^{(1)}$, $\mathsf{S}^{(2)}$, and $\mathsf{S}^{(3)}$ of SU(2). Likewise the total spin operators $\hat{S}^{(1)}_{\rm tot}$, $\hat{S}^{(2)}_{\rm tot}$, and $\hat{S}^{(3)}_{\rm tot}$ in (2.2.7) give a $2|\Lambda|S+1$ dimensional representation of the same generators. Then the corresponding spin rotation operators $\hat{U}^{(\alpha)}_\theta$ give representations of elements of SU(2). It is common to make a slight abuse of terminology and refer to a representation of an element of G simply as an element of G. See, e.g., the remarks that follow (2.1.16) and (2.2.11).

We finally discuss a representation of SU(2) which sheds light on the relation between SU(2) and the rotation group SO(3). Let X be an arbitrary 2×2 traceless Hermitian matrix and write is as $\mathsf{X} = x\,\mathsf{S}^{(1)} + y\,\mathsf{S}^{(2)} + z\,\mathsf{S}^{(3)}$ with $x, y, z \in \mathbb{R}$. Take an arbitrary element U of SU(2), and consider a matrix $\mathsf{X}' = \mathsf{U}^\dagger \mathsf{X} \mathsf{U}$. It is clear that X' is also Hermitian. It is also traceless since $\mathrm{Tr}[\mathsf{X}'] = \mathrm{Tr}[\mathsf{U}^\dagger \mathsf{X} \mathsf{U}] =$

[15] In mathematics it is standard to regard $i\mathsf{A}$ as forming the Lie algebra.

[16] A representation is sometimes called a genuine representation, as opposed to a projective representation. A projective representation of a group G is a map ρ from G to the set of square matrices with a fixed degree that satisfies $\rho(e) = \mathsf{I}$ and $\rho(a)\rho(b) = e^{i\phi(a,b)}\rho(ab)$ for any $a, b \in G$, where $\phi(a, b) \in \mathbb{R}$ is a phase factor that satisfies the condition (8.3.26). See the remarks below (2.1.31) and (8.3.24) for more about the notion of projective representation..

$\mathrm{Tr}[\mathsf{X}\mathsf{U}\mathsf{U}^\dagger] = \mathrm{Tr}[\mathsf{X}] = 0$. We thus find that the new matrix is again written as $\mathsf{X}' = x'\mathsf{S}^{(1)} + y'\mathsf{S}^{(2)} + z'\mathsf{S}^{(3)}$ with $x', y', z' \in \mathbb{R}$. Since x', y', z' depend linearly on x, y, z, there exists a 3×3 matrix $\rho(\mathsf{U})$ with real components such that

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \rho(\mathsf{U}) \begin{pmatrix} x \\ y \\ z \end{pmatrix}. \tag{A.5.6}$$

This defines a representation of SU(2), known as the adjoint representation. By using the properties of $\mathsf{S}^{(1)}$, $\mathsf{S}^{(2)}$, and $\mathsf{S}^{(3)}$ described just below (2.1.7) (or by a direct simple calculation) one confirms that $\mathsf{X}^2 = \{(x^2 + y^2 + z^2)/4\}\mathsf{I}$. It then follows that $(\mathsf{X}')^2 = \mathsf{U}^\dagger \mathsf{X}^2 \mathsf{U} = \{(x^2 + y^2 + z^2)/4\}\mathsf{I}$, and hence $(x')^2 + (y')^2 + (z')^2 = x^2 + y^2 + z^2$. This fact suggests that the matrix $\rho(\mathsf{U})$ describes a rotation in the three dimensional euclidean space. In fact it can be shown that $\rho(\mathsf{U})$ covers the whole SO(3) when U is taken from the whole SU(2). We have already made a key observation for this fact in (2.1.16). It should be noted however that SU(2) and SO(3) are not isomorphic. As can be seen from the fact that $\exp[-2\pi i \mathsf{S}^{(\alpha)}] = -\mathsf{I}$, the group SU(2) is in a sense "twice larger" than the group SO(3).

A.6 Wigner's Theorem

In 1931, Wigner proved a famous theorem (Theorem A.22) which asserts that any symmetry in a quantum system is represented by a unitary or antiunitary operator on the Hilbert space. (The theorem is proved in the appendix to Chap. 20 of his book [10, 11].) Our treatment of symmetry in quantum physics is fundamentally based on this theorem.

For us Wigner's theorem is not logically necessary since we always start with an explicit construction of a unitary or antiunitary transformation that describes the relevant symmetry. We nevertheless believe that the understanding of the theorem, especially its variant for automorphisms (Theorem A.21), gives a clearer perspective on symmetry transformations.

A.6.1 Statement and the Proof

Let $\mathscr{H}$ be a D dimensional Hilbert space, and denote by $M(\mathscr{H})$ the set of all (linear) operators on $\mathscr{H}$. We consider a map $\Gamma : M(\mathscr{H}) \to M(\mathscr{H})$ with the following properties.

(A1) Γ is one-to-one
(A2) For any $\hat{A}, \hat{B} \in M(\mathscr{H})$, we have $\Gamma(\hat{A}\hat{B}) = \Gamma(\hat{A})\Gamma(\hat{B})$
(A3) For any $\hat{A} \in M(\mathscr{H})$, we have $\Gamma(\hat{A}^\dagger) = \Gamma(\hat{A})^\dagger$

(A4) Γ is linear, i.e., $\Gamma(\alpha\hat{A}+\beta\hat{B})=\alpha\Gamma(\hat{A})+\beta\Gamma(\hat{B})$ for any $\hat{A}$, $\hat{B}\in M(\mathscr{H})$ and $\alpha,\beta\in\mathbb{C}$

or

(A4') Γ is antilinear, i.e., $\Gamma(\alpha\hat{A}+\beta\hat{B})=\alpha^*\Gamma(\hat{A})+\beta^*\Gamma(\hat{B})$ for any $\hat{A}$, $\hat{B}\in M(\mathscr{H})$ and $\alpha,\beta\in\mathbb{C}$.

When (A1), (A2), (A3), and (A4) hold, the map Γ is called a linear $*$-automorphism of $M(\mathscr{H})$, and when (A1), (A2), (A3), and (A4') hold, Γ is called an antilinear $*$-automorphism.[17,18]

Then we have the following theorem.[19]

Theorem A.21 (A variant of Wigner's theorem for automorphisms) *If Γ satisfies (A1), (A2), (A3), and (A4), then there exists a unitary operator $\hat{U}$ such that*

$$\Gamma(\hat{A})=\hat{U}^\dagger\hat{A}\hat{U}\quad \textit{for any } \hat{A}\in M(\mathscr{H}). \tag{A.6.1}$$

The unitary operator is unique up to a phase factor. If Γ satisfies (A1), (A2), (A3), and (A4'), then there exists an antiunitary operator $\hat{V}$ such that[20]

$$\Gamma(\hat{A})=\hat{V}^{-1}\hat{A}\hat{V}\quad \textit{for any } \hat{A}\in M(\mathscr{H}). \tag{A.6.2}$$

The antiunitary operator is unique up to a phase factor.

This theorem is closely related to but different from the original theorem proved by Wigner [10, 11], which treats a map between rays (or, equivalently, one-dimensional projections) and assumes the invariance of the inner product of two rays. See Theorem A.22 below. But Theorem A.21 is often called Wigner's theorem.

Proof We shall show that the properties (A1), (A2), and (A3), with (A4) or (A4') imply that there are two orthonormal bases $\{|\Phi_j\rangle\}_{j=1,\dots,D}$ and $\{|\Phi'_j\rangle\}_{j=1,\dots,D}$ such that

$$\Gamma(|\Phi_j\rangle\langle\Phi_k|)=|\Phi'_j\rangle\langle\Phi'_k|\quad \text{for any } j,k=1,\dots,D. \tag{A.6.3}$$

We then define $\hat{U}=\sum_{j=1}^{D}|\Phi_j\rangle\langle\Phi'_j|$, which is unitary and satisfies $\hat{U}^\dagger|\Phi_j\rangle\langle\Phi_k|\hat{U}=|\Phi'_j\rangle\langle\Phi'_k|$. When Γ satisfies (A4), we get the desired (A.6.1) from linearity. To see the uniqueness of $\hat{U}$, suppose that there is $\hat{U}'$ which also satisfies $\Gamma(\hat{A})=(\hat{U}')^\dagger\hat{A}\hat{U}'$ for any $\hat{A}\in M(\mathscr{H})$. But this and (A.6.1) imply $\hat{A}=\Gamma^{-1}(\Gamma(\hat{A}))=\hat{U}(\hat{U}')^\dagger\hat{A}\hat{U}'\hat{U}^\dagger$ for

[17] Note that (A1) and (A2) imply $\Gamma(\hat{1})=\hat{1}$.

[18] When (A3) is not required, Γ is called an automorphism. Here the symbol $*$ denotes the conjugate (in mathematicians' notation), which we denote as $\dagger$.

[19] The theorem is well-known, and can be found, e.g., in [1]. Although we only treat finite dimensional Hilbert spaces for simplicity, the theorem applies to infinite dimensional Hilbert spaces as well.

[20] See Appendix A.4.3 for antiunitary operators.

any $\hat{A} \in M(\mathscr{H})$, and hence $\hat{U}'\hat{U}^\dagger = e^{i\theta}\hat{1}$. When Γ satisfies (A4'), we set $\hat{V} = \hat{U}\hat{K}$ and $\hat{V}^{-1} = \hat{K}\hat{U}^\dagger$, where the complex-conjugation map $\hat{K}$ is defined by[21]

$$\hat{K}\Big(\sum_{j=1}^{D}\alpha_j|\Phi'_j\rangle\Big) = \sum_{j=1}^{D}(\alpha_j)^*|\Phi'_j\rangle. \tag{A.6.4}$$

The proof of the uniqueness is the same.

Let us prove (A.6.3). We note that $\Gamma(0) = 0$ because of (A4) or (A4'). Fix an arbitrary orthonormal basis $\{|\Phi_j\rangle\}_{j=1,\dots,D}$, and let $\hat{P}_j = \Gamma(|\Phi_j\rangle\langle\Phi_j|)$. Since $\hat{P}_j \neq 0$ by (A1), $(\hat{P}_j)^2 = \Gamma(|\Phi_j\rangle\langle\Phi_j||\Phi_j\rangle\langle\Phi_j|) = \Gamma(|\Phi_j\rangle\langle\Phi_j|) = \hat{P}_j$ by (A2), and $\hat{P}_j^\dagger = \hat{P}_j$ by (A3), we find that $\hat{P}_j$ is an orthogonal projection operator. Moreover since $\hat{P}_j\hat{P}_k = \Gamma(|\Phi_j\rangle\langle\Phi_j||\Phi_k\rangle\langle\Phi_k|) = 0$ if $j \neq k$, we see that $\hat{P}_j$ with $j = 1, \dots, D$ must be projections to mutually orthogonal one-dimensional subspaces. Thus there exists an orthonormal basis $\{|\widetilde{\Phi}_j\rangle\}_{j=1,\dots,D}$ such that $\hat{P}_j = \Gamma(|\Phi_j\rangle\langle\Phi_j|) = |\widetilde{\Phi}_j\rangle\langle\widetilde{\Phi}_j|$. Our goal is to modify the phases of the basis states $|\widetilde{\Phi}_j\rangle$ to get the desired $\{|\Phi'_j\rangle\}_{j=1,\dots,D}$. To begin with we set $|\Phi'_1\rangle = |\widetilde{\Phi}_1\rangle$. We thus have $\Gamma(|\Phi_1\rangle\langle\Phi_1|) = |\Phi'_1\rangle\langle\Phi'_1|$.

Let us note here that $\Gamma(|\Phi\rangle\langle\Phi|)$ is a one-dimensional projection for any $|\Phi\rangle$ such that $\|\Phi\| = 1$. To see this we only need to take an orthonormal basis which contains $|\Phi\rangle$, and repeat the above argument.

For $\ell = 2, \dots, D$, let $|\Xi_\ell\rangle = (|\Phi_1\rangle + |\Phi_\ell\rangle)/\sqrt{2}$. Then there is $|\widetilde{\Xi}_\ell\rangle$ such that $\|\widetilde{\Xi}_\ell\| = 1$, and $\Gamma(|\Xi_\ell\rangle\langle\Xi_\ell|) = |\widetilde{\Xi}_\ell\rangle\langle\widetilde{\Xi}_\ell|$. From the definition, we have

$$|\Phi_1\rangle\langle\Phi_1|\Xi_\ell\rangle\langle\Xi_\ell|\Phi_1\rangle\langle\Phi_1| = \frac{1}{2}|\Phi_1\rangle\langle\Phi_1|. \tag{A.6.5}$$

Applying Γ to the left-hand side, we get

$$\begin{aligned}\Gamma(|\Phi_1\rangle\langle\Phi_1|\Xi_\ell\rangle\langle\Xi_\ell|\Phi_1\rangle\langle\Phi_1|) &= \Gamma(|\Phi_1\rangle\langle\Phi_1|)\Gamma(|\Xi_\ell\rangle\langle\Xi_\ell|)\Gamma(|\Phi_1\rangle\langle\Phi_1|)\\ &= |\Phi'_1\rangle\langle\Phi'_1|\widetilde{\Xi}_\ell\rangle\langle\widetilde{\Xi}_\ell|\Phi'_1\rangle\langle\Phi'_1|\\ &= |\langle\widetilde{\Xi}_\ell|\Phi'_1\rangle|^2\,|\Phi'_1\rangle\langle\Phi'_1|,\end{aligned} \tag{A.6.6}$$

where we used (A2). Since this is equal to $|\Phi'_1\rangle\langle\Phi'_1|/2$ because of (A4) or (A4'), we see that $|\langle\widetilde{\Xi}_\ell|\Phi'_1\rangle| = 1/\sqrt{2}$. Then by setting $|\Xi'_\ell\rangle = e^{i\theta_\ell}|\widetilde{\Xi}_\ell\rangle$ with suitable $\theta_\ell \in \mathbb{R}$, we have $\Gamma(|\Xi_\ell\rangle\langle\Xi_\ell|) = |\Xi'_\ell\rangle\langle\Xi'_\ell|$ and $\langle\Xi'_\ell|\Phi'_1\rangle = 1/\sqrt{2}$ for any $\ell = 2, \dots, D$.

Repeating the same argument starting from another trivial identity

$$|\Phi_\ell\rangle\langle\Phi_\ell|\Xi_\ell\rangle\langle\Xi_\ell|\Phi_\ell\rangle\langle\Phi_\ell| = \frac{1}{2}|\Phi_\ell\rangle\langle\Phi_\ell|, \tag{A.6.7}$$

we find $|\langle\Xi'_\ell|\widetilde{\Phi}_\ell\rangle| = 1/\sqrt{2}$. Then setting $|\Phi'_\ell\rangle = e^{i\varphi_\ell}|\widetilde{\Phi}_\ell\rangle$ with suitable $\varphi_\ell \in \mathbb{R}$, we have $\Gamma(|\Phi_\ell\rangle\langle\Phi_\ell|) = |\Phi'_\ell\rangle\langle\Phi'_\ell|$ and $\langle\Xi'_\ell|\Phi'_\ell\rangle = 1/\sqrt{2}$ for any $\ell = 2, \dots, D$.

[21] Note that the map $\hat{K}$ is defined with respect to the basis $\{|\Phi'_j\rangle\}_{j=1,\dots,D}$.

Now we are ready to demonstrate (A.6.3). Noting that $\langle\Phi_1|\Xi_\ell\rangle\langle\Xi_\ell|\Phi_\ell\rangle = 1/2$ for $\ell = 2, \ldots, D$, we observe that

$$\begin{aligned} \Gamma(|\Phi_1\rangle\langle\Phi_\ell|) &= 2\,\Gamma(|\Phi_1\rangle\langle\Phi_1|\Xi_\ell\rangle\langle\Xi_\ell|\Phi_\ell\rangle\langle\Phi_\ell|) \\ &= 2\,|\Phi_1'\rangle\langle\Phi_1'|\Xi_\ell'\rangle\langle\Xi_\ell'|\Phi_\ell'\rangle\langle\Phi_\ell'| \\ &= |\Phi_1'\rangle\langle\Phi_\ell'|, \end{aligned} \tag{A.6.8}$$

and from (A3) that $\Gamma(|\Phi_\ell\rangle\langle\Phi_1|) = |\Phi_\ell'\rangle\langle\Phi_1'|$. We then have, for any $j, k = 1, \ldots, D$, that

$$\Gamma(|\Phi_j\rangle\langle\Phi_k|) = \Gamma(|\Phi_j\rangle\langle\Phi_1|\Phi_1\rangle\langle\Phi_k|) = |\Phi_j'\rangle\langle\Phi_1'|\Phi_1'\rangle\langle\Phi_k'| = |\Phi_j'\rangle\langle\Phi_k'|, \tag{A.6.9}$$

which is the desired (A.6.3). ∎

For the reader's reference, we discuss the original theorem of Wigner's. Consider a D dimensional Hilbert space $\mathscr{H}$ with $D \geq 2$, and let $\mathscr{P}_1$ be the set of all one-dimensional orthogonal projection operators on $\mathscr{H}$. Note that $|\Phi\rangle\langle\Phi| \in \mathscr{P}_1$ and $|\Psi\rangle\langle\Psi| \in \mathscr{P}_1$ are regarded as the same element if $|\Phi\rangle = e^{i\theta}|\Psi\rangle$. Also note that, for $\hat{P} = |\Phi\rangle\langle\Phi| \in \mathscr{P}_1$ and $\hat{P}' = |\Phi'\rangle\langle\Phi'| \in \mathscr{P}_1$, we have $\mathrm{Tr}[\hat{P}\,\hat{P}'] = |\langle\Phi|\Phi'\rangle|^2$.

Theorem A.22 (Wigner's theorem) *Suppose that there is a map $\widetilde{\Gamma} : \mathscr{P}_1 \to \mathscr{P}_1$ such that $\mathrm{Tr}[\hat{P}\,\hat{P}'] = \mathrm{Tr}[\widetilde{\Gamma}(\hat{P})\,\widetilde{\Gamma}(\hat{P}')]$ for any $\hat{P}, \hat{P}' \in \mathscr{P}_1$. Then there exists an operator $\hat{V}$, which is either unitary or antiunitary, such that*

$$\widetilde{\Gamma}(\hat{P}) = \hat{V}\,\hat{P}\,\hat{V}^{-1} \quad \textit{for any } \hat{P} \in \mathscr{P}_1. \tag{A.6.10}$$

The (anti)unitary operator $\hat{V}$ is unique up to a phase factor.

For details, we recommend Bargmann's paper [2], which contains a clear and readable proof as well as a careful discussion of the statement.

A.6.2 Applications

Theorem A.21 guarantees the existence of an (anti)unitary operator once we write down an (anti)linear $*$-automorphism of operators. This is certainly useful.

Spin systems Consider a general quantum spin system, as formulated in Sect. 2.2. We first recall that any operator of a quantum spin system is written as a polynomial of the spin operators $\hat{S}_x^{(\alpha)}$ with $x \in \Lambda$ and $\alpha = 1, 2, 3$. See Problem 2.1.a. Therefore to define a $*$-automorphism for a spin system, one only needs to specify the transformation of $\hat{S}_x^{(\alpha)}$ for each $x \in \Lambda$ and $\alpha = 1, 2, 3$. Here one also has to check whether the transformation is consistent with the commutation relations (2.2.6), such as $[\hat{S}_x^{(1)}, \hat{S}_x^{(2)}] = i\,\hat{S}_x^{(3)}$.

As a simple example, define the linear $*$-automorphism Γ_1 by $\Gamma_1(\hat{S}_x^{(1)}) = \hat{S}_x^{(1)}$, $\Gamma_1(\hat{S}_x^{(2)}) = -\hat{S}_x^{(2)}$, and , $\Gamma_1(\hat{S}_x^{(3)}) = -\hat{S}_x^{(3)}$. It is obvious from (2.1.21) that this automorphism is realized by the π rotation about the 1-axis, but the existence of a unitary transformation is guaranteed by Theorem A.21 once we check that the above transformation and linearity is consistent with the commutation relations. Similarly, we can be sure that the linear $*$-automorphism defined by $\Gamma_{231}(\hat{S}_x^{(1)}) = \hat{S}_x^{(2)}$, $\Gamma_{231}(\hat{S}_x^{(2)}) = \hat{S}_x^{(3)}$, and $\Gamma_{231}(\hat{S}_x^{(3)}) = \hat{S}_x^{(1)}$ can be realized by a unitary transformation, without examining how it can be done by combining $\pi/2$-rotations.

An important example is the time-reversal transformation discussed in detail in Sect. 2.3. In this case, corresponding to (2.3.23), we start from the basic transformation rules $\Gamma_{\rm tr}(\hat{S}_x^{(1)}) = -\hat{S}_x^{(1)}$, $\Gamma_{\rm tr}(\hat{S}_x^{(2)}) = -\hat{S}_x^{(2)}$, and $\Gamma_{\rm tr}(\hat{S}_x^{(3)}) = -\hat{S}_x^{(3)}$. Now it is clear that this rule is consistent with the commutation relations only when we assume $\Gamma_{\rm tr}$ is an antilinear $*$-automorphism. Then the theorem shows that the time-reversal transformation is realized by an antiunitary operator, which we called $\hat{\Theta}$ in Sect. 2.3. This approach is illuminating since the definition of $\hat{\Theta}$ in Sect. 2.3 looks rather ad hoc; given only the definition, one hardly understands the basic principle which guarantees the existence of the operator. Similarly we see, without any examination, that the antilinear $*$-automorphism defined by $\Gamma_{321}(\hat{S}_x^{(1)}) = \hat{S}_x^{(3)}$, $\Gamma_{321}(\hat{S}_x^{(2)}) = \hat{S}_x^{(2)}$, and $\Gamma_{321}(\hat{S}_x^{(3)}) = \hat{S}_x^{(1)}$ can be realized by an antiunitary operator.

Electron systems Theorem A.21 also sheds light on the transformations for the Hubbard model discussed in Sect. 9.3.3. As a rather trivial example, the gauge transformation (9.3.37) is characterize by the liner $*$-automorphism Γ_θ specified by $\Gamma_\theta(\hat{c}_{x,\sigma}^\dagger) = e^{i\theta_x}\,\hat{c}_{x,\sigma}^\dagger$. Much more complicated Shiba transformation, for example, can also be fully characterized by only specifying the transformation rule (9.3.51) and checking its consistency with the anticommutation relations (9.2.27) and (9.2.28).

Let us finally formulate the time-reversal transformation for electron systems, although we do not make use of the transformation in the main text. It is convenient to first define an antilinear $*$-automorphism $\Gamma_{\rm tr}$ by $\Gamma_{\rm tr}(\hat{c}_{x,\uparrow}) = \hat{c}_{x,\downarrow}$ and $\Gamma_{\rm tr}(\hat{c}_{x,\downarrow}) = -\hat{c}_{x,\uparrow}$. The transformation is clearly consistent with the anticommutation relations (9.2.27) and (9.2.28). In this case the corresponding antiunitary operator $\hat{\Theta}$ is constructed explicitly, without invoking Wigner's theorem, by demanding $\hat{\Theta}|\Phi_{\rm vac}\rangle = |\Phi_{\rm vac}\rangle$ and $\hat{\Theta}(\hat{A}|\Phi_{\rm vac}\rangle) = \Gamma_{\rm tr}(\hat{A})|\Phi_{\rm vac}\rangle$ for any operator $\hat{A}$. It is easily checked that the resulting $\hat{\Theta}$ is consistent with that defined in Sect. 2.3.

A.7 Operator Algebraic Formulation of Infinite Systems

In this appendix, we present a brief description of the operator algebraic formulation of quantum spin systems on infinite lattices. Although we have mostly avoided the use of this mathematical formulation in the book, it plays important roles in Sects. 4.3, 7.1.1, and 8.3.6. It is probably a good idea to discuss basic notions for the interested reader. We here describe basic definitions and theorems, without going into proofs. The motivated reader is invited to study Bratteli and Robinson's definitive textbook [4, 5] on the operator algebraic approach to quantum many-body systems.

Operator algebra We consider a quantum spin system with spin quantum number S on the infinite d-dimensional hypercubic lattice $\mathbb{Z}^d$. As in Sect. 2.2, we associate a local Hilbert space $\mathfrak{h}_x \cong \mathbb{C}^{2S+1}$ with each site $x \in \mathbb{Z}^d$. We do not however introduce the Hilbert space of the whole system. We again denote by $\hat{S}_x^{(\alpha)}$ for $x \in \mathbb{Z}^d$ and $\alpha = 1, 2, 3$ the α-component of the spin operator at site x. It acts as the operator $\hat{S}^{(\alpha)}$ determined by (2.1.2) and (2.1.3) on the space $\mathfrak{h}_x$ and as the identity operator on other $\mathfrak{h}_y$ with $y \in \mathbb{Z}^d \backslash \{x\}$. We can thus consider products and linear combinations of the operators $\hat{S}_x^{(\alpha)}$ for $x \in \mathbb{Z}^d$ and $\alpha = 1, 2, 3$. We can also take the conjugation (i.e., the mapping $\hat{A} \to \hat{A}^\dagger$) of all such operators. The set of operators formed in this manner plays a central role in this formulation.

Let $\mathfrak{A}_{\mathrm{loc}}$ be the algebra of local operators, i.e., the set of all polynomials (with complex coefficients) of the spin operators $\hat{S}_x^{(\alpha)}$ with $x \in \mathbb{Z}^d$ and $\alpha = 1, 2, 3$. By definition, each $\hat{A} \in \mathfrak{A}_{\mathrm{loc}}$ is an operator which depends only on a finite number of spins, but there is no limit for this finite number. For $\hat{A} \in \mathfrak{A}_{\mathrm{loc}}$ let $\mathrm{supp}\, \hat{A}$ be its support, i.e., the set of sites on which $\hat{A}$ acts nontrivially. For example, $\mathrm{supp}\, \hat{S}_x^{(\alpha)} = \{x\}$ and $\mathrm{supp}(a\, \hat{S}_x^{(\alpha)} + b\, \hat{S}_y^{(\beta)} \hat{S}_z^{(\gamma)}) = \{x, y, z\}$. (We define $\mathrm{supp}\, \hat{1} = \emptyset$.) Note that we can define the operator norm $\|\hat{A}\|$ for $\hat{A} \in \mathfrak{A}_{\mathrm{loc}}$ by identifying $\hat{A}$ with the corresponding operator on the finite dimensional Hilbert space $\bigotimes_{x \in \mathrm{supp}\, \hat{A}} \mathfrak{h}_x$ and by using the definition (A.2.3).

Physically speaking, $\mathfrak{A}_{\mathrm{loc}}$ is all we need to describe quantum spin systems on $\mathbb{Z}^d$. However it is mathematically convenient to slightly enlarge $\mathfrak{A}_{\mathrm{loc}}$ to make it into a C^*-algebra[22] as

$$\mathfrak{A} := \overline{\mathfrak{A}_{\mathrm{loc}}}, \tag{A.7.1}$$

where the bar denotes the completion with respect to the operator norm.

States Let us discuss the notion of states on the C^*-algebra $\mathfrak{A}$. Since we have not introduced Hilbert spaces, we are not able to talk about vector states such as $|\Phi\rangle$. Instead we shall characterize a state by specifying the corresponding expectation value of any operator in $\mathfrak{A}$.

Definition A.23 A state $\rho(\cdot)$ of a quantum spin system is a linear map from $\mathfrak{A}$ to $\mathbb{C}$ that satisfies $\rho(\hat{1}) = 1$ and $\rho(\hat{A}^\dagger \hat{A}) \geq 0$ for any $\hat{A} \in \mathfrak{A}$.

It follows from the definition that $|\rho(\hat{A})| \leq \|\hat{A}\|$ for any $\hat{A} \in \mathfrak{A}$.

The idea behind the definition is that $\rho(\hat{A})$ is the expectation value of the operator $\hat{A}$ in the state $\rho(\cdot)$. To give a simple (but important) class of examples, let $|\Phi\rangle$ be an arbitrary state in the Hilbert space $\bigotimes_{x \in \Lambda} \mathfrak{h}_x$, where Λ is a finite subset of $\mathbb{Z}^d$. Take an arbitrary monomial $\prod_{x \in S} (\hat{S}_x^{(\alpha_x)})^{n_x}$ of spin operators and define

$$\rho\Big(\prod_{x \in S} (\hat{S}_x^{(\alpha_x)})^{n_x}\Big) = \langle \Phi | \prod_{x \in S \cap \Lambda} (\hat{S}_x^{(\alpha_x)})^{n_x} | \Phi \rangle \prod_{x \in S \backslash \Lambda} \frac{\mathrm{Tr}_x\big[(\hat{S}_x^{(\alpha_x)})^{n_x}\big]}{\mathrm{Tr}_x[1]}, \tag{A.7.2}$$

[22] In general a C^*-algebra is a Banach *-algebra with the property $\|A^* A\| = \|A\|^2$ for any A.

where the trace is taken over the single spin Hilbert space $\mathfrak{h}_x$. Then we can define $\rho(\hat{A})$ for any $\hat{A} \in \mathfrak{A}_{\rm loc}$ by linearity (and then extend $\rho(\cdot)$ to the whole $\mathfrak{A}$).

We have the following abstract but useful property of the set of all states.

Theorem A.24 (Banach–Alaoglu theorem) *The set of all states on $\mathfrak{A}$ is compact with respect to the weak-$*$ topology.*

The above statement probably does not make sense to most readers. Here is an elementary interpretation (in the case of quantum spin systems). Let $\rho_j(\cdot)$ with $j = 1, 2, \dots$ be an arbitrary infinite sequence of states on $\mathfrak{A}$. Then there always exist a state ρ_∞ and a subsequence $j(i)$ with $i = 1, 2, \dots$ and $j(i) < j(i+1)$ such that

$$\lim_{i \uparrow \infty} \rho_{j(i)}(\hat{A}) = \rho_\infty(\hat{A}), \tag{A.7.3}$$

for any $\hat{A} \in \mathfrak{A}$. This property is useful for us when considering infinite volume limits. See (4.3.7).

Ground states In order to define the notion of ground states, we need to introduce the Hamiltonian of the system. The central object is the local Hamiltonian $\hat{h}_x \in \mathfrak{A}_{\rm loc}$ associated with each site $x \in \mathbb{Z}^d$. We assume, for any $x \in \mathbb{Z}^d$, that $\operatorname{supp} \hat{h}_x \subset \{y \in \mathbb{Z}^d \mid |y - x| \le R\}$ for a fixed constant R, and $\|\hat{h}_x\| \le h_0$ for another fixed constant h_0. Note that all the Hamiltonians for quantum spin systems studied in the book (except for that of the toy model (2.5.10)) can be written as a sum of such local Hamiltonians. We can formally write the total Hamiltonian as $\hat{H} = \sum_{x \in \mathbb{Z}^d} \hat{h}_x$, but note that $\hat{H}$ belongs neither to $\mathfrak{A}_{\rm loc}$ nor $\mathfrak{A}$. More importantly we can define the commutator between the Hamiltonian and an arbitrary local operator $\hat{A} \in \mathfrak{A}_{\rm loc}$ as

$$[\hat{H}, \hat{A}] := \Big[\sum_{x \in \Lambda_L} \hat{h}_x, \hat{A} \Big] \in \mathfrak{A}_{\rm loc}, \tag{A.7.4}$$

for sufficiently large L, where Λ_L is the $L \times \cdots \times L$ hypercubic lattice defined in (3.1.2). We here noted that the commutator in the right-hand side does not depend on L when L is taken sufficiently large so that $[\hat{A}, \hat{h}_x] = 0$ for any x outside Λ_L. Then the following is the standard definition of a ground state.

Definition A.25 A state $\omega(\cdot)$ is a ground state of a quantum spin system on $\mathbb{Z}^d$ with the Hamiltonian $\hat{H}$ if and only if $\omega(\hat{A}^\dagger[\hat{H}, \hat{A}]) \ge 0$ for any $\hat{A} \in \mathfrak{A}_{\rm loc}$.

The motivation for the definition is easily understood by noting that the finite volume version of the condition reads $\langle \Phi_{\rm GS} | \hat{A}^\dagger [\hat{H}, \hat{A}] | \Phi_{\rm GS} \rangle \ge 0$, which is rewritten as $\langle \Phi_{\rm GS} | \hat{A}^\dagger \hat{H} \hat{A} | \Phi_{\rm GS} \rangle \ge E_{\rm GS} \langle \Phi_{\rm GS} | \hat{A}^\dagger \hat{A} | \Phi_{\rm GS} \rangle$. When $\hat{A} | \Phi_{\rm GS} \rangle \ne 0$, this inequality becomes

$$\langle \Psi | \hat{H} | \Psi \rangle \ge E_{\rm GS}, \tag{A.7.5}$$

with a normalized state $|\Psi\rangle = \hat{A}|\Phi_{\rm GS}\rangle / \|\hat{A}|\Phi_{\rm GS}\rangle\|$. Thus the condition in the definition simply says that one cannot lower the energy of the state ω by a local perturbation

$\hat{A}$. It is remarkable that Definition A.25 fully characterizes a state of the infinite system only in terms of the expectation values of local operators.

Let us give another characterization of the ground states in terms of the variational principle. For each $L = 1, 2, \ldots$, let

$$\hat{H}_L := \sum_{x \in \overline{\Lambda}_L} \hat{h}_x, \tag{A.7.6}$$

where $\overline{\Lambda}_L := \{x \in \mathbb{Z}^d \,\big|\, |x - y| \leq R \text{ for some } y \in \Lambda_L\}$. Note that we have enlarged the lattice so that to include in the sum all $\hat{h}_x$ whose support may overlap with Λ_L. We also define $\mathscr{C}_L^\omega$ to be the set of all states that coincide with $\omega(\cdot)$ outside Λ_L. More precisely, $\mathscr{C}_L^\omega$ consists of states $\omega'(\cdot)$ such that $\omega(\hat{A}) = \omega'(\hat{A})$ for any $\hat{A} \in \mathfrak{A}_{\text{loc}}$ such that $\operatorname{supp} \hat{A} \cap \Lambda_L = \emptyset$.

Theorem A.26 *A state $\omega(\cdot)$ is a ground state of a quantum spin system on $\mathbb{Z}^d$ with the Hamiltonian $\hat{H}$ if and only if*

$$\omega(\hat{H}_L) = \inf_{\omega' \in \mathscr{C}_L^\omega} \omega'(\hat{H}_L), \tag{A.7.7}$$

for any L.

The theorem states that a ground state is a state that minimizes the partial Hamiltonian $\hat{H}_L$ for any L. The reader with background in physics probably find this characterization plausible. For a proof, see the Proof of Theorem 6.2.52 in [5].

Let us finally state what we mean by a unique ground state with a nonzero gap.

Definition A.27 Let $\omega(\cdot)$ be a ground state of a quantum spin system on $\mathbb{Z}^d$ with the Hamiltonian $\hat{H}$, and further assume that $\omega(\cdot)$ is the unique ground state.[23] We say that $\omega(\cdot)$ is accompanied by a nonzero energy gap if and only if there is a constant $\gamma > 0$, and $\omega(\hat{A}^\dagger[\hat{H}, \hat{A}]) \geq \gamma\, \omega(\hat{A}^\dagger \hat{A})$ for any $\hat{A} \in \mathfrak{A}_{\text{loc}}$ such that $\omega(\hat{A}) = 0$.

The motivation of the definition becomes clear again by considering the corresponding relations in a finite system. By using the same $|\Psi\rangle$ as in (A.7.5), we see that the conditions read $\langle\Psi|\hat{H}|\Psi\rangle \geq E_{\text{GS}} + \gamma$ and $\langle\Phi_{\text{GS}}|\Psi\rangle = 0$. These are the conditions that $|\Phi_{\text{GS}}\rangle$ is a unique ground state with a nonzero gap.

Gelfand–Naimark–Segal (GNS) construction Let $\mathscr{H}$ be a Hilbert space, and denote by $B(\mathscr{H})$ the set of all bounded operators on $\mathscr{H}$. A pair $(\mathscr{H}, \pi)$, where π is a map from a C^*-algebra $\mathfrak{A}$ to $B(\mathscr{H})$, is said to be a representation of $\mathfrak{A}$ if

[23] Here it is only necessary in general to require that $\omega(\cdot)$ is the unique ground state in the corresponding GNS Hilbert space. This means that the energy gap associated with a symmetry breaking ground state of the quantum Ising model (see Sect. 3.3) can be characterized by this definition.

$$\pi(\alpha\hat{A} + \beta\hat{B}) = \alpha\,\pi(\hat{A}) + \beta\,\pi(\hat{B}), \tag{A.7.8}$$

$$\pi(\hat{A}\hat{B}) = \pi(\hat{A})\pi(\hat{B}), \tag{A.7.9}$$

$$\pi(\hat{A}^\dagger) = \pi(\hat{A})^\dagger, \tag{A.7.10}$$

for any $\alpha, \beta \in \mathbb{C}$ and $\hat{A}, \hat{B} \in \mathfrak{A}$.

When a C^*-algebra and a state are given, one can go through a standard procedure known as the Gelfand–Naimark–Segal (GNS) construction to define a representation of the C^*-algebra. In the present context, we get the following.

Theorem A.28 (GNS construction) *Let $\rho(\cdot)$ be a state on $\mathfrak{A}$. Then there exist a separable Hilbert space $\mathscr{H}_\rho$, a map $\pi_\rho : \mathfrak{A} \to B(\mathscr{H}_\rho)$, and a vector Ω_ρ such that $(\mathscr{H}_\rho, \pi_\rho)$ is a representation of $\mathfrak{A}$, and*

$$\rho(\hat{A}) = \langle \Omega_\rho, \pi_\rho(\hat{A})\,\Omega_\rho \rangle, \tag{A.7.11}$$

for any $\hat{A} \in \mathfrak{A}$. Here $\langle \cdot, \cdot \rangle$ denotes the inner product of $\mathscr{H}_\rho$. The set of vectors $\{\pi_\rho(\hat{A})\,\Omega_\rho \mid \hat{A} \in \mathfrak{A}\}$ is dense in the Hilbert space $\mathscr{H}_\rho$.

$(\mathscr{H}_\rho, \pi_\rho, \Omega_\rho)$ is called the GNS triple for the state $\rho(\cdot)$.

Remarkably (A.7.11) shows that an arbitrary state $\rho(\cdot)$ can be expressed as a vector state Ω_ρ in the Hilbert space $\mathscr{H}_\rho$. Physically speaking, $\mathscr{H}_\rho$ may be interpreted as a Hilbert space that contains the original state $\rho(\cdot)$ (now represented as Ω_ρ) and other states obtained by locally perturbing it. Such a "small" Hilbert space is indeed suitable for various applications in physics problems.

The Idea of the Proof of Theorem A.28 Let us discuss the basic idea of the GNS construction. We believe it is illuminating also to the readers who are not interested in abstract mathematical theories. See, e.g., Sect. 2.3.3 of [4] for a complete proof.

To construct the Hilbert space $\mathscr{H}_\rho$, we recall that the C^*-algebra $\mathfrak{A}$ itself is a linear space. We shall regard its elements $\hat{A}, \hat{B}, \ldots$ as "vectors", and define their inner products by using the state $\rho(\cdot)$ as

$$\langle \hat{A}, \hat{B} \rangle := \rho(\hat{A}^\dagger \hat{B}). \tag{A.7.12}$$

Of course $\mathfrak{A}$ is not yet a proper vector space with an inner product since there may be a nonzero $\hat{A}$ such that $\langle \hat{A}, \hat{A} \rangle = 0$. We thus define an equivalence relation $\sim$ by

$$\hat{A} \sim \hat{B} \iff \langle (\hat{A} - \hat{B}), (\hat{A} - \hat{B}) \rangle = 0. \tag{A.7.13}$$

The desired Hilbert space is then obtained as the completion of the quotient space as $\mathscr{H}_\rho := \overline{\mathfrak{A}/\!\sim}$.

By definition the quotient space $\mathfrak{A}/\!\sim$ consists of equivalence classes $\psi_{\hat{B}} = \{\hat{B}' \mid \hat{B}' \sim \hat{B}\}$, whose inner products are given by $\langle \psi_{\hat{B}}, \psi_{\hat{C}} \rangle = \langle \hat{B}, \hat{C} \rangle$. We can naturally define the representation π_ρ by $\pi_\rho(\hat{A})\psi_{\hat{B}} = \psi_{\hat{A}\hat{B}}$ for any $\hat{A}, \hat{B} \in \mathfrak{A}$. It is

automatic to extend π_ρ to the whole Hilbert space $\mathscr{H}_\rho$. Finally we set $\Omega_\rho = \psi_{\hat{1}}$. Then for any $\hat{A} \in \mathfrak{A}$, we see that

$$\langle \Omega_\rho, \pi_\rho(\hat{A})\Omega_\rho \rangle = \langle \psi_{\hat{1}}, \psi_{\hat{A}} \rangle = \langle \hat{1}, \hat{A} \rangle = \rho(\hat{A}), \tag{A.7.14}$$

which is the desired (A.7.11). ∎

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Solutions

Problems of Chap. 2

2.1.a (p. 15) Note first that the projection operator onto the basis state $|\psi^\sigma\rangle$ is written as

$$|\psi^\sigma\rangle\langle\psi^\sigma| = \prod_{\substack{\tau=-S \\ (\tau\neq\sigma)}}^{S} \left(\frac{\hat{S}^{(3)} - \tau\hat{1}}{\sigma - \tau} \right). \tag{S.1}$$

This is easily verified by applying the right-hand side to any basis state $|\psi^{\sigma'}\rangle$. Then, by suitably applying $\hat{S}^{\pm}$ and normalizing, one gets $|\psi^\tau\rangle\langle\psi^\sigma|$ for any τ and σ. Since any matrix can be written as a linear combination of $|\psi^\tau\rangle\langle\psi^\sigma|$, we see that the desired property holds.

2.1.b (p. 18) From (2.1.7) one finds $(2\hat{S}^{(\alpha)})^n = \hat{1}$ for even n and $(2\hat{S}^{(\alpha)})^n = 2\hat{S}^{(\alpha)}$ for odd n. By using the definition (A.2.16) of the exponential, we find

$$\begin{aligned} e^{-i\theta\hat{S}^{(\alpha)}} &= \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{-i\theta}{2} \right)^n (2\hat{S}^{(\alpha)})^n = \sum_{n:\text{even}} \frac{1}{n!} \left(\frac{-i\theta}{2} \right)^n \hat{1} + \sum_{n:\text{odd}} \frac{1}{n!} \left(\frac{-i\theta}{2} \right)^n 2\hat{S}^{(\alpha)} \\ &= \left(\cos\frac{\theta}{2} \right) \hat{1} - 2i \left(\sin\frac{\theta}{2} \right) \hat{S}^{(\alpha)}. \end{aligned} \tag{S.2}$$

See the solution to Problem 2.1.c below for two other strategies.

2.1.c (p. 18) For $S = 1$, (2.1.9) implies $(\hat{S}^{(\alpha)})^3 = \hat{S}^{(\alpha)}$. One can then proceed as in the solution to Problem 2.1.b above, but let us show another derivation. The relation $(\hat{S}^{(\alpha)})^3 = \hat{S}^{(\alpha)}$ implies that one has $e^{-i\theta\hat{S}^{(\alpha)}} = a(\theta)\hat{1} + b(\theta)\hat{S}^{(\alpha)} + c(\theta)(\hat{S}^{(\alpha)})^2$ with coefficients $a(\theta)$, $b(\theta)$, and $c(\theta)$ whose initial conditions are $a(0) = 1$ and $b(0) = c(0) = 0$. By noting that $de^{-i\theta\hat{S}^{(\alpha)}}/d\theta = -i\hat{S}^{(\alpha)}e^{-i\theta\hat{S}^{(\alpha)}}$, we find that the coefficients satisfy the set of differential equations $a'(\theta) = 0$, $b'(\theta) = -i\{a(\theta) + c(\theta)\}$, and $c'(\theta) = -ib(\theta)$, whose unique solution is $a(\theta) = 1, b(\theta) = -i\sin\theta$, and $c(\theta) =$

H. Tasaki, *Physics and Mathematics of Quantum Many-Body Systems*,
Graduate Texts in Physics, https://doi.org/10.1007/978-3-030-41265-4

$\cos\theta - 1$. We thus find

$$\hat{U}_\theta^{(\alpha)} = \hat{1} - i(\sin\theta)\hat{S}^{(\alpha)} + (\cos\theta - 1)(\hat{S}^{(\alpha)})^2. \tag{S.3}$$

Let us show the third derivation which is the simplest (but may look a bit tricky). From (2.1.9), one readily finds that $e^{-i\theta\hat{S}^{(3)}} = \begin{pmatrix} e^{-i\theta} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & e^{i\theta} \end{pmatrix}$, from which one can read off the desired relation (S.3) for $\alpha = 3$. But this implies (S.3) for $\alpha = 1$ and 2 as well, since all the spin operators have the same algebraic properties.

2.1.d (p. 18) Substituting (2.1.7) into (2.1.26) we obtain

$$\hat{U}_\theta^{(1)} = \begin{pmatrix} \cos\frac{\theta}{2} & -i\sin\frac{\theta}{2} \\ -i\sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{pmatrix}, \ \hat{U}_\theta^{(2)} = \begin{pmatrix} \cos\frac{\theta}{2} & -\sin\frac{\theta}{2} \\ \sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{pmatrix}, \ \hat{U}_\theta^{(3)} = \begin{pmatrix} e^{-i\theta/2} & 0 \\ 0 & e^{i\theta/2} \end{pmatrix}. \tag{S.4}$$

By using this we find

$$|\psi_{\theta,\varphi}\rangle = \begin{pmatrix} e^{-i\theta/2} & 0 \\ 0 & e^{i\theta/2} \end{pmatrix} \begin{pmatrix} \cos\frac{\theta}{2} & -\sin\frac{\theta}{2} \\ \sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} e^{-i\varphi/2}\cos\frac{\theta}{2} \\ e^{i\varphi/2}\sin\frac{\theta}{2} \end{pmatrix}. \tag{S.5}$$

We next see from (2.1.7) that

$$\hat{\boldsymbol{S}} \cdot \boldsymbol{n}(\theta,\varphi) = \frac{1}{2} \begin{pmatrix} \cos\theta & e^{-i\varphi}\sin\theta \\ e^{i\varphi}\sin\theta & -\cos\theta \end{pmatrix}. \tag{S.6}$$

Then the desired relation $\{\hat{\boldsymbol{S}} \cdot \boldsymbol{n}(\theta,\varphi)\}|\psi_{\theta,\varphi}\rangle = (1/2)|\psi_{\theta,\varphi}\rangle$ can be checked directly (with a little bit of calculation). Another (more illuminating) way to confirm the relation is to first note that (2.1.20) implies $\hat{U}\hat{S}^{(3)}\hat{U}^\dagger = \hat{\boldsymbol{S}} \cdot \boldsymbol{n}(\theta,\varphi)$ where $\hat{U} = \hat{U}_\varphi^{(3)}\hat{U}_\theta^{(2)}$. We then have

$$\{\hat{\boldsymbol{S}} \cdot \boldsymbol{n}(\theta,\varphi)\}|\psi_{\theta,\varphi}\rangle = \hat{U}\hat{S}^{(3)}\hat{U}^\dagger\hat{U}|\psi^\uparrow\rangle = \frac{1}{2}\hat{U}|\psi^\uparrow\rangle = \frac{1}{2}|\psi_{\theta,\varphi}\rangle. \tag{S.7}$$

2.1.e (p. 18) From (S.5), we have $|\psi_{(0,1,0)}\rangle = (e^{-i(\pi/4)}, e^{i(\pi/4)})^{\mathrm{t}}/\sqrt{2}$. By using (S.4), we find that

$$|\psi'_{(0,1,0)}\rangle = \hat{U}_{-\pi/2}^{(1)}|\psi^\uparrow\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & i \\ i & 1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ i \end{pmatrix}. \tag{S.8}$$

We see that $|\psi'_{(0,1,0)}\rangle = e^{i(\pi/4)}|\psi_{(0,1,0)}\rangle$.

To work out the case with $S = 1$ explicitly, we use (S.3) and (2.1.9) to see that

$$\hat{U}^{(1)}_{-\pi/2} = \frac{1}{2}\begin{pmatrix} 1 & \sqrt{2}\,i & -1 \\ \sqrt{2}\,i & 0 & \sqrt{2}\,i \\ -1 & \sqrt{2}\,i & 1 \end{pmatrix}, \quad \hat{U}^{(2)}_{\pi/2} = \frac{1}{2}\begin{pmatrix} 1 & -\sqrt{2} & 1 \\ \sqrt{2} & 0 & -\sqrt{2} \\ 1 & \sqrt{2} & 1 \end{pmatrix},$$

$$\hat{U}^{(3)}_{\pi/2} = \frac{1}{\sqrt{2}}\begin{pmatrix} -i & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & i \end{pmatrix}. \tag{S.9}$$

Recalling that $|\psi^1\rangle = (1, 0, 0)^{\mathrm{t}}$, we find

$$|\psi_{(0,1,0)}\rangle = \hat{U}^{(3)}_{\pi/2}\,\hat{U}^{(2)}_{\pi/2}|\psi^1\rangle = \frac{1}{2}\begin{pmatrix} -i \\ \sqrt{2} \\ i \end{pmatrix}, \tag{S.10}$$

$$|\psi'_{(0,1,0)}\rangle = \hat{U}^{(1)}_{-\pi/2}|\psi^1\rangle = \frac{1}{2}\begin{pmatrix} 1 \\ \sqrt{2}\,i \\ -1 \end{pmatrix}, \tag{S.11}$$

which shows that $|\psi'_{(0,1,0)}\rangle = i\,|\psi_{(0,1,0)}\rangle$. In fact the final relation can be obtained from the result for $S = 1/2$ by noting that a spin with $S = 1$ can be represented by two spins with $S = 1/2$. See Appendix A.3.3 and the expression (2.4.11).

2.1.f (p. 19) A 180° rotation about the y-axis followed by a 180° rotation about the x-axis is equivalent to a 180° rotation about the z-axis. One my confirm this fact easily by, for example, turning a box around.

2.1.g (p. 20) The expression (2.1.34) for $\hat{u}_3$ is obvious. The basis state $|\psi^\sigma\rangle$ (with $\sigma = -S, \ldots, S$) of a spin S can be represented as

$$|\psi^\sigma\rangle = \binom{2S}{n_\uparrow}^{-1/2} \sum_{\substack{\sigma_1,\ldots,\sigma_{2S}=\pm 1/2 \\ (\sum \sigma_j = \sigma)}} |\psi_1^{\sigma_1}\rangle \otimes \cdots \otimes |\psi_{2S}^{\sigma_{2S}}\rangle, \tag{S.12}$$

where $|\psi_j^{\sigma_j}\rangle$ (with $\sigma_j = \pm 1/2$ and $j = 1, \ldots, 2S$) is the basis state of a spin 1/2. There are $n_\uparrow = S + \sigma$ spins with $\sigma_j = 1/2$, and $n_\downarrow = S - \sigma$ spins with $\sigma_j = -1/2$ in each term of (S.12). The expression (S.12) is nothing but (2.4.11). The original spin operator $\hat{S}^{(\alpha)}$ (which is the total spin operator in the present context) is then represented as $\hat{S}^{(\alpha)} = \sum_{j=1}^{2S} \hat{S}_j^{(\alpha)}$, where $\hat{S}_j^{(\alpha)}$ acts on $|\psi_j^\sigma\rangle$. Since $e^{-i\pi \hat{S}_j^{(\alpha)}} = -2i\,\hat{S}_j^{(\alpha)}$, one finds

$$e^{-i\pi \hat{S}^{(\alpha)}} = \prod_{j=1}^{2S}(-2i\,\hat{S}_j^{(\alpha)}) = \begin{cases} (-i)^{2S}\prod_{j=1}^{2S}(\hat{S}_j^+ + \hat{S}_j^-) & \text{if } \alpha = 1, \\ \prod_{j=1}^{2S}(-\hat{S}_j^+ + \hat{S}_j^-) & \text{if } \alpha = 2. \end{cases} \tag{S.13}$$

Recalling that $\hat{S}_j^\pm |\psi_j^{\mp 1/2}\rangle = |\psi_j^{\pm 1/2}\rangle$, one gets (2.1.34) by inspection.

2.2.a (p. 23) The first part is obvious from (2.1.25) for a single spin and the definition (2.2.11). To show the orthogonality, suppose that $\hat{U}_\pi^{(\alpha)}|\Phi\rangle = c|\Phi\rangle$. Note that we have $|c| = 1$. Then observe that $\hat{U}_\pi^{(\alpha)}(\hat{U}_\pi^{(\beta)}|\Phi\rangle) = -\hat{U}_\pi^{(\beta)}\hat{U}_\pi^{(\alpha)}|\Phi\rangle = -c\hat{U}_\pi^{(\beta)}|\Phi\rangle$. Thus $\hat{U}_\pi^{(\beta)}|\Phi\rangle$ is also an eigenstate of $\hat{U}_\pi^{(\alpha)}$ with eigenvalue $-c$. We thus see that $|\Phi\rangle$ and $\hat{U}_\pi^{(\beta)}|\Phi\rangle$ are orthogonal.

2.2.b (p. 23) From the solution to Problem 2.1.d (and a similar computation of $e^{-i\varphi\hat{S}^{(3)}}e^{-i\theta\hat{S}^{(2)}}|\psi^\downarrow\rangle$) we find

$$\begin{aligned}\hat{U}_\varphi^{(3)}\hat{U}_\theta^{(2)}\,|\uparrow\rangle_1|\downarrow\rangle_2 =&\big(e^{-i\varphi/2}\cos\tfrac{\theta}{2}|\uparrow\rangle_1 + e^{i\varphi/2}\sin\tfrac{\theta}{2}|\downarrow\rangle_1\big)\\ &\otimes\big(-e^{-i\varphi/2}\sin\tfrac{\theta}{2}|\uparrow\rangle_2 + e^{i\varphi/2}\cos\tfrac{\theta}{2}|\downarrow\rangle_2\big)\\ =&-e^{-i\varphi}\cos\tfrac{\theta}{2}\sin\tfrac{\theta}{2}|\uparrow\rangle_1|\uparrow\rangle_2 + e^{i\varphi}\cos\tfrac{\theta}{2}\sin\tfrac{\theta}{2}|\downarrow\rangle_1|\downarrow\rangle_2\\ &+(\cos\tfrac{\theta}{2})^2|\uparrow\rangle_1|\downarrow\rangle_2 - (\sin\tfrac{\theta}{2})^2|\downarrow\rangle_1|\uparrow\rangle_2. \qquad \text{(S.14)}\end{aligned}$$

Then (2.2.14) follows by elementary integrations. Similarly we have

$$\begin{aligned}\hat{U}_\varphi^{(3)}\hat{U}_\theta^{(2)}\,|\uparrow\rangle_1|\uparrow\rangle_2 =&\big(e^{-i\varphi/2}\cos\tfrac{\theta}{2}|\uparrow\rangle_1 + e^{i\varphi/2}\sin\tfrac{\theta}{2}|\downarrow\rangle_1\big)\\ &\otimes\big(e^{-i\varphi/2}\cos\tfrac{\theta}{2}|\uparrow\rangle_2 + e^{i\varphi/2}\sin\tfrac{\theta}{2}|\downarrow\rangle_2\big)\\ =&-e^{-i\varphi}(\cos\tfrac{\theta}{2})^2|\uparrow\rangle_1|\uparrow\rangle_2 + e^{i\varphi}(\sin\tfrac{\theta}{2})^2|\downarrow\rangle_1|\downarrow\rangle_2\\ &+\cos\tfrac{\theta}{2}\sin\tfrac{\theta}{2}(|\uparrow\rangle_1|\downarrow\rangle_2 + |\downarrow\rangle_1|\uparrow\rangle_2), \qquad \text{(S.15)}\end{aligned}$$

which gives (2.2.15) upon integration.

2.2.c (p. 23) The representation in the footnote and $\hat{U}|\Phi_{0,0}\rangle = |\Phi_{0,0}\rangle$ imply

$$\begin{aligned}\hat{U}|\uparrow\rangle_1|\downarrow\rangle_2 &= \sqrt{2}(\tfrac{1}{2} + \hat{U}\hat{S}_1^{(3)}\hat{U}^\dagger)(\tfrac{1}{2} - \hat{U}\hat{S}_2^{(3)}\hat{U}^\dagger)|\Phi_{0,0}\rangle\\ &= \sqrt{2}(\tfrac{1}{2} + \hat{\boldsymbol{S}}_1\cdot\boldsymbol{n})(\tfrac{1}{2} - \hat{\boldsymbol{S}}_2\cdot\boldsymbol{n})|\Phi_{0,0}\rangle, \qquad \text{(S.16)}\end{aligned}$$

where the final expression clearly depends only on $\boldsymbol{n}$.

2.3.a (p. 31) Since V is antiunitary, we have $\langle\mathsf{V}\boldsymbol{u},\mathsf{V}\boldsymbol{v}\rangle = \langle\boldsymbol{v},\boldsymbol{u}\rangle$ for any $\boldsymbol{u}$ and $\boldsymbol{v}$. See (A.4.17). Setting $\boldsymbol{u} = \mathsf{V}\boldsymbol{v}$, we find $\langle\boldsymbol{v},\mathsf{V}\boldsymbol{v}\rangle = \langle\mathsf{V}^2\boldsymbol{v},\mathsf{V}\boldsymbol{v}\rangle = -\langle\boldsymbol{v},\mathsf{V}\boldsymbol{v}\rangle$, which implies $\langle\boldsymbol{v},\mathsf{V}\boldsymbol{v}\rangle = 0$.

2.4.a (p. 34) In each subspace $\mathscr{H}_M$ there is at least one ground state, i.e., $|\Phi_M\rangle$. It suffices to show the uniqueness of ground state in each $\mathscr{H}_M$. This is easily done by applying the Perron–Frobenius theorem to the matrix representation $\langle\Psi^\sigma|\hat{H}|\Psi^\sigma\rangle$ of the Hamiltonian.

2.4.b (p. 34) Such an expression is not unique. Here is a simple construction. Fix $\theta \in (0,\pi)$ and write $\hat{U}_\theta^{(2)}|\Phi^\uparrow\rangle = \sum_{M=-|\Lambda|S}^{|\Lambda|S} c_M|\Phi_M\rangle$. It is found that $c_M \neq 0$ for any M. Then we have

$$\int_0^{2\pi} d\varphi\, e^{iM\varphi}|\Xi_{\theta,\varphi}\rangle = \int_0^{2\pi} d\varphi \sum_{M'=-|\Lambda|S}^{|\Lambda|S} c_{M'}\, e^{i(M-M')\varphi}|\Phi_{M'}\rangle = 2\pi\, c_M|\Phi_M\rangle. \tag{S.17}$$

2.4.c (p. 34) Denoting the copy of $|\psi_{\theta,\varphi}\rangle$ (see Problem 2.1.d) on site $x \in \Lambda$ as $|\psi_{\theta,\varphi}\rangle_x$ we have

$$|\Xi_{\theta,\varphi}\rangle = \bigotimes_{x\in\Lambda} |\psi_{\theta,\varphi}\rangle_x = \bigotimes_{x\in\Lambda} \left\{ e^{-i\varphi/2} \cos\tfrac{\theta}{2}\, |\psi_x^{\uparrow}\rangle + e^{i\varphi/2} \sin\tfrac{\theta}{2}\, |\psi_x^{\downarrow}\rangle \right\} \tag{S.18}$$

By expanding and using (2.4.11), we find

$$\begin{aligned} |\Xi_{\theta,\varphi}\rangle &= \sum_{M=-S_{\max}}^{S_{\max}} e^{-iM\varphi/2} (\cos\tfrac{\theta}{2})^{S_{\max}+M} (\sin\tfrac{\theta}{2})^{S_{\max}-M} \sum_{\substack{\boldsymbol{\sigma} \\ (\overline{\boldsymbol{\sigma}}=M)}} |\Psi^{\boldsymbol{\sigma}}\rangle \\ &= \sum_{M=-S_{\max}}^{S_{\max}} \sqrt{\frac{(2S_{\max})!}{(S_{\max}+M)!\,(S_{\max}-M)!}}\; e^{-iM\varphi/2} (\cos\tfrac{\theta}{2})^{S_{\max}+M} (\sin\tfrac{\theta}{2})^{S_{\max}-M} |\Phi_M\rangle. \end{aligned} \tag{S.19}$$

2.4.d (p. 35) Expanding the right-hand side of (2.4.14), one finds

$$\begin{aligned} (\mathrm{RHS}) &= \sum_{\{x,y\}\in\mathscr{B}} \{-|g_x|^2 - |g_y|^2 + g_x^* g_y + g_x g_y^*\} \\ &= -\sum_{x\in\Lambda} |\mathscr{N}(x)|\, |g_x|^2 + \sum_{\substack{x,y\in\Lambda \\ (\{x,y\}\in\mathscr{B})}} g_x^* g_y, \end{aligned} \tag{S.20}$$

which is identical to the left-hand side.

2.5.a (p. 38) This problem can be solved by using basic facts about addition of angular momenta. Note that $\hat{h}_0 = \hat{\boldsymbol{S}}_0 \cdot \hat{\boldsymbol{J}} = \{(\hat{\boldsymbol{S}}_0 + \hat{\boldsymbol{J}})^2 - (\hat{\boldsymbol{S}}_0)^2 - (\hat{\boldsymbol{J}})^2\}/2$ with $\hat{\boldsymbol{J}} = \sum_{j=1}^{z} \hat{\boldsymbol{S}}_j$. Consider a sector in which $\hat{\boldsymbol{J}}^2 = J(J+1)$. Then in order to minimize $(\hat{\boldsymbol{S}}_0 + \hat{\boldsymbol{J}})^2$ the whole system should have the minimum possible total angular momentum $|J - S|$. Then the eigenvalue of $\hat{h}_0$ is

$$\frac{1}{2}\Big\{ |J-S|\big(|J-S|+1\big) - S(S+1) - J(J+1) \Big\} = -JS - \min\{J, S\}. \tag{S.21}$$

This is minimized when $J = zS$, and the minimum energy is $-S(1+zS)$.

2.5.b (p. 38) To get a lower bound for E_{GS}, note that $\hat{H} = \sum_{x\in A} \hat{h}_x$ with $\hat{h}_x = \sum_{y\in\mathscr{N}(x)} \hat{\boldsymbol{S}}_x \cdot \hat{\boldsymbol{S}}_y$. Here $\mathscr{N}(x) \subset B$ is the set of sites connected to x. Since the above estimate shows that the ground state energy of $\hat{h}_x$ is $-S(1 + |\mathscr{N}(x)|\, S)$, we find

that $E_{\rm GS} \geq -\sum_{x\in A} S(1+|\mathscr{N}(x)|\,S)$. In the d-dimensional hypercubic lattice with $\mathscr{N}(x) = 2d$ and $|\Lambda| = L^d$ (see p. 51), we get $E_{\rm GS} \geq -L^d S(1+2dS)/2$.

2.5.c (p. 39) The uniqueness of the ground state and the SU(2) invariance of the Hamiltonian implies $\langle\Phi_{\rm GS}|(\hat{S}_x^{(1)})^2|\Phi_{\rm GS}\rangle = \langle\Phi_{\rm GS}|(\hat{S}_x^{(2)})^2|\Phi_{\rm GS}\rangle = \langle\Phi_{\rm GS}|(\hat{S}_x^{(3)})^2|\Phi_{\rm GS}\rangle$ for each x. Since $(\hat{S}_x^{(1)})^2 + (\hat{S}_x^{(2)})^2 + (\hat{S}_x^{(3)})^2 = S(S+1)$, one readily gets (2.5.6).

2.5.d (p. 40) An essential observation is that the SU(2) invariance implies

$$\begin{aligned}\langle\Phi_{\rm GS}|\hat{\boldsymbol{S}}_x\cdot\hat{\boldsymbol{S}}_y|\Phi_{\rm GS}\rangle &= \frac{3}{2}\langle\Phi_{\rm GS}|(\hat{S}_x^{(1)}\hat{S}_y^{(1)}+\hat{S}_x^{(2)}\hat{S}_y^{(2)})|\Phi_{\rm GS}\rangle \\ &= \frac{3}{4}\langle\Phi_{\rm GS}|(\hat{S}_x^{+}\hat{S}_y^{-}+\hat{S}_x^{-}\hat{S}_y^{+})|\Phi_{\rm GS}\rangle. \end{aligned} \tag{S.22}$$

Therefore it suffices to show that $\langle\Phi_{\rm GS}|\hat{S}_x^{+}\hat{S}_y^{-}|\Phi_{\rm GS}\rangle$ is nonzero and has the sign specified in (2.5.7). It is easily found that $\hat{U}\,\hat{S}_x^{\pm}\hat{U} = (-1)^x\hat{S}_x^{\pm}$ for the unitary operator defined in the hint, where we set $(-1)^x = 1$ if $x\in A$ and $(-1)^x = -1$ if $x\in B$. Since $\hat{U}^2 = \hat{1}$, we have $\hat{U}|\Phi_{\rm GS}\rangle = \sum_{\boldsymbol{\sigma}\,(\overline{\boldsymbol{\sigma}}=0)} c_{\boldsymbol{\sigma}}\,|\Psi^{\boldsymbol{\sigma}}\rangle$. We then find

$$\begin{aligned}(-1)^x(-1)^y\langle\Phi_{\rm GS}|\hat{S}_x^{+}\hat{S}_y^{-}|\Phi_{\rm GS}\rangle &= \langle\Phi_{\rm GS}|\hat{U}\,\hat{S}_x^{+}\hat{S}_y^{-}\hat{U}|\Phi_{\rm GS}\rangle \\ &= \sum_{\substack{\boldsymbol{\sigma},\boldsymbol{\tau}\\(\overline{\boldsymbol{\sigma}}=\overline{\boldsymbol{\tau}}=0)}} c_{\boldsymbol{\sigma}}\,c_{\boldsymbol{\tau}}\langle\Psi^{\boldsymbol{\sigma}}|\hat{S}_x^{+}\hat{S}_y^{-}|\Psi^{\boldsymbol{\tau}}\rangle, \end{aligned} \tag{S.23}$$

where the right-hand side is clearly positive. This is nothing but the desired result.

Problems of Chap. 3

3.3.a (p. 59) We start by examining the matrix elements of the Hamiltonian (3.3.1) with respect to these basis states. Diagonal elements are

$$\langle\Phi^{\uparrow}|\hat{H}|\Phi^{\uparrow}\rangle = \langle\Phi^{\downarrow}|\hat{H}|\Phi^{\downarrow}\rangle = E_{\rm GS}^{(0)} = -\frac{L-1}{4}, \tag{S.24}$$

$$\langle\Phi_j^{\uparrow\downarrow}|\hat{H}|\Phi_j^{\uparrow\downarrow}\rangle = \langle\Phi_j^{\downarrow\uparrow}|\hat{H}|\Phi_j^{\downarrow\uparrow}\rangle = E_{\rm GS}^{(0)} + \frac{1}{2}, \tag{S.25}$$

for $j = 1,\ldots,L-1$. Off-diagonal elements, which come from the spin flip by $\hat{S}_x^{(1)}$, are

$$\langle\Phi_j^{\uparrow\downarrow}|\hat{H}|\Phi_{j+1}^{\uparrow\downarrow}\rangle = \langle\Phi_j^{\downarrow\uparrow}|\hat{H}|\Phi_{j+1}^{\downarrow\uparrow}\rangle = -\frac{\lambda}{2}, \tag{S.26}$$

for $j = 1,\ldots,L-2$, and

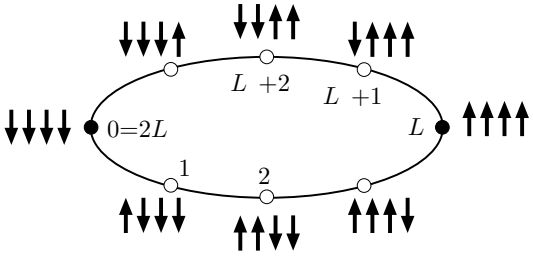


Fig. A.1 The tight-binding model (S.30) which describes low energy properties of the quantum Ising model (3.3.1). The black dots represent sites with potential energy 0, and white dots represent sites with potential energy 1/2. The spin configuration corresponding to each site is also shown ()

$$\langle \Phi^{\uparrow}|\hat{H}|\Phi_1^{\downarrow\uparrow}\rangle = \langle \Phi^{\uparrow}|\hat{H}|\Phi_{L-1}^{\uparrow\downarrow}\rangle = \langle \Phi^{\downarrow}|\hat{H}|\Phi_1^{\uparrow\downarrow}\rangle = \langle \Phi^{\downarrow}|\hat{H}|\Phi_{L-1}^{\downarrow\uparrow}\rangle = -\frac{\lambda}{2}. \quad \text{(S.27)}$$

Matrix elements are symmetric, e.g., $\langle \Phi^{\uparrow}|\hat{H}|\Phi_1^{\downarrow\uparrow}\rangle = \langle \Phi_1^{\downarrow\uparrow}|\hat{H}|\Phi^{\uparrow}\rangle$. All other matrix elements are vanishing.

Let us expand low energy states (approximately) as

$$|\Phi\rangle = \varphi_0|\Phi^{\downarrow}\rangle + \sum_{j=1}^{L-1}\varphi_j|\Phi_j^{\uparrow\downarrow}\rangle + \varphi_L|\Phi^{\uparrow}\rangle + \sum_{j=1}^{L-1}\varphi_{j+L}|\Phi_j^{\downarrow\uparrow}\rangle, \quad \text{(S.28)}$$

and demand that it satisfies the Schrödinger equation

$$\hat{H}|\Phi\rangle = (E_{\mathrm{GS}}^{(0)} + \varepsilon)|\Phi\rangle. \quad \text{(S.29)}$$

By using the matrix elements obtained above, we can write down equations which determine the energy eigenvalues ε and the corresponding eigenstates $(\varphi_j)_{j=1,\dots,2L-1}$, i.e.,

$$\varepsilon\,\varphi_j = -\frac{\lambda}{2}(\varphi_{j-1} + \varphi_{j+1}) + v_j\,\varphi_j, \quad \text{(S.30)}$$

for any $j = 1, \dots, 2L-1$, where we use periodic boundary conditions $\varphi_{j+2L} = \varphi_j$. The potential is given by $v_0 = v_L = 0$ and $v_j = 1/2$ for $j \neq 0, L$.

Note that (S.30) is nothing but the standard tight-binding Schrödinger equation (see Sect. 9.3.1) on a periodic chain with two potential wells at $j = 0$ and L, which correspond to $|\Phi^{\uparrow}\rangle$ and $|\Phi^{\downarrow}\rangle$. See Fig. A.1. The Schrödinger equation (S.30) can be solved easily as similar exercises in elementary quantum mechanics.

The equation (S.30) is trivial for $j \neq 0, L$ and we see that $e^{\pm\kappa j}$ are independent solutions, where $\kappa > 0$ is a constant to be determined. The corresponding energy is

$$\varepsilon = -\frac{\lambda}{2}(e^{\kappa} + e^{-\kappa}) + \frac{1}{2}. \quad \text{(S.31)}$$

From the symmetry we see that there are two independent low energy eigenstates in which the "particle" is bound at $j = 0$ and L. They are the symmetric solution with $\varphi_0 = \varphi_L$, and the antisymmetric solution with $\varphi_0 = -\varphi_L$. We can thus write down the (unnormalized) solutions as

$$\varphi_j = \begin{cases} e^{-\kappa j} \pm e^{-\kappa(L-j)} & \text{for } j = 0, \dots, L, \\ \pm e^{-\kappa(j-L)} + e^{-\kappa(2L-j)} & \text{for } j = L, \dots, 2L, \end{cases} \tag{S.32}$$

where the signs + and − correspond to the symmetric and antisymmetric solutions, respectively. By substituting (S.32) into the Schrödinger equation (S.30) with $j = 0$ or L, we get another expression of the energy:

$$\varepsilon\,(1 \pm e^{-\kappa L}) = -\lambda\,(e^{-\kappa} \pm e^{-\kappa(L-1)}). \tag{S.33}$$

By substituting (S.31) into (S.33), we get an equation for κ alone, which, after some work, can be organized as

$$e^{\kappa} - e^{-\kappa} = \lambda^{-1}\,\frac{1 \pm e^{-\kappa L}}{1 \mp e^{-\kappa L}}. \tag{S.34}$$

If we let $L \uparrow \infty$, the right-hand side becomes λ^{-1}, and we get the same constant κ for the symmetric and antisymmetric eigenstates. This implies, as expected, that the two energy eigenvalues degenerate. We write the solution of (S.34) for $L \uparrow \infty$ as κ_∞, i.e.,

$$e^{\kappa_\infty} - e^{-\kappa_\infty} = \lambda^{-1}. \tag{S.35}$$

Because $0 < \lambda \ll 1$, we have $e^{\kappa_\infty} \simeq \lambda^{-1}$, or $\kappa_\infty \simeq -\log\lambda$.

We wish to find the lowest order correction to κ satisfying (S.34) for $0 < \lambda \ll 1$ and $L \gg 1$.[1] Writing $\kappa = \kappa_\infty + \delta$, we have

$$e^{\kappa_\infty+\delta} - e^{-\kappa_\infty-\delta} \simeq \lambda^{-1}\,(1 \pm 2\,e^{-\kappa_\infty L}). \tag{S.36}$$

Expanding the left-hand side in δ to the lowest order, we get

$$\delta \simeq \pm\lambda^{-1}\,\frac{2\,e^{-\kappa_\infty L}}{e^{\kappa_\infty} + e^{-\kappa_\infty}}. \tag{S.37}$$

Now, by substituting $\kappa = \kappa_\infty + \delta$ into (S.31), and expanding in δ, we get

$$\varepsilon = -\frac{\lambda}{2}(e^{\kappa_\infty+\delta} + e^{-\kappa_\infty-\delta}) + \frac{1}{2} \simeq \varepsilon_\infty - \frac{\lambda}{2}(e^{\kappa_\infty} - e^{-\kappa_\infty})\,\delta, \tag{S.38}$$

where

[1] More precisely we fix small λ, and then make L large so that $\lambda^{-1}e^{-\kappa_\infty L}$ is small.

$$\varepsilon_\infty = -\frac{\lambda}{2}(e^{\kappa_\infty} + e^{-\kappa_\infty}) + \frac{1}{2} = -\frac{\sqrt{1+4\lambda^2}}{2} + \frac{1}{2} \simeq -\lambda^2 \tag{S.39}$$

is the energy for $L \uparrow \infty$. Substituting (S.37), we find

$$\varepsilon_\pm \simeq \varepsilon_\infty \mp \frac{e^{\kappa_\infty} - e^{-\kappa_\infty}}{e^{\kappa_\infty} + e^{-\kappa_\infty}}\, e^{-\kappa_\infty L}. \tag{S.40}$$

We see that the symmetric solution has a lower energy, as it should be. The energy difference is given by

$$E_{1\mathrm{st}} - E_{\mathrm{GS}} = \varepsilon_- - \varepsilon_+ \simeq 2\frac{e^{\kappa_\infty} - e^{-\kappa_\infty}}{e^{\kappa_\infty} + e^{-\kappa_\infty}}\, e^{-\kappa_\infty L} \simeq 2\,\lambda^L. \tag{S.41}$$

We finally note that these eigenstates are concentrated at two sites $j = 0$ and L. Observe that $|\varphi_0| = |\varphi_L| \simeq 1$, while other components are smaller, e.g., $\varphi_1 \simeq e^{-\kappa} \simeq \lambda$, $\varphi_2 \simeq e^{-2\kappa} \simeq \lambda^2$. This confirms (3.3.8) and (3.3.9).

3.4.a (p. 67) Note that $[\hat{o}_z, [\hat{h}_x, \hat{o}_y]] \neq 0$ only when $|x - y| \leq r$ and $|x - z| \leq 2r$. For a fixed x, the numbers of such y and z do not exceed $(2r+1)^2$ and $(4r+1)^d$, respectively. Since there are L^d choices of x, we get the desired (3.4.13) by recalling that $\|[\hat{o}_z, [\hat{h}_x, \hat{o}_y]]\| \leq 4h_0(o_0)^2$. We note that (3.4.13) is a very crude upper bound, and can be improved by estimating more efficiently the numbers of y and z with nonzero contributions.

3.4.b (p. 69) Observe, exactly as in (3.4.15), that

$$\begin{aligned}\langle \Xi_+|(\hat{\mathcal{O}}_L)^2|\Xi_+\rangle &= \frac{1}{2}\left\{\left(\langle \Phi_{\mathrm{GS}}| + \frac{\langle \Phi_{\mathrm{GS}}|\hat{\mathcal{O}}_L}{\|\hat{\mathcal{O}}_L|\Phi_{\mathrm{GS}}\rangle\|}\right)(\hat{\mathcal{O}}_L)^2\left(|\Phi_{\mathrm{GS}}\rangle + \frac{\hat{\mathcal{O}}_L|\Phi_{\mathrm{GS}}\rangle}{\|\hat{\mathcal{O}}_L|\Phi_{\mathrm{GS}}\rangle\|}\right)\right\} \\ &= \frac{1}{2}\left\{\langle \Phi_{\mathrm{GS}}|(\hat{\mathcal{O}}_L)^2|\Phi_{\mathrm{GS}}\rangle + \frac{\langle \Phi_{\mathrm{GS}}|(\hat{\mathcal{O}}_L)^4|\Phi_{\mathrm{GS}}\rangle}{\langle \Phi_{\mathrm{GS}}|(\hat{\mathcal{O}}_L)^2|\Phi_{\mathrm{GS}}\rangle}\right\},\end{aligned} \tag{S.42}$$

which, with (3.4.15), implies

$$\begin{aligned}&\langle \Xi_+|\left(\frac{\hat{\mathcal{O}}_L}{L^d}\right)^2|\Xi_+\rangle - \left\{\langle \Xi_+|\frac{\hat{\mathcal{O}}_L}{L^d}|\Xi_+\rangle\right\}^2 \\ &= \frac{1}{2}\left\{\langle \Phi_{\mathrm{GS}}|\left(\frac{\hat{\mathcal{O}}_L}{L^d}\right)^2|\Phi_{\mathrm{GS}}\rangle\right\}^{-1}\left[\langle \Phi_{\mathrm{GS}}|\left(\frac{\hat{\mathcal{O}}_L}{L^d}\right)^4|\Phi_{\mathrm{GS}}\rangle - \left\{\langle \Phi_{\mathrm{GS}}|\left(\frac{\hat{\mathcal{O}}_L}{L^d}\right)^2|\Phi_{\mathrm{GS}}\rangle\right\}^2\right].\end{aligned} \tag{S.43}$$

Problems of Chap. 4

4.2.1.a (p. 104) The expression (2.5.11) of the toy Hamiltonian is still valid. We denote the eigenvalues of $(\hat{\boldsymbol{S}}_{\rm tot})^2$, $(\hat{\boldsymbol{S}}_A)^2$, and $(\hat{\boldsymbol{S}}_B)^2$ as $S_{\rm tot}(S_{\rm tot}+1)$, $S^A_{\rm tot}(S^A_{\rm tot}+1)$, and $S^B_{\rm tot}(S^B_{\rm tot}+1)$, respectively. We then have $S^A_{\rm tot} = |A|S - k$, $S^B_{\rm tot} = |B|S - \ell$, and $S_{\rm tot} = |S^A_{\rm tot} - S^B_{\rm tot}| + m$, where $k, \ell, m = 0, 1, 2, \ldots$. Thus the energy eigenvalues are given by

$$E_{k,\ell,m} = \frac{1}{2|\Lambda|}\Big\{\big(\big|(|A|-|B|)S - k + \ell\big| + m\big)\big(\big|(|A|-|B|)S - k + \ell\big| + m + 1\big) - (|A|S-k)(|A|S-k+1) - (|B|S-\ell)(|B|S-\ell+1)\Big\}. \tag{S.44}$$

Clearly the ground state is attained with $k = \ell = m = 0$. Let us write $\Delta E_{k,\ell,m} = E_{k,\ell,m} - E_{0,0,0}$.

To confirm that there is a gap it suffices to check that $\Delta E_{1,0,0} = |B|S/|\Lambda|$, $\Delta E_{0,1,0} = |A|S/|\Lambda| + |\Lambda|^{-1}$, and $\Delta E_{0,0,1} = (|A|-|B|)S/|\Lambda| + |\Lambda|^{-1} = aS + |\Lambda|^{-1}$. It is useful to note that

$$\Delta E_{0,0,m} = aSm + \frac{m(m+1)}{2|\Lambda|}, \tag{S.45}$$

which, with $m = 1, 2, \ldots$, are the lowest excited energies when a is sufficiently small. We also recover the "tower" structure (4.2.8) when $a = 0$.

4.4.3.a (p. 130) First note that the basic inequality (4.4.36) is valid for any lattice geometry. In one-dimensional models with nearest neighbor interactions, it is convenient to chose the classical field configuration as

$$\varphi_x = \begin{cases} 2\mu\,(\ell - |x|) & \text{if } |x| \le \ell, \\ 0 & \text{if } |x| \ge \ell, \end{cases} \tag{S.46}$$

where $\mu > 0$ is a constant and ℓ is a positive integer. Note that $|\varphi_x - \varphi_y|$ is either 2μ or 0 for any $\{x, y\} \in \mathscr{B}_L$.

To show the decay of correlation, we set $h = 0$ and note that (4.4.37) is valid as it is. We set $\ell = |z|$, and observe that $\varphi_0 = 2\mu\ell$ and $\varphi_z = 0$ to get

$$\big|\langle \hat{S}^+_o \hat{S}^-_z \rangle^L_{\beta,0}\big| \le 4S^2 \exp\big[-2\mu\ell + 2\beta S^2 \times 2\ell\{\cosh(2\mu) - 1\}\big]. \tag{S.47}$$

Let $\mu(\beta)$ be the positive solution of $\mu = 4\beta S^2\{\cosh(2\mu) - 1\}$, which behaves as $\mu(\beta) \simeq (8S^2\beta)^{-1}$ if $\beta \gg 1$. Then (S.47) yields

$$\big|\langle \hat{S}^+_o \hat{S}^-_z \rangle^L_{\beta,0}\big| \le 4S^2\, e^{-\mu(\beta)\,|z|}, \tag{S.48}$$

which establishes that the correlation function decays (at least) exponentially. In particular $1/\mu(\beta)$ is a rigorous upper bound of the correlation length.

To control the magnetization, we use (4.4.47) to see that

$$\big|\langle \hat{S}_o^+ \rangle_{\beta,h}^L\big| \le 2S \, \exp\big[-\mu(\beta)\,\ell + h\, G(\beta,\ell)\big], \tag{S.49}$$

with

$$G(\beta,\ell) = 2\beta S \sum_{x=-\ell}^{\ell} \cosh\big[2\mu(\beta)\,(\ell - |x|)\big]. \tag{S.50}$$

We then get (4.4.22) exactly as in the two-dimensional case.

Problems of Chap. 5

5.2.a (p. 138) The single-particle Schrödinger equation corresponding to the Hamiltonian (5.1.3) is

$$\varepsilon\, \varphi_x = - \sum_{\substack{y\in\Lambda_L \\ (\{x,y\}\in\mathscr{B}_L)}} \varphi_y. \tag{S.51}$$

For details, see Sects. 9.2, 9.3, and 9.4, where we discuss the basics of the Hubbard model. The ground state of (S.51) is given by $\varphi_x = |\Lambda_L|^{-1/2}$ for all $x \in \Lambda_L$. Let $\hat{b}^\dagger = |\Lambda_L|^{-1/2} \sum_{x\in\Lambda_L} \hat{a}_x^\dagger$ be the corresponding creation operator of the single-particle ground state. The ground state of the free N boson system is

$$|\Phi_{\rm GS}\rangle = \frac{1}{\sqrt{N!}} (\hat{b}^\dagger)^N |\Phi_{\rm vac}\rangle, \tag{S.52}$$

which is normalized because $\langle \Phi_{\rm vac}|\hat{b}^N (\hat{b}^\dagger)^N|\Phi_{\rm vac}\rangle = N!$. From the commutation relation (5.1.1), we find that $[\hat{a}_x, \hat{b}^\dagger] = |\Lambda_L|^{-1/2}$. We then see

$$\hat{a}_x|\Phi_{\rm GS}\rangle = \frac{1}{\sqrt{N!}} \hat{a}_x (\hat{b}^\dagger)^N |\Phi_{\rm vac}\rangle = \frac{1}{\sqrt{N!}} \frac{N}{\sqrt{|\Lambda_L|}} (\hat{b}^\dagger)^{N-1} |\Phi_{\rm vac}\rangle. \tag{S.53}$$

We thus find for any $x, y \in \Lambda_L$ that

$$\langle \Phi_{\rm GS}|\hat{a}_x^\dagger \hat{a}_y|\Phi_{\rm GS}\rangle = \frac{1}{N!} \frac{N^2}{|\Lambda_L|} \langle \Phi_{\rm vac}|\hat{b}^{N-1} (\hat{b}^\dagger)^{N-1}|\Phi_{\rm vac}\rangle = \frac{N}{|\Lambda_L|}, \tag{S.54}$$

which is the desired (5.2.1).

5.4.a (p. 143) Take any normalized state $|\mathscr{E}_M\rangle$ of the second (external) system which has $N_{\rm tot} - M$ particles. Then recalling (5.3.5), we define

$$|\Phi_{\rm tot}\rangle = \frac{1}{\sqrt{2M_{\max}(L)+1}} \sum_{M=-M_{\max}(L)}^{M_{\max}(L)} |\Gamma_M\rangle \otimes |\mathscr{E}_M\rangle. \tag{S.55}$$

We then have

$$\langle \Phi_{\rm tot}|(\hat{A}\otimes\hat{1})|\Phi_{\rm tot}\rangle = \frac{1}{2M_{\max}(L)+1} \sum_{M=-M_{\max}(L)}^{M_{\max}(L)} \langle \Gamma_M|\hat{A}|\Gamma_M\rangle, \tag{S.56}$$

where the right-hand side is identical to (5.4.1).

Problems of Chap. 6

6.1.a (p. 157) Let $\hat{\mathscr{O}}'_L = \sum_{x\,(|x|\le BL/2)} \hat{o}_x$, and define a trial state by $|\Gamma\rangle = \hat{\mathscr{O}}'_L|\Phi_{\rm GS}\rangle/\|\hat{\mathscr{O}}'_L|\Phi_{\rm GS}\rangle\|$ as in (3.4.7). Note that the assumption (6.1.4) implies

$$\langle \Phi_{\rm GS}|(\hat{\mathscr{O}}'_L)^2|\Phi_{\rm GS}\rangle = \sum_{\substack{x,y\in\Lambda_L \\ (|x|,|y|\le BL/2)}} \langle \Phi_{\rm GS}|\hat{o}_x\hat{o}_y|\Phi_{\rm GS}\rangle \ge C'L^{d+\kappa}, \tag{S.57}$$

and that the estimate as in Problem 3.4.a (p. 67) implies $\|[\hat{\mathscr{O}}'_L,[\hat{H},\hat{\mathscr{O}}'_L]]\| \le C''L^d$. Then, exactly as in (3.4.8), (3.4.9), (3.4.10), and (3.4.11), we find

$$\langle\Gamma|\hat{H}|\Gamma\rangle - E_{\rm GS} = \frac{\langle \Phi_{\rm GS}|[\hat{\mathscr{O}}'_L,[\hat{H},\hat{\mathscr{O}}'_L]]|\Phi_{\rm GS}\rangle}{2\langle \Phi_{\rm GS}|(\hat{\mathscr{O}}'_L)^2|\Phi_{\rm GS}\rangle} \le \frac{C''L^d}{2C'L^{d+\kappa}} = CL^{-\kappa}, \tag{S.58}$$

which, with the variational principle, implies the desired bound.

Problems of Chap. 7

7.1.2.a (p. 184) We use the (standard) abbreviation $|\sigma\rangle_x$ for $|\psi^\sigma_x\rangle$. From the definition (7.1.11), we get

$$\begin{aligned}|\Phi_{\text{pre-VBS}}\rangle &= \frac{1}{2}\Big(|\uparrow\rangle_{1,\rm R}|\downarrow\rangle_{2,\rm L} - |\downarrow\rangle_{1,\rm R}|\uparrow\rangle_{2,\rm L}\Big)\Big(|\uparrow\rangle_{2,\rm R}|\downarrow\rangle_{1,\rm L} - |\downarrow\rangle_{2,\rm R}|\uparrow\rangle_{1,\rm L}\Big) \\ &= \frac{1}{2}\Big(|\downarrow\rangle_{1,\rm L}|\uparrow\rangle_{1,\rm R}|\downarrow\rangle_{2,\rm L}|\uparrow\rangle_{2,\rm R} - |\downarrow\rangle_{1,\rm L}|\downarrow\rangle_{1,\rm R}|\uparrow\rangle_{2,\rm L}|\uparrow\rangle_{2,\rm R} \\ &\quad - |\uparrow\rangle_{1,\rm L}|\uparrow\rangle_{1,\rm R}|\downarrow\rangle_{2,\rm L}|\downarrow\rangle_{2,\rm R} + |\uparrow\rangle_{1,\rm L}|\downarrow\rangle_{1,\rm R}|\uparrow\rangle_{2,\rm L}|\downarrow\rangle_{2,\rm R}\Big).\end{aligned} \tag{S.59}$$

By using the definition (7.1.12) and the projection (7.1.9), one finds

$$|\Phi_{\rm VBS}\rangle = \frac{1}{2}\Big(|0\rangle_1|0\rangle_2 - |+\rangle_1|-\rangle_2 - |-\rangle_1|+\rangle_2\Big). \tag{S.60}$$

Recalling (2.2.18), (2.2.16), (2.1.2), and (2.1.3), one easily checks that[2]

$$(\hat{\boldsymbol{S}}_1 + \hat{\boldsymbol{S}}_2)^2|\Phi_{\rm VBS}\rangle = 0, \tag{S.61}$$

which means $|\Phi_{\rm VBS}\rangle$ has $S_{\rm tot} = 0$. This is of course a sufficient condition for $\hat{P}_2[\hat{\boldsymbol{S}}_1 + \hat{\boldsymbol{S}}_2]\,|\Phi_{\rm VBS}\rangle = 0$.

7.1.2.b (p. 184) As in the above problem, we find from (7.1.11) that

$$\begin{aligned}
&2\sqrt{2}\,|\Phi_{\text{pre-VBS}}\rangle \\
&=\Big(|\uparrow\rangle_{1,\rm R}|\downarrow\rangle_{2,\rm L} - |\downarrow\rangle_{1,\rm R}|\uparrow\rangle_{2,\rm L}\Big)\Big(|\uparrow\rangle_{2,\rm R}|\downarrow\rangle_{3,\rm L} - |\downarrow\rangle_{2,\rm R}|\uparrow\rangle_{3,\rm L}\Big) \\
&\quad\Big(|\uparrow\rangle_{3,\rm R}|\downarrow\rangle_{1,\rm L} - |\downarrow\rangle_{3,\rm R}|\uparrow\rangle_{1,\rm L}\Big) \\
&=|\downarrow\rangle_{1,\rm L}|\uparrow\rangle_{1,\rm R}|\downarrow\rangle_{2,\rm L}|\uparrow\rangle_{2,\rm R}|\downarrow\rangle_{3,\rm L}|\uparrow\rangle_{3,\rm R} - |\uparrow\rangle_{1,\rm L}|\uparrow\rangle_{1,\rm R}|\downarrow\rangle_{2,\rm L}|\uparrow\rangle_{2,\rm R}|\downarrow\rangle_{3,\rm L}|\downarrow\rangle_{3,\rm R} \\
&-|\downarrow\rangle_{1,\rm L}|\uparrow\rangle_{1,\rm R}|\downarrow\rangle_{2,\rm L}|\downarrow\rangle_{2,\rm R}|\uparrow\rangle_{3,\rm L}|\uparrow\rangle_{3,\rm R} + |\uparrow\rangle_{1,\rm L}|\uparrow\rangle_{1,\rm R}|\downarrow\rangle_{2,\rm L}|\downarrow\rangle_{2,\rm R}|\uparrow\rangle_{3,\rm L}|\downarrow\rangle_{3,\rm R} \\
&-|\downarrow\rangle_{1,\rm L}|\downarrow\rangle_{1,\rm R}|\uparrow\rangle_{2,\rm L}|\uparrow\rangle_{2,\rm R}|\downarrow\rangle_{3,\rm L}|\uparrow\rangle_{3,\rm R} + |\uparrow\rangle_{1,\rm L}|\downarrow\rangle_{1,\rm R}|\uparrow\rangle_{2,\rm L}|\uparrow\rangle_{2,\rm R}|\downarrow\rangle_{3,\rm L}|\downarrow\rangle_{3,\rm R} \\
&+|\downarrow\rangle_{1,\rm L}|\downarrow\rangle_{1,\rm R}|\uparrow\rangle_{2,\rm L}|\downarrow\rangle_{2,\rm R}|\uparrow\rangle_{3,\rm L}|\uparrow\rangle_{3,\rm R} - |\uparrow\rangle_{1,\rm L}|\downarrow\rangle_{1,\rm R}|\uparrow\rangle_{2,\rm L}|\downarrow\rangle_{2,\rm R}|\uparrow\rangle_{3,\rm L}|\downarrow\rangle_{3,\rm R}.
\end{aligned} \tag{S.62}$$

Then from (7.1.12) and (7.1.9), we get

$$\begin{aligned}
|\Phi_{\rm VBS}\rangle =&\frac{1}{4}\Big(-|+\rangle_1|0\rangle_2|-\rangle_3 - |0\rangle_1|-\rangle_2|+\rangle_3 + |+\rangle_1|-\rangle_2|0\rangle_3 \\
&- |-\rangle_1|+\rangle_2|0\rangle_3 + |0\rangle_1|+\rangle_2|-\rangle_3 + |-\rangle_1|0\rangle_2|+\rangle_3\Big) \\
=&\frac{1}{4}\Big(|+\rangle_1|-\rangle_2|0\rangle_3 + |0\rangle_1|+\rangle_2|-\rangle_3 + |-\rangle_1|0\rangle_2|+\rangle_3 \\
&- |-\rangle_1|+\rangle_2|0\rangle_3 - |0\rangle_1|-\rangle_2|+\rangle_3 - |+\rangle_1|0\rangle_2|-\rangle_3\Big),
\end{aligned} \tag{S.63}$$

where we have rearranged the terms to see the structure. To determine the total spin on sites 1 and 2, we further rewrite (S.63) as

$$\begin{aligned}
|\Phi_{\rm VBS}\rangle = \frac{1}{4}\Big(&\big\{|+\rangle_1|-\rangle_2 - |-\rangle_1|+\rangle_2\big\}|0\rangle_3 + \big\{|-\rangle_1|0\rangle_2 - |0\rangle_1|-\rangle_2\big\}|+\rangle_3 \\
&+ \big\{|0\rangle_1|+\rangle_2 - |+\rangle_1|0\rangle_2\big\}|-\rangle_3\Big).
\end{aligned} \tag{S.64}$$

[2] It is useful to note that (2.1.3) reads $\hat{S}^+|-\rangle = \sqrt{2}|0\rangle$, $\hat{S}^+|0\rangle = \sqrt{2}|+\rangle$, $\hat{S}^-|+\rangle = \sqrt{2}|0\rangle$, and $\hat{S}^-|0\rangle = \sqrt{2}|-\rangle$.

Recalling that the states with $S_{\rm tot}=2$ on sites 1 and 2 are

$$|+\rangle_1|+\rangle_2,\frac{|+\rangle_1|0\rangle_2+|0\rangle_1|+\rangle_2}{\sqrt{2}},\frac{|+\rangle_1|-\rangle_2+2|0\rangle_1|0\rangle_2+|-\rangle_1|+\rangle_2}{\sqrt{6}},$$
$$\frac{|0\rangle_1|-\rangle_2+|-\rangle_1|0\rangle_2}{\sqrt{2}},|-\rangle_1|-\rangle_2, \tag{S.65}$$

one clearly sees that $|\Phi_{\rm VBS}\rangle$ has no components with $S_{\rm tot}=2$, i.e., is orthogonal to (S.65).

7.1.2.c (p. 186) For $x=1,\dots,L-1$, we have

$$\hat{U}_{\rm LSM}(|\psi_x^\uparrow\rangle|\psi_{x+1}^\downarrow\rangle-|\psi_x^\downarrow\rangle|\psi_{x+1}^\uparrow\rangle)=e^{i\Delta\theta/2}|\psi_x^\uparrow\rangle|\psi_{x+1}^\downarrow\rangle-e^{-i\Delta\theta/2}|\psi_x^\downarrow\rangle|\psi_{x+1}^\uparrow\rangle, \tag{S.66}$$

which means

$$|\Phi'\rangle=\bigotimes_{y=1}^{L/2}\frac{1}{\sqrt{2}}\Big(e^{i\Delta\theta/2}|\psi_{2y-1}^\uparrow\rangle|\psi_{2y}^\downarrow\rangle-e^{-i\Delta\theta/2}|\psi_{2y-1}^\downarrow\rangle|\psi_{2y}^\uparrow\rangle\Big). \tag{S.67}$$

From this one easily finds that

$$\langle\Phi_{\rm dimer}^{\rm odd}|\Phi'\rangle=\big(\cos\frac{\Delta\theta}{2}\big)^{L/2}\simeq\big(1-\frac{2\pi^2}{L^2}\big)^{L/2}\to 1. \tag{S.68}$$

In short we see that $|\Phi'\rangle=\hat{U}_{\rm LSM}|\Phi_{\rm dimer}^{\rm odd}\rangle\simeq|\Phi_{\rm dimer}^{\rm odd}\rangle$, i.e., the state essentially does not change after the twist. This is the same as what is expected for the $S=1$ chain with Haldane gap. See (6.2.22). Lemma 6.2 does not apply here because $|\Phi_{\rm dimer}^{\rm odd}\rangle$ is not translation invariant.

Both Lemmas 6.1 and 6.2 (and hence Theorem 6.3) apply to the translation invariant ground state $|\Phi_{\rm dimer}^{+}\rangle$. Thus we know that $|\Phi''\rangle$ is orthogonal to $|\Phi_{\rm dimer}^{+}\rangle$ and has low energy. To see what $|\Phi''\rangle$ look like, we note that (S.66) should be modified (only) for $x=L$ as

$$\begin{aligned}\hat{U}_{\rm LSM}(|\psi_L^\uparrow\rangle|\psi_1^\downarrow\rangle-|\psi_L^\downarrow\rangle|\psi_1^\uparrow\rangle)&=e^{-i(\theta_L-\theta_1)/2}|\psi_L^\uparrow\rangle|\psi_1^\downarrow\rangle-e^{i(\theta_L-\theta_1)/2}|\psi_L^\downarrow\rangle|\psi_1^\uparrow\rangle\\&=-(e^{i\Delta\theta/2}|\psi_L^\uparrow\rangle|\psi_1^\downarrow\rangle-e^{-i\Delta\theta/2}|\psi_L^\downarrow\rangle|\psi_1^\uparrow\rangle),\end{aligned} \tag{S.69}$$

where we noted that $\theta_L-\theta_1=2\pi-\Delta\theta$. We thus find

$$\hat{U}_{\rm LSM}|\Phi_{\rm dimer}^{\rm even}\rangle=-\bigotimes_{y=1}^{L/2}\frac{1}{\sqrt{2}}\Big(e^{i\Delta\theta/2}|\psi_{2y}^\uparrow\rangle|\psi_{2y+1}^\downarrow\rangle-e^{-i\Delta\theta/2}|\psi_{2y}^\downarrow\rangle|\psi_{2y+1}^\uparrow\rangle\Big)\simeq-|\Phi_{\rm dimer}^{\rm even}\rangle, \tag{S.70}$$

which implies $|\Phi''\rangle\simeq|\Phi_{\rm dimer}^{\rm odd}\rangle-|\Phi_{\rm dimer}^{\rm even}\rangle$.

7.2.2.a (p. 196) Since $\mathsf{A}^-(1,0)^{\mathrm{t}} = (0,0)^{\mathrm{t}}$, we may multiply $(1,0)^{\mathrm{t}}$ either by A^+ or A^0. Multiplying n times by A^0, we get $(2^{-n},0)^{\mathrm{t}}$. This generates n contiguous sequence of 0's. Multiplying by A^+, which corresponds to the insertion of a single $+$, the vector becomes a constant times $(0,1)^{\mathrm{t}}$. Then we may multiply the vector either by A^0 or A^-. The process can be repeated to generate the whole configuration with complete hidden antiferromagnetic order.

7.2.2.b (p. 196) By using the standard formula $|\psi^\sigma\rangle = \sum_{\gamma=1,2,3} |p^{(\gamma)}\rangle\langle p^{(\gamma)}|\psi^\sigma\rangle$, the matrix product representation (7.2.14) is rewritten as

$$|\Phi_{\mathrm{VBS}}\rangle = \sum_{\boldsymbol{\gamma}} \mathrm{Tr}[\mathsf{B}^{(\gamma_1)}\mathsf{B}^{(\gamma_2)} \cdots \mathsf{B}^{(\gamma_L)}]\, |\mathscr{P}^{\boldsymbol{\gamma}}\rangle, \tag{S.71}$$

with $\mathsf{B}^{(\gamma)} = \sum_{\sigma=0,\pm} \langle p^{(\gamma)}|\psi^\sigma\rangle\, \mathsf{A}^\sigma$. Explicit calculations with (7.2.12) and (7.2.16) show, rather remarkably, that

$$\mathsf{B}^{(1)} = \frac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \mathsf{B}^{(2)} = \frac{1}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \mathsf{B}^{(3)} = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{S.72}$$

Thus the matrices $\mathsf{B}^{(\gamma)}$ in the matrix product representation (S.71) are exactly identical to the spin operators (2.1.7) for $S = 1/2$.

7.2.2.c (p. 200) Exactly as in (7.2.26), $\langle \Phi_{\mathrm{VBS}}|\hat{P}^0_{x_1} \cdots \hat{P}^0_{x_n}|\Phi_{\mathrm{VBS}}\rangle$ is written as the trace of the product of $L-n$ copies of $\tilde{\mathsf{A}}$ and n copies of $\tilde{\mathsf{C}}$, where

$$(\tilde{\mathsf{C}})_{\alpha,\beta;\alpha',\beta'} = \sum_{\sigma=-1,0,1} (1-\sigma^2) A^\sigma_{\alpha,\alpha'} A^\sigma_{\beta,\beta'}. \tag{S.73}$$

It is easily found that

$$\tilde{\mathsf{C}} = \begin{array}{c} \\ 1,1 \\ 2,2 \\ 1,2 \\ 2,1 \end{array} \begin{array}{c} \begin{array}{cccc} 1,1 & 2,2 & 1,2 & 2,1 \end{array} \\ \begin{pmatrix} \frac{1}{4} & 0 & 0 & 0 \\ 0 & \frac{1}{4} & 0 & 0 \\ 0 & 0 & -\frac{1}{4} & 0 \\ 0 & 0 & 0 & -\frac{1}{4} \end{pmatrix} \end{array}. \tag{S.74}$$

This simple form makes the evaluation of the trace almost trivial (note that $\tilde{\mathsf{A}}$ and $\tilde{\mathsf{C}}$ commute). One finds

$$\begin{aligned} \langle \Phi_{\mathrm{VBS}}|\hat{P}^0_{x_1} \cdots \hat{P}^0_{x_n}|\Phi_{\mathrm{VBS}}\rangle &= \mathrm{Tr}[\tilde{\mathsf{C}}^n\, \tilde{\mathsf{A}}^{L-n}] = \left(\frac{1}{4}\right)^n \mathrm{Tr}\left[\begin{pmatrix} \frac{1}{4} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{4} \end{pmatrix}^{L-n}\right] + 2\left(-\frac{1}{4}\right)^L \\ &= \left(\frac{1}{4}\right)^n \left\{\left(\frac{3}{4}\right)^{L-n} + \left(-\frac{1}{4}\right)^{L-n}\right\} + 2\left(-\frac{1}{4}\right)^L, \end{aligned} \tag{S.75}$$

which implies

$$\lim_{L\uparrow\infty} \frac{\langle \Phi_{\rm VBS}|\hat{P}^0_{x_1}\hat{P}^0_{x_2}\cdots\hat{P}^0_{x_n}|\Phi_{\rm VBS}\rangle}{\langle \Phi_{\rm VBS}|\Phi_{\rm VBS}\rangle} = \left(\frac{1}{3}\right)^n. \tag{S.76}$$

This means that 0's appear independently with probability 1/3 in the VBS state.

7.2.2.d (p. 200) Fix $x < y$. Since 0's appear independently with probability 1/3 (in the $L \uparrow \infty$ limit), the probability that both x and y are occupied by $+$ or $-$ is $(2/3)^2 = 4/9$. Noting that there is complete hidden antiferromagnetic order, one finds $\lim_{L\uparrow\infty} \mathscr{S}^{(3)}_{x,y}(\Phi_{\rm VBS}) = 4/9$, which immediately implies (7.2.8).

7.2.2.e (p. 201) One can take, e.g., $\mathsf{A}^{\uparrow} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$ and $\mathsf{A}^{\downarrow} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$.

7.2.2.f (p. 201) One can take, e.g., $\mathsf{A}^{\uparrow} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$ and $\mathsf{A}^{\downarrow} = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$.

7.2.3.a (p. 207) Since $\hat{S}^{(3)}_{\rm tot}|\Phi^{\sigma_{\rm L},\sigma_{\rm R}}_{\rm VBS}\rangle = (\sigma_{\rm L}+\sigma_{\rm R})|\Phi^{\sigma_{\rm L},\sigma_{\rm R}}_{\rm VBS}\rangle$, the independence of $|\Phi^{\uparrow,\uparrow}_{\rm VBS}\rangle$ and $|\Phi^{\downarrow,\downarrow}_{\rm VBS}\rangle$ is obvious. We consider the expansion (7.2.1) for the remaining two states. The state $|\Phi^{\uparrow,\downarrow}_{\rm VBS}\rangle$ leads to configurations where the left-most nonzero spin is $+$ (such as $00{+}0{-}{+}0{-}0$) while the state $|\Phi^{\downarrow,\uparrow}_{\rm VBS}\rangle$ to those where the left-most nonzero spin is $-$ (such as $0{-}0{+}0{-}{+}00$). This proves that the two states are linearly independent. Note that the two states are not orthogonal since the configuration with all 0 appear in the both states.

7.2.3.b (p. 207) Let $|\Phi\rangle$ be a ground state. Then by the same logic as before, we find that the corresponding polynomial satisfies (7.1.24) for $x = 1, \ldots, L-1$. Then the uniqueness of factorization implies

$$\Phi(\boldsymbol{u},\boldsymbol{v}) = (c_1\,u_1u_L + c_2\,u_1v_L + c_3\,v_1u_L + c_4\,v_1v_L)\prod_{x=1}^{L}(u_xv_{x+1} - v_xu_{x+1}), \tag{S.77}$$

where $c_1, c_2, c_3, c_4 \in \mathbb{C}$ are arbitrary. This means that the ground states are exactly four-fold degenerate.

7.2.3.c (p. 207) From the same consideration as $A^{\sigma}_{\alpha,\alpha'}$, the boundary vectors are obtained as $\ell^+_1 = 1$, $\ell^0_2 = 1/\sqrt{2}$, $r^+_2 = -1/\sqrt{2}$, and $r^0_1 = 1/2$. Other components are vanishing. This gives a matrix product representation (7.2.45) of $|\Phi^{\uparrow,\uparrow}_{\rm VBS}\rangle$.

To compute normalization and correlation we need four component vectors $\tilde{\ell}^{\sigma}_{\alpha,\beta} = \sum_{\sigma} \ell^{\sigma}_{\alpha}\,\ell^{\sigma}_{\beta}$, $\tilde{m}^{\sigma}_{\alpha,\beta} = \sum_{\sigma}\sigma\,\ell^{\sigma}_{\alpha}\,\ell^{\sigma}_{\beta}$, and $\tilde{r}^{\sigma}_{\alpha,\beta} = \sum_{\sigma} r^{\sigma}_{\alpha}\,r^{\sigma}_{\beta}$. Using the representation as in (7.2.24), these vectors are written as

$$\tilde{\boldsymbol{\ell}} = (1, \tfrac{1}{2}, 0, 0), \quad \tilde{\boldsymbol{m}} = (1,0,0,0), \quad \tilde{\boldsymbol{r}} = \begin{pmatrix} \frac{1}{4} \\ \frac{1}{2} \\ 0 \\ 0 \end{pmatrix}. \tag{S.78}$$

Then the normalization factor is computed as

$$\langle \Phi^{\uparrow,\uparrow}_{\rm VBS} | \Phi^{\uparrow,\uparrow}_{\rm VBS} \rangle = \tilde{\boldsymbol{\ell}}\, \tilde{\mathsf{A}}^{L-2}\, \tilde{\boldsymbol{r}} = (1, \tfrac{1}{2}) \begin{pmatrix} \frac{1}{4} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{4} \end{pmatrix}^{L-2} \begin{pmatrix} \frac{1}{4} \\ \frac{1}{2} \end{pmatrix}$$
$$= (1, \tfrac{1}{2}) \, \mathsf{O} \begin{pmatrix} (\frac{3}{4})^{L-2} & 0 \\ 0 & (-\frac{1}{4})^{L-2} \end{pmatrix} \mathsf{O} \begin{pmatrix} \frac{1}{4} \\ \frac{1}{2} \end{pmatrix} \simeq \frac{9}{16} \left(\frac{3}{4} \right)^{L-2}. \tag{S.79}$$

To evaluate the expectation value, we note that

$$\langle \Phi^{\uparrow,\uparrow}_{\rm VBS} | \hat{S}^{(3)}_1 | \Phi^{\uparrow,\uparrow}_{\rm VBS} \rangle = \tilde{\boldsymbol{m}}\, \tilde{\mathsf{A}}^{L-2}\, \tilde{\boldsymbol{r}} = (1, 0) \begin{pmatrix} \frac{1}{4} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{4} \end{pmatrix}^{L-2} \begin{pmatrix} \frac{1}{4} \\ \frac{1}{2} \end{pmatrix} \simeq \frac{3}{8} \left(\frac{3}{4} \right)^{L-2} \tag{S.80}$$

and, for $x \geq 2$, that

$$\langle \Phi^{\uparrow,\uparrow}_{\rm VBS} | \hat{S}^{(3)}_x | \Phi^{\uparrow,\uparrow}_{\rm VBS} \rangle = \tilde{\boldsymbol{\ell}}\, \tilde{\mathsf{A}}^{x-2}\, \tilde{\mathsf{B}}\, \tilde{\mathsf{A}}^{L-x-1}\, \tilde{\boldsymbol{r}}$$
$$= (1, \tfrac{1}{2}) \begin{pmatrix} \frac{1}{4} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{4} \end{pmatrix}^{x-2} \begin{pmatrix} 0 & -\frac{1}{2} \\ \frac{1}{2} & 0 \end{pmatrix} \begin{pmatrix} \frac{1}{4} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{4} \end{pmatrix}^{L-x-1} \begin{pmatrix} \frac{1}{4} \\ \frac{1}{2} \end{pmatrix}$$
$$\simeq -\frac{3}{32} \left(-\frac{1}{4} \right)^{x-2} \left(\frac{3}{4} \right)^{L-x-1}, \tag{S.81}$$

which imply the desired (7.2.50).

7.3.1.a (p. 209) We write $\hat{\boldsymbol{S}}_x$, $\hat{\boldsymbol{S}}_{x+1}$ and $\hat{P}_J[\hat{\boldsymbol{S}}_x + \hat{\boldsymbol{S}}_{x+1}]$ as $\hat{\boldsymbol{S}}$, $\hat{\boldsymbol{S}}'$, and $\hat{P}_J$. We note, as in (7.1.6), that

$$\hat{\boldsymbol{S}} \cdot \hat{\boldsymbol{S}}' = \frac{1}{2}(\hat{\boldsymbol{S}} + \hat{\boldsymbol{S}}')^2 - 6 = \frac{1}{2}\big\{4 \times 5\, \hat{P}_4 + 3 \times 4\, \hat{P}_3 + 2 \times 3\, \hat{P}_2 + 2\, \hat{P}_1\big\} - 6$$
$$= 4\, \hat{P}_4 - 3\, \hat{P}_2 - 5\, \hat{P}_1 - 6\, \hat{P}_0, \tag{S.82}$$

which means

$$(\hat{\boldsymbol{S}} \cdot \hat{\boldsymbol{S}}')^2 = 16\, \hat{P}_4 + 9\, \hat{P}_2 + 25\, \hat{P}_1 + 36\, \hat{P}_0, \tag{S.83}$$
$$(\hat{\boldsymbol{S}} \cdot \hat{\boldsymbol{S}}')^3 = 64\, \hat{P}_4 - 27\, \hat{P}_2 - 125\, \hat{P}_1 - 216\, \hat{P}_0. \tag{S.84}$$

It is then easy to check that (7.3.3) gives (7.3.2) with $a = 10$, $b = 10/7$, and $c = -10/7$.

7.3.2.a (p. 213) The representation is not unique, so yours may not be the same as ours. First we need a rule corresponding to (7.1.9). By setting $S_{\rm max} = 2$ in (2.4.11), we find

$$\mathscr{S}[|\uparrow\rangle|\uparrow\rangle|\uparrow\rangle|\uparrow\rangle] = |\psi^2\rangle, \quad \mathscr{S}[|\uparrow\rangle|\uparrow\rangle|\uparrow\rangle|\downarrow\rangle] = \frac{1}{2}|\psi^1\rangle, \quad \mathscr{S}[|\uparrow\rangle|\uparrow\rangle|\downarrow\rangle|\downarrow\rangle] = \frac{1}{\sqrt{6}}|\psi^0\rangle,$$
$$\mathscr{S}[|\uparrow\rangle|\downarrow\rangle|\downarrow\rangle|\downarrow\rangle] = \frac{1}{2}|\psi^{-1}\rangle, \quad \mathscr{S}[|\downarrow\rangle|\downarrow\rangle|\downarrow\rangle|\downarrow\rangle] = |\psi^{-2}\rangle. \tag{S.85}$$

As for the valence bonds $(1/\sqrt{2})\{|\psi_x^{\uparrow}\rangle|\psi_{x+\boldsymbol{e}}^{\downarrow}\rangle - |\psi_x^{\downarrow}\rangle|\psi_{x+\boldsymbol{e}}^{\uparrow}\rangle\}$, where $\boldsymbol{e} = \boldsymbol{e}_{\rm x}$ or $\boldsymbol{e}_{\rm y}$, we again set $\alpha_{x,x+\boldsymbol{e}} = 1$ for the first term and $\alpha_{x,x+\boldsymbol{e}} = 2$ for the second term. We assign the factor $\pm 1/\sqrt{2}$ to A at the site x. Then by inspection one finds

$$\begin{gathered}
A^2_{1122} = \frac{1}{2}, \\
A^1_{1112} = A^1_{1121} = \frac{1}{4}, \quad A^1_{2122} = A^1_{1222} = -\frac{1}{4}, \\
A^0_{2222} = A^0_{1111} = \frac{1}{2\sqrt{6}}, \quad A^0_{1212} = A^0_{1221} = A^0_{2112} = A^0_{2121} = -\frac{1}{2\sqrt{6}}, \\
A^{-1}_{2221} = A^{-1}_{2212} = \frac{1}{4}, \quad A^{-1}_{1211} = A^{-1}_{2111} = -\frac{1}{4}, \\
A^{-2}_{2211} = \frac{1}{2}.
\end{gathered} \tag{S.86}$$

7.3.3.a (p. 217) The identity (7.3.28) is easily confirmed by examining the action on the four basis states $|\psi_x^{\sigma}\rangle|\psi_y^{\sigma'}\rangle$ with $\sigma, \sigma' = \uparrow, \downarrow$. Recall that $|\Phi_{\rm BR}\rangle = (\prod_{y=1}^{L} \hat{C}_{y,y+1})\hat{\sigma}_x^{(1)}|\Phi_{\rightarrow}\rangle$. Clearly $\hat{\sigma}_x^{(1)}$ commutes with $\hat{C}_{y,y+1}$ unless $y = x-1$ or $y = x$. We then use (7.3.28) to see that $\hat{C}_{x-1,x}\,\hat{C}_{x,x+1}\,\hat{\sigma}_x^{(1)} = \hat{C}_{x-1,x}\,\hat{\sigma}_x^{(1)}\hat{\sigma}_{x+1}^{(3)}\,\hat{C}_{x,x+1} = \hat{\sigma}_x^{(1)}\,\hat{\sigma}_{x-1}^{(3)}\hat{C}_{x-1,x}\,\hat{\sigma}_{x+1}^{(3)}\,\hat{C}_{x,x+1} = \hat{\sigma}_{x-1}^{(3)}\hat{\sigma}_x^{(1)}\hat{\sigma}_{x+1}^{(3)}\hat{C}_{x-1,x}\,\hat{C}_{x,x+1}$, which implies the desired (7.3.18).

7.3.3.b (p. 219) Let $\hat{U}_{\hat{A}} = \prod_{c\in\mathscr{C}_{\hat{A}}} \hat{C}_c$ and $\hat{U}_{\hat{B}} = \prod_{c\in\mathscr{C}_{\hat{B}}} \hat{C}_c$. Noting that $\hat{C}_c$ commute with each other and $(\hat{C}_c)^2 = \hat{1}$, we find

$$\begin{aligned}
\langle\Phi_{\mathscr{C}}|\hat{A}\hat{B}|\Phi_{\mathscr{C}}\rangle &= \langle\Phi_{\rightarrow}|(\hat{U}_{\hat{A}}\,\hat{A}\hat{U}_{\hat{A}})(\hat{U}_{\hat{B}}\,\hat{B}\hat{U}_{\hat{B}})|\Phi_{\rightarrow}\rangle \\
&= \langle\Phi_{\rightarrow}|\hat{U}_{\hat{A}}\,\hat{A}\hat{U}_{\hat{A}}|\Phi_{\rightarrow}\rangle\langle\Phi_{\rightarrow}|\hat{U}_{\hat{B}}\,\hat{B}\hat{U}_{\hat{B}}|\Phi_{\rightarrow}\rangle \\
&= \langle\Phi_{\mathscr{C}}|\hat{A}|\Phi_{\mathscr{C}}\rangle\langle\Phi_{\mathscr{C}}|\hat{B}|\Phi_{\mathscr{C}}\rangle,
\end{aligned} \tag{S.87}$$

where we noted that $|\Phi_{\rightarrow}\rangle$ is a trivial product state, and the supports of $\hat{U}_{\hat{A}}\,\hat{A}\hat{U}_{\hat{A}}$ and $\hat{U}_{\hat{B}}\,\hat{B}\hat{U}_{\hat{B}}$ (which are $\bar{\Lambda}_{\hat{A}}$ and $\bar{\Lambda}_{\hat{B}}$, respectively) do not overlap.

7.3.3.c (p. 220) Let us write the Hamiltonian (7.3.34) as $\hat{H}_{\mathscr{C}} = -\sum_{x\in\Lambda} \hat{h}_x$. The local Hamiltonian is $\hat{h}_x = \hat{\sigma}_x^{(1)}\hat{C}_{\{x_1,x_2\}}\hat{C}_{\{x_2,x_3\}}\hat{C}_{\{x_3,x_4\}}\hat{C}_{\{x_4,x_5\}}\hat{C}_{\{x_5,x_6\}}\hat{C}_{\{x_6,x_1\}}$, where $x_1, x_2, \ldots, x_6$ are the sites (ordered in a proper manner) of the hexagon centered at x.

Since $\hat{h}_x|\Phi_{\mathscr{C}}\rangle = |\Phi_{\mathscr{C}}\rangle$ for any x, any product of $\hat{h}_x$'s can be used to detect the hidden order. For example let B be a connected subset of one of the three sublattices. Then the operator $\prod_{x\in B}\hat{h}_x = (\prod_{x\in B}\hat{\sigma}_x^{(1)})(\prod_{j=1}^{M}\hat{C}_{\{x_j,x_{j+1}\}})$, where $x_1, x_2, \ldots, x_M$

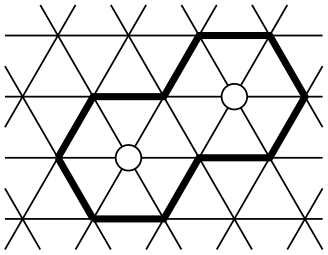


Fig. A.2 A simple example of the operator which measures the hidden order in the generalized cluster state (hyper graph state) on the hexagonal lattice. A white circle represents $\hat{\sigma}_x^{(1)}$ and a gray line represents $\hat{C}_{\{y,y'\}}$. This is operator is the product of two $\hat{h}_x$'s, where two x's correspond to white circles ()

(with $x_{M+1} = x_1$) are sites in other sublattices surrounding the set B, has expectation value 1 in the generalized cluster state $|\Phi_{\mathscr{C}}\rangle$. See Fig. A.2.

Since it is obvious that $[\hat{h}_x, \hat{U}_v] = 0$ when $x \in S_v$, we only need to show that $[\hat{h}_x, \hat{U}_v] = 0$ when $x \notin S_v$. This is equivalent to showing that, for any configuration $\sigma_1, \dots, \sigma_6 = \uparrow, \downarrow$, the sign factor $s(\sigma_1, \sigma_2)s(\sigma_2, \sigma_3) \dots s(\sigma_5, \sigma_6)s(\sigma_6, \sigma_1)$ is invariant under the simultaneous spin flip $\sigma_2 \to -\sigma_2$, $\sigma_4 \to -\sigma_4$, and $\sigma_6 \to -\sigma_6$. By inspection one finds that, under the spin flip $\sigma' \to -\sigma'$, the sign factor $s(\sigma, \sigma')s(\sigma', \sigma'')$ is invariant if $\sigma = \sigma''$, and changes the sign if $\sigma \neq \sigma''$. But, in any configuration $\sigma_1, \dots, \sigma_6$, the latter case does not take place or takes place exactly twice. This proves the desired invariance. It is interesting that one needs to treat the configuration of six spins on a closed loop (i.e., the hexagon) to see the invariance.

Problems of Chap. 8

8.3.3.a (p. 263) We assume that the ground state is $\mathbb{Z}_2 \times \mathbb{Z}_2$ is invariant and hence $\hat{U}_\pi^{(\alpha)} \hat{\rho}_{\mathrm{R}} (\hat{U}_\pi^{(\alpha)})^\dagger = \hat{\rho}_{\mathrm{R}}$ for $\alpha = 1, 2, 3$. This in particular means $[\hat{U}_\pi^{(3)}, \hat{\rho}_{\mathrm{R}}] = 0$, and hence we can assume that each $|\Psi_j\rangle_{\mathrm{R}}$ is an eigenstate of $\hat{U}_\pi^{(3)}$. We also see that the invariance (8.3.9) is valid with $|\Psi'_j\rangle_{\mathrm{R}} = \hat{U}_\pi^{(1)} |\Psi_j\rangle_{\mathrm{R}}$. Now, suppose that $|\Psi_j\rangle_{\mathrm{R}}$ can be regarded as states with half-odd-integer spins. Then from Problem 2.2.a (p. 23) we find that $|\Psi_j\rangle_{\mathrm{R}}$ and $|\Psi'_j\rangle_{\mathrm{R}}$ are orthogonal for each j. The rest is the same as the case with time-reversal symmetry.

8.3.4.a (p. 270) Let $\tilde{\rho}(e) = \rho(e) = \mathsf{I}$ and $\tilde{\rho}(g) = e^{-i\phi(g,g)/2}\rho(g)$ for $g \in \{a, b, c\}$. We see that $\tilde{\rho}(\cdot)$ gives an equivalent projective representation with the property that $\tilde{\rho}(g)\tilde{\rho}(g) = \tilde{\rho}(e)$ (and hence $\tilde{\phi}(g, g) = 0$) for all $g \in \mathbb{Z}_2 \times \mathbb{Z}_2$. Note also that $\tilde{\phi}(g, e) = \tilde{\phi}(e, g) = 0$ for $g \in \{a, b, c\}$ because $\tilde{\rho}(e) = \mathsf{I}$.[1]

[1] *Minor note:* The assumption $\rho(e) = \mathsf{I}$ is indeed not necessary. If $\rho(e) \neq \mathsf{I}$, we set $\tilde{\rho}(e) = e^{-i\phi(e,e)}\rho(e)$ and $\tilde{\rho}(g) = e^{-i\{\phi(g,g)+\phi(e,e)\}/2}\rho(g)$. We then have $\tilde{\rho}(g)\tilde{\rho}(g) = \tilde{\rho}(e)$ (and hence $\tilde{\phi}(g, g) = 0$) for all $g \in \mathbb{Z}_2 \times \mathbb{Z}_2$. Next, multiplying the relation $\tilde{\rho}(g)\tilde{\rho}(e) = e^{i\tilde{\phi}(g,e)}\tilde{\rho}(g)$ by $\tilde{\rho}(e)$

The cocycle condition (8.3.26) for $\tilde{\rho}(\cdot)$ with $(g_1, g_2, g_3) = (a, b, c)$ then reads $\tilde{\phi}(a, b) = \tilde{\phi}(b, c)$. By setting $(g_1, g_2, g_3) = (b, c, a)$, we also see $\tilde{\phi}(b, c) = \tilde{\phi}(c, a)$, and hence that $\tilde{\phi}(a, b) = \tilde{\phi}(b, c) = \tilde{\phi}(c, a) =: \xi$ with some $\xi \in \mathbb{R}$. Similarly we have $\tilde{\phi}(a, c) = \tilde{\phi}(c, b) = \tilde{\phi}(b, a) =: \xi'$ with some $\xi' \in \mathbb{R}$. We next use (8.3.26) with $(g_1, g_2, g_3) = (a, b, b)$ to find $\tilde{\phi}(a, b) + \tilde{\phi}(c, b) = 0$, which implies $\xi + \xi' = 0$. We finally use (8.3.26) with $(g_1, g_2, g_3) = (a, b, a)$ to see that $\tilde{\phi}(a, b) + \tilde{\phi}(c, a) = \tilde{\phi}(b, a) + \tilde{\phi}(a, c) \pmod{2\pi}$, which, with the above results, shows that $4\xi = 0 \pmod{2\pi}$.

It is easily found that we only need to consider the cases with $\xi = 0$ and with $\xi = \pi/2$. (Other cases are equivalent to one of the two.) When $\xi = \xi' = 0$, we readily see that $\tilde{\rho}(\cdot)$ is a genuine representation, and hence the original projective representation $\rho(\cdot)$ is trivial. When $\xi = \pi/2$ and $\xi' = -\pi/2$, we have $\tilde{\rho}(a)\tilde{\rho}(b) = e^{i\pi/2}\tilde{\rho}(c)$ and $\tilde{\rho}(b)\tilde{\rho}(a) = e^{-i\pi/2}\tilde{\rho}(c)$, etc. By setting $\tilde{\tilde{\rho}}(e) = \tilde{\rho}(e) = \mathsf{I}$ and $\tilde{\tilde{\rho}}(g) = e^{-i\pi/2}\tilde{\rho}(g)$ for $g \in \{a, b, c\}$, we get an equivalent projective representation $\tilde{\tilde{\rho}}(\cdot)$, which satisfies $\tilde{\tilde{\rho}}(g)\tilde{\tilde{\rho}}(g) = -\tilde{\tilde{\rho}}(e)$ for $g \in \{a, b, c\}$, and $\tilde{\tilde{\rho}}(a)\tilde{\tilde{\rho}}(b) = -\tilde{\tilde{\rho}}(b)\tilde{\tilde{\rho}}(a) = \tilde{\tilde{\rho}}(c)$, etc. This is nothing but the nontrivial projective representation (2.1.31).

8.3.4.b (p. 271) Noting that $\hat{u}_2 = \exp[-i\pi\hat{S}^{(2)}] = \begin{pmatrix} 0 & 0 & 1 \\ 0 & -1 & 0 \\ 1 & 0 & 0 \end{pmatrix}$ as in (2.1.33), we find that the new matrices are given by

$$\tilde{\mathsf{A}}^{+} = \mathsf{A}^{-}, \quad \tilde{\mathsf{A}}^{0} = -\mathsf{A}^{0}, \quad \tilde{\mathsf{A}}^{-} = \mathsf{A}^{+}. \tag{S.88}$$

8.3.4.c (p. 272) The matrices $\tilde{\mathsf{A}}^{\sigma}$ above are written in the form (8.3.16) with $\mathsf{U}_2 = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$, which is again $\exp[-i\pi\hat{S}^{(2)}]$ for $S = 1/2$. (Note that the choice of the unitary matrix is not unique.) This time we should set the phase factor as $e^{i\eta_L/L} = -1$.

8.3.4.d (p. 274) When no complex conjugation takes place as in the $\mathbb{Z}_2 \times \mathbb{Z}_2$ transformation, the matrices (8.3.39) transform in the same manner as (8.3.28) for the VBS state. This means that we can take the same unitary matrices U_1, U_2, and U_3, and hence the twisted VBS state is associated with the nontrivial projective representation of $\mathbb{Z}_2 \times \mathbb{Z}_2$.

There is a difference in time-reversal transformation (8.3.33) since it involves complex conjugation. One finds that (8.3.33) is recovered by (8.3.34) with $\zeta = \pi$ and $\mathsf{U} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$. We have $\mathsf{U}\mathsf{U}^{*} = \mathsf{U}^2 = \mathsf{I}$, which means that the associated phase is trivial, i.e, $\sigma_{\mathrm{tr}} = 1$.

Finally the VBS and the twisted VBS states can be connected smoothly via the θ-twisted-VBS state defined by the matrices

---

from left and right, one gets $\tilde{\rho}(e)\tilde{\rho}(g)\tilde{\rho}(e) = e^{i\tilde{\phi}(g,e)}\tilde{\rho}(e)\tilde{\rho}(g)\tilde{\rho}(e)$, which implies $\tilde{\phi}(g, e) = 0$. We similarly find $\tilde{\phi}(e, g) = 0$. This means that $\tilde{\rho}(g)\tilde{\rho}(e) = \tilde{\rho}(e)\tilde{\rho}(g) = \tilde{\rho}(g)$ for all $g \in \mathbb{Z}_2 \times \mathbb{Z}_2$. The rest of the proof is the same.

$$\mathsf{A}^{\pm}_{\theta\text{-VBS}} = \mathsf{A}^{\pm}_{\text{VBS}}, \quad \mathsf{A}^{0}_{\theta\text{-VBS}} = e^{i\theta}\,\mathsf{A}^{0}_{\text{VBS}}. \tag{S.89}$$

It can be checked easily that the state violates time-reversal symmetry except for $\theta = 0$ or π, but has $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry for any θ.

8.4.a (p. 295) The conditions (8.4.2), (8.4.3) for ground states are written as $\hat{A}_v|\Phi_{\text{GS}}\rangle = |\Phi_{\text{GS}}\rangle$ and $\hat{B}_p|\Phi_{\text{GS}}\rangle = |\Phi_{\text{GS}}\rangle$ for any v and p. Since it is obvious that $\hat{A}_v|\Phi_\uparrow\rangle = |\Phi_\uparrow\rangle$, we find $\hat{A}_v|\Phi_0\rangle = |\Phi_0\rangle$ from $[\hat{A}_v, \hat{B}_p] = 0$. Note also that $(\hat{B}_p)^2 = \hat{1}$ means $\hat{B}_p(\hat{1} + \hat{B}_p) = \hat{1} + \hat{B}_p$, which implies $\hat{B}_p|\Phi_0\rangle = |\Phi_0\rangle$. Thus $|\Phi_0\rangle$ is a ground state. The state $|\Phi_\uparrow\rangle$ corresponds to the empty graph with $\nu = \nu' = 0$. Since the action of $\hat{B}_p$ precisely corresponds to the local modification (8.4.17), we see that $|\Phi_0\rangle = \text{const.}\,|\Phi_{0,0}\rangle$.

8.4.b (p. 295) We give an elementary constructive proof,[2] which may not be elegant.[3] We prove that any graph with $\nu = \nu' = 0$ can be modified into the empty graph. Other cases can be treated similarly (or can be reduced to this case).

Given a graph, concentrate on the configuration of vertical thick bonds which cross the horizontal line in Fig. 8.18. By using the rules (8.4.17) repeatedly, one can move the thick bonds to the left or right, and let them pairwise annihilate. Since there are even number of thick bonds to begin with, we can get a configuration with no thick vertical bonds passing through the horizontal line. By repeating the procedure for all horizontal lines, we end up with a graph with no thick vertical lines. Remaining horizontal thick bonds must form horizontal loops wrapping around the lattice. Note that the number of the loops must be even. By moving these loops and letting them pairwise annihilate, we get the empty graph.

8.4.c (p. 297) We shall evaluate the correlation

$$\langle \hat{Z}_{\text{hor}} \hat{Z}'_{\text{hor}} \rangle_{\beta,L} := \frac{\text{Tr}[\hat{Z}_{\text{hor}} \hat{Z}'_{\text{hor}}\, e^{-\beta \hat{H}_{\text{tc}}}]}{\text{Tr}[e^{-\beta \hat{H}_{\text{tc}}}]}. \tag{S.90}$$

Write the Hamiltonian (8.4.1) as $\hat{H}_{\text{tc}} = -\sum_{v\in\mathscr{V}} \hat{A}_v - \sum_{p\in\mathscr{P}} \hat{B}_p$ by using (8.4.18). Noting that all $\hat{A}_v$ and $\hat{B}_p$ commute, and using the relation in footnote 72 (p. 297), we find

$$\begin{aligned} e^{-\beta \hat{H}_{\text{tc}}} &= (\cosh\beta)^{2L^2} \prod_{v\in\mathscr{V}} \{\hat{1} + (\tanh\beta)\hat{A}_v\} \prod_{p\in\mathscr{P}} \{\hat{1} + (\tanh\beta)\hat{B}_p\} \\ &= (\cosh\beta)^{2L^2} \sum_{\substack{V\subset\mathscr{V} \\ P\subset\mathscr{P}}} (\tanh\beta)^{|V|+|P|} \Big(\prod_{v\in V} \hat{A}_v\Big)\Big(\prod_{p\in P} \hat{B}_p\Big), \end{aligned} \tag{S.91}$$

[2] Or a "destructive proof" since we shall eliminate loops.

[3] The reader looking for an elegant proof may try to show that graphs (of loops) with $\nu = \nu' = 0$ must be a boundary of a region in the square lattice.

where V and P are summed over all subsets (including the empty set) of $\mathscr{V}$ and $\mathscr{P}$, respectively. Note that $\left(\prod_{v\in V}\hat{A}_v\right)\left(\prod_{p\in P}\hat{B}_p\right)$ is a monomial in $\hat{\sigma}_x^{(1)}$ and $\hat{\sigma}_x^{(3)}$ with $x\in\mathscr{E}$. The trace of a monomial is easily calculated as

$$\mathrm{Tr}\Big[\prod_{x\in\mathscr{E}}\{(\hat{\sigma}_x^{(1)})^{n_x^{(1)}}(\hat{\sigma}_x^{(3)})^{n_x^{(3)}}\}\Big]=\begin{cases}2^{2L^d} & \text{when all } n_x^{(1)} \text{ and } n_x^{(3)} \text{ are even,}\\ 0 & \text{otherwise.}\end{cases} \tag{S.92}$$

By using (S.91) and (S.92), one can evaluate (S.90) easily. For the partition function $\mathrm{Tr}[e^{-\beta\hat{H}_{\mathrm{tc}}}]$ the only nonvanishing contribution from the expansion (S.91) come from terms with $(V,P)=(\emptyset,\emptyset)$, $(\mathscr{V},\emptyset)$, $(\emptyset,\mathscr{P})$, or $(\mathscr{V},\mathscr{P})$. We thus get

$$\mathrm{Tr}[e^{-\beta\hat{H}_{\mathrm{tc}}}]=(2\cosh\beta)^{2L^2}\{1+2(\tanh\beta)^{L^2}+(\tanh\beta)^{2L^2}\}. \tag{S.93}$$

For $\mathrm{Tr}[\hat{Z}_{\mathrm{hor}}\hat{Z}'_{\mathrm{hor}}\,e^{-\beta\hat{H}_{\mathrm{tc}}}]$, nonvanshing contribution come from $(V,P)=(V_1,\emptyset)$, $(V_2,\emptyset)$, $(V,P)=(V_1,\mathscr{P})$, or $(V_2,\mathscr{P})$ where V_1 and V_2 are the two regions in $\mathscr{V}$ which have the two horizontal lines as boundaries. We thus find

$$\mathrm{Tr}[\hat{Z}_{\mathrm{hor}}\hat{Z}'_{\mathrm{hor}}\,e^{-\beta\hat{H}_{\mathrm{tc}}}]=(2\cosh\beta)^{2L^2}\{(\tanh\beta)^{\ell L}+(\tanh\beta)^{(L-\ell)L}\}\{1+(\tanh\beta)^{L^2}\}, \tag{S.94}$$

which implies

$$\langle\hat{Z}_{\mathrm{hor}}\hat{Z}'_{\mathrm{hor}}\rangle_{\beta,L}=\frac{(\tanh\beta)^{\ell L}+(\tanh\beta)^{(L-\ell)L}}{1+(\tanh\beta)^{L^2}}. \tag{S.95}$$

Problems of Chap. 9

9.2.3.a (p. 318) From the matrix elements listed above (9.2.38), one finds

$$\hat{S}_x^{(1)}=\frac{1}{2}(\hat{c}_{x,\uparrow}^\dagger\hat{c}_{x,\downarrow}+\hat{c}_{x,\downarrow}^\dagger\hat{c}_{x,\uparrow}),\ \ \hat{S}_x^{(2)}=\frac{1}{2i}(\hat{c}_{x,\uparrow}^\dagger\hat{c}_{x,\downarrow}-\hat{c}_{x,\downarrow}^\dagger\hat{c}_{x,\uparrow}),$$
$$\hat{S}_x^{(3)}=\frac{1}{2}(\hat{c}_{x,\uparrow}^\dagger\hat{c}_{x,\uparrow}-\hat{c}_{x,\downarrow}^\dagger\hat{c}_{x,\downarrow}), \tag{S.96}$$

from which one gets (9.2.44). Then an explicit calculation shows that

$$(\hat{\boldsymbol{S}}_x)^2=\frac{3}{4}(\hat{n}_{x,\uparrow}+\hat{n}_{x,\downarrow}-2\hat{n}_{x,\uparrow}\hat{n}_{x,\downarrow})=\frac{3}{4}\hat{n}_x(2-\hat{n}_x), \tag{S.97}$$

where we repeatedly used $(\hat{n}_{x,\sigma})^2=\hat{n}_{x,\sigma}$. We thus see that if a state $|\Phi\rangle$ satisfies $\hat{n}_x|\Phi\rangle=|\Phi\rangle$ then there is a spin $S=1/2$ at x, while if it satisfies $\hat{n}_x|\Phi\rangle=0$ or $\hat{n}_x|\Phi\rangle=2|\Phi\rangle$ then there is no spin at x. In the latter case the two electrons at x are forming a spin-singlet. (See Appendix A.3.3.)

9.2.3.b (p. 319) We use the notation of Sect. 9.2.1, and write $u=(x,\sigma)$ etc. Thus $\hat{B}(\mathsf{A})=\sum_{u,v}\hat{c}_u^\dagger(\mathsf{A})_{u,v}\hat{c}_v$ and $\hat{C}^\dagger(\boldsymbol{\varphi})=\sum_u\varphi(u)\hat{c}_u^\dagger$. By using the anticommutation relations (9.2.27) and (9.2.28), one finds $\hat{c}_u^\dagger\hat{c}_v\hat{c}_w^\dagger=-\hat{c}_u^\dagger\hat{c}_w^\dagger\hat{c}_v+\hat{c}_u^\dagger\delta_{v,w}=$

$\hat{c}_w^\dagger \hat{c}_u^\dagger \hat{c}_v + \hat{c}_u^\dagger \delta_{v,w}$, which means $[\hat{c}_u^\dagger \hat{c}_v, \hat{c}_w^\dagger] = \delta_{v,w} \hat{c}_u^\dagger$. Then one gets $[\hat{B}(\mathsf{A}), \hat{C}^\dagger(\boldsymbol{\varphi})] = \sum_{u,v,w} (\mathsf{A})_{u,v} \varphi(w)\, [\hat{c}_u^\dagger \hat{c}_v, \hat{c}_w^\dagger] = \sum_{u,v} (\mathsf{A})_{u,v} \varphi(v) \hat{c}_u^\dagger = \hat{C}^\dagger(\mathsf{A}\boldsymbol{\varphi})$.

Similarly one finds that $[\hat{c}_u^\dagger \hat{c}_v, \hat{c}_w^\dagger \hat{c}_z] = \delta_{v,w} \hat{c}_u^\dagger \hat{c}_z - \delta_{u,z} \hat{c}_w^\dagger \hat{c}_v$. Then one gets

$$
\begin{aligned}
[\hat{B}(\mathsf{A}), \hat{B}(\mathsf{B})] &= \sum_{u,v,w,z} (\mathsf{A})_{u,v} (\mathsf{B})_{w,z} [\hat{c}_u^\dagger \hat{c}_v, \hat{c}_w^\dagger \hat{c}_z] \\
&= \sum_{u,z} (\mathsf{AB})_{u,z} \hat{c}_u^\dagger \hat{c}_z - \sum_{v,w} (\mathsf{BA})_{w,v} \hat{c}_w^\dagger \hat{c}_v = \hat{B}([\mathsf{A}, \mathsf{B}]). \qquad \text{(S.98)}
\end{aligned}
$$

9.2.3.c (p. 323) From the commutation relations (9.2.67), one finds $\hat{S}_{\rm tot}^{\pm} \hat{S}_{\rm tot}^{\mp} \hat{c}_{x,\uparrow}^\dagger \hat{c}_{y,\downarrow}^\dagger |\Phi_{\rm vac}\rangle = (\hat{c}_{x,\uparrow}^\dagger \hat{c}_{y,\downarrow}^\dagger + \hat{c}_{x,\downarrow}^\dagger \hat{c}_{y,\uparrow}^\dagger)|\Phi_{\rm vac}\rangle$ and $\hat{S}_{\rm tot}^{(3)} \hat{c}_{x,\uparrow}^\dagger \hat{c}_{y,\downarrow}^\dagger |\Phi_{\rm vac}\rangle = 0$. We thus get

$$
\begin{aligned}
(\hat{\boldsymbol{S}}_{\rm tot})^2 |\xi\rangle &= \left\{ \frac{\hat{S}_{\rm tot}^+ \hat{S}_{\rm tot}^- + \hat{S}_{\rm tot}^- \hat{S}_{\rm tot}^+}{2} + (\hat{S}_{\rm tot}^{(3)})^2 \right\} \sum_{x,y \in \Lambda} \xi(x,y)\, \hat{c}_{x,\uparrow}^\dagger \hat{c}_{y,\downarrow}^\dagger |\Phi_{\rm vac}\rangle \\
&= \sum_{x,y \in \Lambda} \xi(x,y) \{ \hat{c}_{x,\uparrow}^\dagger \hat{c}_{y,\downarrow}^\dagger + \hat{c}_{x,\downarrow}^\dagger \hat{c}_{y,\uparrow}^\dagger \} |\Phi_{\rm vac}\rangle \\
&= \sum_{x,y \in \Lambda} \big\{ \xi(x,y) - \xi(y,x) \big\} \hat{c}_{x,\uparrow}^\dagger \hat{c}_{y,\downarrow}^\dagger |\Phi_{\rm vac}\rangle, \qquad \text{(S.99)}
\end{aligned}
$$

which implies $(\hat{\boldsymbol{S}}_{\rm tot})^2 |\xi\rangle = 0$ if $\xi(\cdot,\cdot)$ is symmetric, and $(\hat{\boldsymbol{S}}_{\rm tot})^2 |\xi\rangle = 2|\xi\rangle$ if $\xi(\cdot,\cdot)$ is antisymmetric. The two cases correspond to spin-singlet with $S_{\rm tot} = 0$, and spin-triplet with $S_{\rm tot} = 1$, respectively. See Appendix A.3.3. This relation between the total spin $S_{\rm tot}$ and the symmetry of the spatial wave function $\xi(x, y)$ is essential for determining magnetic properties of many-electron systems.[1]

9.3.2.a (p. 329) The anticommutation relations (9.3.25) and (9.3.26) are straightforward consequences of (9.2.63) and (9.2.64). To show (9.3.27) we use the definition of $\hat{a}_{j,\sigma}$ and the Schrödinger equation (9.3.3) to observe

$$
\begin{aligned}
\sum_j \varepsilon_j \hat{\tilde{n}}_{j,\sigma} &= \sum_{j,x,y} \varepsilon_j\, \psi_x^{(j)} (\psi_y^{(j)})^*\, \hat{c}_{x,\sigma}^\dagger \hat{c}_{y,\sigma} = \sum_{j,x,y,z} t_{x,z}\, \psi_z^{(j)} (\psi_y^{(j)})^*\, \hat{c}_{x,\sigma}^\dagger \hat{c}_{y,\sigma} \\
&= \sum_{x,y,z} t_{x,z}\, \delta_{z,y}\, \hat{c}_{x,\sigma}^\dagger \hat{c}_{y,\sigma} = \sum_{x,y} t_{x,y}\, \hat{c}_{x,\sigma}^\dagger \hat{c}_{y,\sigma}. \qquad \text{(S.100)}
\end{aligned}
$$

[1] The standard explanation in terms of wave function language is as follows: The total wave function of two electrons must be antisymmetric with respect to the change of the labels of the two electrons. If the spatial part of the wave function is symmetric (*resp.* antisymmetric), then the spin part must be antisymmetric (*resp.* symmetric), which means that the total spin is 0 (*resp.* 1). Note that the necessary symmetry is automatically satisfied in the Fock space representation.

From (9.3.25) and (9.3.26), we find that $[\hat{\tilde{n}}_{j,\sigma}, \hat{a}^\dagger_{k,\tau}] = \delta_{j,k}\delta_{\sigma,\tau}\,\hat{a}^\dagger_{j,\sigma}$ exactly as in (9.2.31). By applying $\hat{H}_{\rm hop}$ represented as (9.3.27) onto (9.3.22), and using the above commutation relation repeatedly and noting $\hat{\tilde{n}}_{j,\sigma}|\Phi_{\rm vac}\rangle = 0$, we recover (9.3.23).

9.3.3.a (p. 335) By rewriting $\hat{U}^{{\rm ph},\theta}_{x,\sigma} = \hat{c}_{x,\sigma} - e^{-i\theta}\,\hat{c}^\dagger_{x,\sigma}$, one readily finds $(\hat{U}^{{\rm ph},\theta}_{x,\sigma})^\dagger\,\hat{c}_{x,\sigma}\,\hat{U}^{{\rm ph},\theta}_{x,\sigma} = -e^{-i\theta}\,\hat{c}^\dagger_{x,\sigma}$ and $(\hat{U}^{{\rm ph},\theta}_{x,\sigma})^\dagger\,\hat{c}^\dagger_{x,\sigma}\,\hat{U}^{{\rm ph},\theta}_{x,\sigma} = -e^{i\theta}\,\hat{c}_{x,\sigma}$.

9.3.3.b (p. 336) From (9.2.44) and (9.3.51), one readily finds $\hat{\eta}^+_x = (-1)^x\,\hat{c}_{x,\uparrow}\,\hat{c}_{x,\downarrow}$, $\hat{\eta}^-_x = (-1)^x\,\hat{c}^\dagger_{x,\downarrow}\,\hat{c}^\dagger_{x,\uparrow}$, and $\hat{\eta}^{(3)}_x = (1-\hat{n}_x)/2$.

To show that $[\hat{\eta}^{(\alpha)}_{\rm tot}, \hat{S}^{(\beta)}_{\rm tot}] = 0$, it suffices to check that $\hat{\eta}^\pm_x$ and $\hat{\eta}^{(3)}_x$ are SU(2) invariant (with respect to the spin rotations). From (A.2.2), we see that

$$[\hat{c}_{x,\uparrow}\,\hat{c}_{x,\downarrow}, \hat{S}^+_{\rm tot}] = [\hat{c}_{x,\uparrow}, \hat{S}^+_{\rm tot}]\hat{c}_{x,\downarrow} + \hat{c}_{x,\uparrow}[\hat{c}_{x,\downarrow}, \hat{S}^+_{\rm tot}] = (\hat{c}_{x,\downarrow})^2 = 0, \tag{S.101}$$

where we used the commutation relations (9.3.36). Similarly,

$$[\hat{c}_{x,\uparrow}\,\hat{c}_{x,\downarrow}, \hat{S}^-_{\rm tot}] = [\hat{c}_{x,\uparrow}, \hat{S}^-_{\rm tot}]\hat{c}_{x,\downarrow} + \hat{c}_{x,\uparrow}[\hat{c}_{x,\downarrow}, \hat{S}^-_{\rm tot}] = (\hat{c}_{x,\uparrow})^2 = 0, \tag{S.102}$$

where we used $[\hat{c}_{x,\uparrow}, \hat{S}^-_{\rm tot}] = 0$ and $[\hat{c}_{x,\downarrow}, \hat{S}^-_{\rm tot}] = \hat{c}_{x,\uparrow}$, which follow by taking the conjugate of (9.3.36). We also see from (9.2.31) that

$$\begin{aligned}[\hat{c}_{x,\uparrow}\,\hat{c}_{x,\downarrow}, \hat{S}^{(3)}_{\rm tot}] &= \frac{1}{2}\Big([\hat{c}_{x,\uparrow}\,\hat{c}_{x,\downarrow}, \hat{n}_{x,\uparrow}] - [\hat{c}_{x,\uparrow}\,\hat{c}_{x,\downarrow}, \hat{n}_{x,\downarrow}]\Big) \\ &= \frac{1}{2}(\hat{c}_{x,\uparrow}\,\hat{c}_{x,\downarrow} - \hat{c}_{x,\uparrow}\,\hat{c}_{x,\downarrow}) = 0.\end{aligned} \tag{S.103}$$

We have thus shown that $\hat{\eta}^+_x = (-1)^x\,\hat{c}_{x,\uparrow}\,\hat{c}_{x,\downarrow}$ is SU(2) invariant. Clearly $\hat{\eta}^-_x = (\hat{\eta}^+_x)^\dagger$ is also SU(2) invariant. Finally $\hat{\eta}^{(3)}_x = (1-\hat{n}_x)/2$ is SU(2) invariant since we have shown that $\hat{n}_x$ is SU(2) invariant.

We have already shown that $[\hat{H}_{\rm hop}, \hat{S}^{(\alpha)}_{\rm tot}] = 0$ and $[\hat{H}'_{\rm int}, \hat{S}^{(\alpha)}_{\rm tot}] = 0$ for $\alpha = 1, 2, 3$. By applying the Shiba transformation, these relations immediately imply $[\hat{H}_{\rm hop}, \hat{\eta}^{(\alpha)}_{\rm tot}] = 0$ and $[-\hat{H}'_{\rm int}, \hat{\eta}^{(\alpha)}_{\rm tot}] = 0$.

Problems of Chap. 10

10.1.a (p. 342) From (10.1.3) and (10.1.4), we see that the Schrödinger equation $\hat{H}|\Phi\rangle = E|\Phi\rangle$ is

$$t(\beta+\gamma) = E\alpha, \quad 2t\alpha + U\beta = E\beta, \quad 2t\alpha + U\gamma = E\gamma. \tag{S.104}$$

This is an eigenvalue equation of a 3×3 matrix, but can be solved easily by using the symmetry between the two sites. Assume first that $\beta = \gamma$. Then (S.104) reduces to $2t\beta = E\alpha$, $2t\alpha + U\beta = E\beta$, which implies $E^2 - UE - 4t^2 = 0$. We thus find two energy eigenvalues $E = (U \pm \sqrt{U^2+16t^2})/2$, one of which is the ground state energy. The other energy eigenvalue behaves as $E \simeq U + 4t^2/U$ if $|t| \ll U$. Next

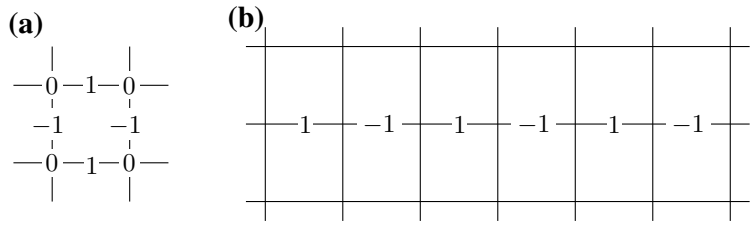


Fig. A.3 **a** A zero energy state that is localized on a single plaquette. **b** A nonlocal zero energy state that raps around the whole lattice ()

by assuming $\beta = -\gamma$ in (S.104), we get a trivial solution with $\alpha = 0$, in which case the energy eigenvalue is exactly U.

10.2.3.a (p. 358) For each plaquette (i.e., a unit square which has four black sites on the corners), consider the state depicted in Fig. A.3a, which is localized at the plaquette and has nonzero components only on the A sublattice. The state is clearly the energy eigenstate with zero energy. It seems like we are done since there are exactly L^2 plaquettes while Proposition 10.7 requires L^2 zero energy eigenstates.[1] However we find that these L^2 states are not linearly independent because we can take a linear combination of all these states to get zero. Thus we have found only $L^2 - 1$ zero energy states. One more is missing.

In fact there is a nonlocal zero energy eigenstate that lives on the horizontal line and has nonvanishing components only on the A sublattice. See Fig. A.3b. Such a state is well defined since we assume periodic boundary conditions. One may have noticed that the construction is somewhat similar to that of the ground states of Kitaev's toric code model discussed in Sect. 8.4. We have thus found one more eigenstate, but there clearly is one more independent state that raps around the lattice in the vertical direction. We now have $L^2 + 1$ zero energy eigenstates. Proposition 10.7 does not inhibit a model from having more than L^2 zero energy states, but the symmetry $-\varepsilon_j = \varepsilon_{|\Lambda|-j}$ requires the number of the zero-energy states to be even. So there must be at least $L^2 + 2$ zero energy states! What is one more state?[2]

Problems of Chap. 11

11.3.1.a (p. 399) The unit cell of this model consists of $d + 1$ sites. We can take one of them as the origin, and the rest as $\boldsymbol{e}_j/2$ with $j = 1, \dots, d$, where $\boldsymbol{e}_j$ is the unit vector in the j-direction. We shall abbreviate them as 0 and j, respectively, and write $\mathscr{U} = \{0, 1, 2, \dots, d\}$. See Fig. A.4.

[1] Probably this is sufficient when L is odd.

[2] Hint: How many zero energy eigenstates does the single-electron Schrödinger equation (10.2.18) have? The answer is L if L is odd, but is $L + 2$ if L is even.

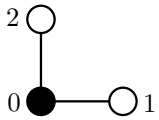


Fig. A.4 The unit cell of the flat-band model with $d = 2$ in Fig. 11.11 consists of three sites, which we call 0, 1, and 2 ()

From (11.3.22) we see that the nonzero components of the effective hopping (9.3.12) are $S^{(\boldsymbol{k})}_{0,0} = 2\nu^2 t \sum_{j=1}^{d}(1+\cos k_j)$, $S^{(\boldsymbol{k})}_{j,j} = t$, and $S^{(\boldsymbol{k})}_{0,j} = (S^{(\boldsymbol{k})}_{j,0})^* = \nu t(1+e^{-ik_j})$, where $j = 1, 2, \dots, d$. The effective hopping matrix thus looks like

$$\mathsf{S}^{(\boldsymbol{k})} = \begin{pmatrix} S^{(\boldsymbol{k})}_{0,0} & S^{(\boldsymbol{k})}_{0,1} & S^{(\boldsymbol{k})}_{0,2} & \cdots & S^{(\boldsymbol{k})}_{0,d} \\ S^{(\boldsymbol{k})}_{1,0} & t & 0 & \cdots & 0 \\ S^{(\boldsymbol{k})}_{2,0} & 0 & t & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ S^{(\boldsymbol{k})}_{d,0} & 0 & 0 & \cdots & t \end{pmatrix} \tag{S.105}$$

One then finds by inspection that

$$\begin{aligned} \det[\mathsf{S}^{(\boldsymbol{k})} - \varepsilon \mathsf{I}] &= (S^{(\boldsymbol{k})}_{0,0} - \varepsilon)(t-\varepsilon)^d - \sum_{j=1}^{d} |S^{(\boldsymbol{k})}_{0,j}|^2 (t-\varepsilon)^{d-1} \\ &= \varepsilon\{\varepsilon - (t + S^{(\boldsymbol{k})}_{0,0})\}(t-\varepsilon)^{d-1}, \end{aligned} \tag{S.106}$$

where we used the identity $\sum_{j=1}^{d} |S^{(\boldsymbol{k})}_{0,j}|^2 = t\, S^{(\boldsymbol{k})}_{0,0}$. The desired dispersion relations (11.3.23) readily follows from the eigenvalue equation $\det[\mathsf{S}^{(\boldsymbol{k})} - \varepsilon \mathsf{I}] = 0$.

11.3.2.a (p. 403) The d-dimensional checkerboard lattice Λ is identical to the set of internal sites $\mathscr{I}$ in the decorated hypercubic lattice considered in Sect. 11.3.1. See Fig. 11.10. Consider the single-electron Schrödinger equation for the Tasaki model

$$\hat{H}_{\mathrm{hop}} \sum_{u\in\mathscr{I}} \varphi(u)\, \hat{b}^{\dagger}_{u,\sigma} |\Phi_{\mathrm{vac}}\rangle = \varepsilon \sum_{u\in\mathscr{I}} \varphi(u)\, \hat{b}^{\dagger}_{u,\sigma} |\Phi_{\mathrm{vac}}\rangle, \tag{S.107}$$

which describes the bands other than the lowest flat-band. The definition (11.3.5) of $\hat{H}_{\mathrm{hop}}$ and the anticommutation relation

$$\{\hat{b}_{u,\sigma}, \hat{b}^{\dagger}_{v,\tau}\} = \begin{cases} (1+2\nu^2)\,\delta_{\sigma,\tau} & \text{if } u = v, \\ \nu^2\,\delta_{\sigma,\tau} & \text{if } \exists p \in \mathscr{E} \text{ s.t. } |p-u| = |p-v| = 1/2, \\ 0 & \text{otherwise} \end{cases} \tag{S.108}$$

imply that (S.107) becomes

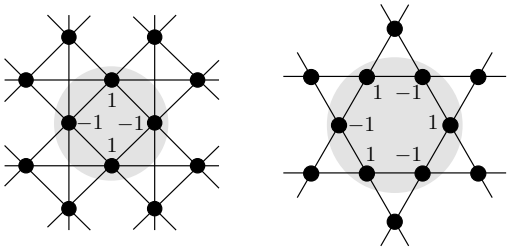
$$(1+2\nu^2)t\,\varphi(u)+t\nu\sum_{\substack{v\in\mathscr{I}\\ \{u,v\}\in\mathscr{B}}}\varphi(v)=\tilde{\varepsilon}\varphi(u), \tag{S.109}$$

where $\mathscr{B}$ is the set of bonds for the generalized checkerboard lattice. The single-electron Schrödinger equation for the d-dimensional checkerboard lattice that we want to solve, on the other hand, reads

$$2t\,\varphi(u)+t\sum_{\substack{v\in\mathscr{I}\\ \{u,v\}\in\mathscr{B}}}\varphi(v)=\varepsilon\varphi(u). \tag{S.110}$$

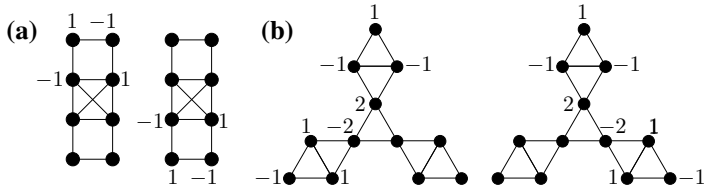
Note that (S.109) reduces to (S.110) if we set $\nu=1$ and $\tilde{\varepsilon}=\varepsilon+t$. We thus get the desired (11.3.33) from (11.3.23).

11.3.2.b (p. 403) Nonzero components of the zero energy states are as in the following.



These localized states may or may not span the whole zero-energy subspace, depending on the boundary conditions. In fact the situation is quite similar to those for the zero-energy states in the Lieb lattice. See Problem 10.2.3.a.

11.3.2.c (p. 405) Nonzero components of the desired zero energy states are obtained by inspection as follows.



For each case, let $\hat{a}_{1,\sigma}$ and $\hat{a}_{2,\sigma}$ denote the fermion operators of the two states. For model (a), one finds that the state $\hat{a}^\dagger_{1,\sigma}\hat{a}^\dagger_{2,\tau}|\Phi_{\rm GS}\rangle$ with any $\sigma,\tau=\uparrow,\downarrow$ is a ground state for any $U>0$. Thus the ground states have both $S_{\rm tot}=0$ and 1. For model (b), one can repeat the proof of Tasaki's flat-band ferromagnetism in Sect. 11.3.1 by using the $\hat{a}^\dagger$ operators to prove that the model exhibits ferromagnetism.

11.4.1.a (p. 417) We can assume that $\omega_u(x)=O(\nu^3)$ if $|x-u|>1$. Then by writing $\omega_u(u)=A$ and $\omega_u(u\pm\frac{1}{2})=A\alpha$ (where α is expected to be of order ν), we find from the requirement $\langle\boldsymbol{\omega}_u,\boldsymbol{\omega}_{u+1}\rangle=0$ that $\omega_u(u\pm1)=-A\alpha^2/2+O(\nu^3)$. Now by demanding that $\langle\boldsymbol{\omega}_u,\boldsymbol{\omega}_{u+\frac{1}{2}}\rangle=0$, where $\boldsymbol{\omega}_{u+\frac{1}{2}}$ is given by (11.4.5), we find $\alpha=\nu/(1+\gamma)+O(\nu^3)$. We therefore get

$$\omega_u(x) = \left(1 + \frac{2\nu^2}{(1+\gamma)^2}\right)^{-1/2} \times \begin{cases} 1 + O(\nu^3) & \text{if } x = u, \\ \dfrac{\nu}{1+\gamma} + O(\nu^3) & \text{if } |x-u| = \frac{1}{2}, \\ -\dfrac{1}{2}\left(\dfrac{\nu}{1+\gamma}\right)^2 + O(\nu^3) & \text{if } |x-u| = 1, \\ O(\nu^3) & \text{otherwise.} \end{cases} \tag{S.111}$$

By operating the hopping matrix (11.4.1) explicitly, one finds

$$\mathsf{T}\boldsymbol{\omega}_u = (1+\gamma)\, t\, \boldsymbol{\omega}_u + \frac{\nu^2}{1+\gamma}\, t\, \{2\boldsymbol{\omega}_u + \boldsymbol{\omega}_{u-1} + \boldsymbol{\omega}_{u+1}\} + O(\nu^3), \tag{S.112}$$

which is consistent with the dispersion relation (11.4.3).