Progress of Theoretical Physics, Vol. 99, No. 4, April 1998

From Nagaoka's Ferromagnetism to Flat-Band Ferromagnetism and Beyond

— *An Introduction to Ferromagnetism in the Hubbard Model* —

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(Received January 12, 1998)

It is believed that strong ferromagnetic interactions in some solids are generated by subtle interplay between quantum many-body effects and spin-independent Coulomb interactions between electrons. It is a challenging problem to verify this scenario in the Hubbard model, which is an idealized model for strongly interacting electrons in a solid.

Nagaoka's ferromagnetism is a well-known rigorous example of ferromagnetism in the Hubbard model. It deals with the limiting situation in which there is one fewer electron than in the half-filling and the on-site Coulomb interaction is infinitely large. There are relatively new rigorous examples of ferromagnetism in Hubbard models called flat-band ferromagnetism. Flat-band ferromagnetism takes place in carefully prepared models in which the lowest bands (in the single-electron spectra) are "flat." Usually, these two approaches are regarded as two complimentary routes to ferromagnetism in the Hubbard model.

In the present paper we describe Nagaoka's ferromagnetism and flat-band ferromagnetism in detail, giving all the necessary background as well as complete (but elementary) mathematical proofs. By studying an intermediate model called the long-range hopping model, we also demonstrate that there is indeed a deep relation between these two seemingly different approaches to ferromagnetism.

We further discuss some attempts to go beyond these approaches. We briefly discuss recent rigorous example of ferromagnetism in the Hubbard model which has neither infinitely large parameters nor completely flat bands. We give preliminary discussion regarding possible experimental realizations of the (nearly-)flat-band ferromagnetism. Finally, we focus on some theoretical attempts to understand metallic ferromagnetism. We discuss three artificial one-dimensional models in which the existence of metallic ferromagnetism can be easily proved.

We have tried to make the present paper as self-contained as possible, keeping in mind readers who are new to the field. Although the present paper is written as a review, it contains some material which appears for the first time.

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§1. Introduction

1.1. *Hubbard model and the origin of ferromagnetism*

The origin of strong ferromagnetic ordering observed in some materials has been a mystery in physical science for a long time. Since quantum mechanical many-electron systems without interactions universally exhibit paramagnetism, the origin of ferromagnetism should be sought in electron-electron interactions. In most solids, however, the dominant part of the interaction between electrons is the Coulomb interaction, which is perfectly spin-independent. We are thus faced with a very interesting and fundamental problem in theoretical physics to determine *whether spin-independent interactions in an itinerant electron system can be the origin of ferromagnetic ordering.* This problem is important not only because ferromagnetism is a very common (and useful) phenomenon, but because it focuses on the fundamental role of nonlinear interactions in many-body quantum mechanical systems.

It was Heisenberg [1] who first realized that ferromagnetism is an intrinsically quantum mechanical phenomenon. In Heisenberg's approach to ferromagnetism, one starts from the picture that each electron (relevant to magnetism) is almost localized in an atomic orbit. By treating the effect of the Coulomb interaction and overlap between nearby atomic orbits in a perturbative manner as in the Heitler-London theory, Heisenberg concluded that there appears an "exchange interaction" between nearby electronic spins which determines the magnetic properties of the system.

In a different approach to the problem of ferromagnetism, which was originated by Bloch, [2] one starts from the quantum mechanical free electron gas, in which electrons are in plane-wave like states. One then treats the effect of the Coulomb interaction perturbatively, and tries to find instabilities against certain magnetic ordering. When combined with the Hartree-Fock approximation (or a mean-field theory), this approach leads to the picture that there is an instability with respect to ferromagnetism when the density of states at the fermi energy and the Coulomb interaction are sufficiently large.

In spite of a considerable number of attempts to improve these ideas, neither of these two approaches has yet produced a truly convincing explanation about the origin of ferromagnetism.

A modern version of the problem of the origin of ferromagnetism was formulated by Kanamori, [3] Gutzwiller, [4] and Hubbard [5] in the 1960's.*) They studied simple tight-binding models of electrons with on-site Coulomb interaction. This model is usually called the 'Hubbard model.' When there is no electron-electron interaction, the model exhibits paramagnetism as an inevitable consequence of the Pauli exclusion principle. Among other things, Kanamori, Gutzwiller and Hubbard asked *whether the paramagnetism found for a non-interacting system can be converted into ferromagnetism when there is a sufficiently large Coulomb interaction.* This is a concrete formulation of the fundamental problem that we alluded to in the opening of the previous subsection.

It is worth noting that the on-site Coulomb interaction itself is completely in-

*) A similar formulation was given earlier, for example, in Ref. 6).

dependent of electronic spins, and it does not favor any magnetic ordering. One does not find any terms in the Hubbard Hamiltonian which explicitly favor ferromagnetism (or any other ordering). Our theoretical goal is to show that magnetic ordering arises as a consequence of the subtle interplay between the kinetic motion of electrons and the short-ranged Coulomb interaction. It is interesting to compare this situation with that in spin systems, where one is often given a Hamiltonian which favors some kind of magnetic ordering, and the major task is to investigate if such ordering really takes place. We can say that the Hubbard model formulation goes deeper into fundamental mechanisms of magnetism than that of spin systems. It offers a challenging problem to theoretical physicists to derive magnetic interaction from models which do not explicitly contain such interactions.

From a more global point of view, the importance of the Hubbard model may be understood from the philosophy of "universality", which, in our opinion, is at the very heart of contemporary physics. We believe that nontrivial physical phenomena or mechanisms found in a suitable idealized model can also be found in other systems in the same "universality class" as the idealized model. We expect that the universality class is often large and rich enough to contain various realistic systems with complicated details which are ignored in the idealized model. As for strongly interacting electron systems, the Hubbard model is regarded as one of the most promising candidates for an idealized model to be used in our search of possible universality classes.

Perhaps the best justification of the Hubbard model as a standard model of itinerant electron systems comes from such theoretical considerations, rather than its accuracy in modeling narrow band electron systems.

1.2. *Rigorous results*

The problem of ferromagnetism in the Hubbard model was studied extensively using various heuristic methods. The Hartree-Fock approximation discussed above leads one to the so-called Stoner criterion. It states that the Hubbard model exhibits ferromagnetism when the condition $UD_{\mathrm{F}} > 1$ is satisfied, where U is the strength of the on-site Coulomb interaction and D_{F} is the density of states of the corresponding single-electron problem measured at the fermi level (of the corresponding noninteracting system). Although the criterion cannot be trusted literally,*) it guides us to look for ferromagnetism in models in which U is large and/or the density of states is large.

The first rigorous result about ferromagnetism in the Hubbard model, which is one of the main topics of the present paper, was provided by Nagaoka.**), [10] It was proved that certain Hubbard models have ground states with saturated ferromagnetism when there is exactly one hole and the Coulomb repulsion U is infinite.

In 1989, Lieb proved an important general theorem for the Hubbard model on a bipartite lattice at half-filling. [11] As a corollary of this theorem, Lieb showed that

*) There are many systems which fully satisfy the criterion but do not exhibit ferromagnetism. Flat-band Hubbard models with low electron densities [7),8)] are typical examples.

**) Thouless [9] reached a similar but slightly weaker conclusion.

a rather general class of Hubbard model exhibits ferrimagnetism.*) (See also Ref. 12).)

In 1991, Mielke[13),14)] found a new class of rigorous examples of ferromagnetism in the Hubbard model. He showed that the Hubbard models on a general class of line graphs have ferromagnetic ground states. A special feature of Mielke's models is that the corresponding single-electron Schrödinger equation has highly degenerate ground states. In other words, Mielke's models have flat (or dispersionless) bands. Mielke's original results were for the case in which the number of electrons corresponds to the half-filling of the lowest flat band, but later it was extended to different electron densities in two-dimensional models.[15)]

A similar but different class of examples of ferromagnetism in Hubbard models, which we will discuss in detail in the present paper, were proposed in Refs. 7) and 8). These models are defined on a class of decorated lattices with "cell structures", and are also characterized by flat bands at the bottom of the single-electron spectrum. In a class of models in two and higher dimensions, it was proved that the ferromagnetism is stable against fluctuations in the electron number.[7),8)] The ferromagnetism in Mielke's models and those in Refs. 7) and 8) is now called "flat-band ferromagnetism", and regarded as one of reliable starting points for the problem of ferromagnetism.

There are also rigorous results for ferromagnetism in 'nearly-flat-band models' obtained by perturbing the flat-band models of Refs. 7) and 8). In a general situation, local stability of ferromagnetism is known,[16),17)] and for a special class of models, global stability of ferromagnetism has been established.[18),19)] We shall also briefly discuss the latter results in the present paper.

Nagaoka's ferromagnetism takes place in models with $U \to \infty$, while (nearly-) flat-band ferromagnetism takes place in models characterized by large (or infinite) density of states D_{F}. One might say that these two rigorous results realize the Stoner criterion $UD_{\mathrm{F}} > 1$ through complementary paths.

1.3. *About the present paper*

One of the main aims of the present paper is to give complete descriptions of Nagaoka's ferromagnetism and flat-band ferromagnetism of Refs. 7) and 8). In particular, the proof of the generalized version of Nagaoka's theorem is described in complete detail for the first time. Another important aim is to show that there is a close relation between these two approaches which are usually regarded as complementary. We demonstrate this fact by studying an artificial model which we call the 'long range hopping model.' Our hope is that a clarification of the relation between the two approaches will lead us to a more global view of ferromagnetism in the Hubbard model, and that this might lead us in the long run to a better understanding of the essence of the fascinating phenomenon of ferromagnetism.

We also discuss three topics related to these results. First, we briefly discuss important attempts to go beyond flat-band ferromagnetism by treating non-singular Hubbard models. One of the main achievements in this direction is a proof of the existence of ferromagnetism in a Hubbard model which has a finite Coulomb

*) Ferrimagnetism is a kind of antiferromagnetism on a bipartite lattice such that the numbers of sites in two sublattices are different.

repulsion U and a finite density of states D_F. Next, we give a preliminary discussion of some experimental results which may be relevant to flat-band ferromagnetism. The ferromagnetism seen in $La_4Ba_2Cu_2O_{10}$, which was discovered back in 1990, shows some striking similarities with flat-band ferromagnetism. Finally we describe some attempts to obtain theoretical examples of metallic ferromagnetism. There are strong indications that some one-dimensional Hubbard models exhibit metallic ferromagnetism, but there are no rigorous results yet. We discuss three artificial models in one-dimension which are easily shown to exhibit metallic ferromagnetism. The results for the third model, the limiting U-V model, are perhaps new.

We have tried to make the present paper as self-contained as possible.*) We carefully start from basic assumptions and definition of the Hubbard model, keeping in mind readers who are new to the field. We give complete proofs to all the theorems which are directly related to the main subjects of the paper. The proofs, however, may not be optimally organized from a mathematical point of view. Instead, we have tried to present "readable" proofs from which the readers can learn physical mechanisms underlying the theorems. (This comment applies even to the proof of purely mathematical theorems such as Theorem 4.3.)

The present paper is organized as follows. In §2, we give a complete definition of the Hubbard model. We start from the description of the single-electron problem, and proceed by defining fermion operators, many-body Hilbert space, and the Hubbard Hamiltonian. An expert can safely skip this entire section, provided that he/she takes a brief look at §§2.1 and 2.3 to note our notation in the coordinate-free formalism of fermion operators.

Section 3 is also introductory and standard. We define the spin angular momenta of the model, and give a precise definition (Definition 3.1) of what we mean by ferromagnetism. We also present some results which rule out the possibility of ferromagnetism under several conditions.

In §4, we present a complete description and a proof of Nagaoka's ferromagnetism in its most generalized form.

In §5, we introduce and discuss an artificial model that we call the 'long-range hopping model.' Ferromagnetism in this model is first regarded as a special case of Nagaoka's ferromagnetism, but a different point of view is presented. This new picture naturally leads us to flat-band ferromagnetism.

In §6, we introduce flat-band ferromagnetism as a natural generalization of the long-range hopping model. We also discuss some results for the nearly-flat-band models obtained by adding a perturbation to the flat-band models.

In §7, we focus on experimental results which may be relevant to flat-band ferromagnetism.

In §8, we present some results about the possibility of metallic ferromagnetism in the Hubbard model. Preliminary rigorous results for related models in one-dimension are discussed.

*) For related reviews of mathematically rigorous results in the Hubbard model, see Refs. 20) and 21). Unfortunately there are many interesting related topics that we do not even mention in the present paper. For recent reviews of related topics from complementary points of view, see Refs. 22) ~ 25).

Technical material is contained in the Appendices. In Appendices A and B, we discuss the gauge transformation and the hole-particle transformation, respectively. In Appendix C, we summarize some useful properties of positive semidefinite operators. In Appendix D, we present (mainly for mathematicians) an explicit construction of the Hilbert space and fermion operators. In Appendix E, we explain (for readers without background in condensed matter physics) the elementary notion of band structures for a single-electron in a tight-binding description. In Appendix F, we present technical calculations required in the proof of Theorem 3.3.

§2. Definition of the Hubbard model

2.1. *Tight-binding description of a single electron*

Before introducing the Hubbard model, we describe the corresponding single-electron problem. Let lattice Λ be a collection of N_{s} sites. Lattice sites $x, y, \ldots \in \Lambda$ represent atomic sites in a solid. In the tight-binding description, which is a kind of low-energy effective theory, we declare that *electrons can live only on lattice sites.* In the *single-orbital model* that we study here, we further assume that each atomic site carries a single non-degenerate*) orbital state. Of course, actual atoms can have more than one orbit (or band). The philosophy behind the model building is that those electrons in other states do not play significant roles in determining the low-energy physics in which we are interested, and can be "forgotten" for the moment. (See Fig. 1.)

Then, a quantum mechanical state of a single electron (with a fixed spin) is described by a vector state $\boldsymbol{\varphi} = (\varphi_x)_{x\in\Lambda}$ with $\varphi_x \in \mathbb{C}$. We denote by $\mathfrak{h} \cong \mathbb{C}^{N_{\mathrm{s}}}$ ($\cong \ell^2(\Lambda;\mathbb{C})$) the N_{s}-dimensional Hilbert space formed by such $\boldsymbol{\varphi}$. The inner product of two states $\boldsymbol{\varphi}$ and $\boldsymbol{\psi} = (\psi_x)_{x\in\Lambda} \in \mathfrak{h}$ is

$$\langle \boldsymbol{\varphi}, \boldsymbol{\psi} \rangle = \sum_{x\in\Lambda} (\varphi_x)^* \psi_x. \tag{2·1}$$

For $x, y \in \Lambda$ with $x \neq y$, we denote by $t_{x,y}$ the quantum mechanical amplitude that an electron hops (i.e., tunnels) from the site y to x. We assume $t_{x,y}$ is real**) and symmetric as $t_{x,y} = t_{y,x}$. For $x \in \Lambda$, we denote by $t_{x,x}$ the (real valued) potential energy***) (which we usually write V_x) for the electron at site x. Then the Schrödinger equation for stationary states becomes

$$\varepsilon\varphi_x = \sum_{y\in\Lambda} t_{x,y}\,\varphi_y \quad \text{for any } x \in \Lambda, \tag{2·2}$$

*) In some solids, the degeneracy in the original atomic orbit is lifted by crystalline anisotropy.

**) In a system under magnetic field, $t_{x,y}$ is generally complex and satisfies $(t_{x,y})^* = t_{y,x}$.

***) We do not want to refer to $V_x (= t_{x,x})$ as "site-dependent chemical potential." The notion of the chemical potential makes sense in the contexts of thermodynamics or statistical physics. This notion, in our opinion, should be distinguished from the purely quantum mechanical notion of the potential (although there is a relation between the two).

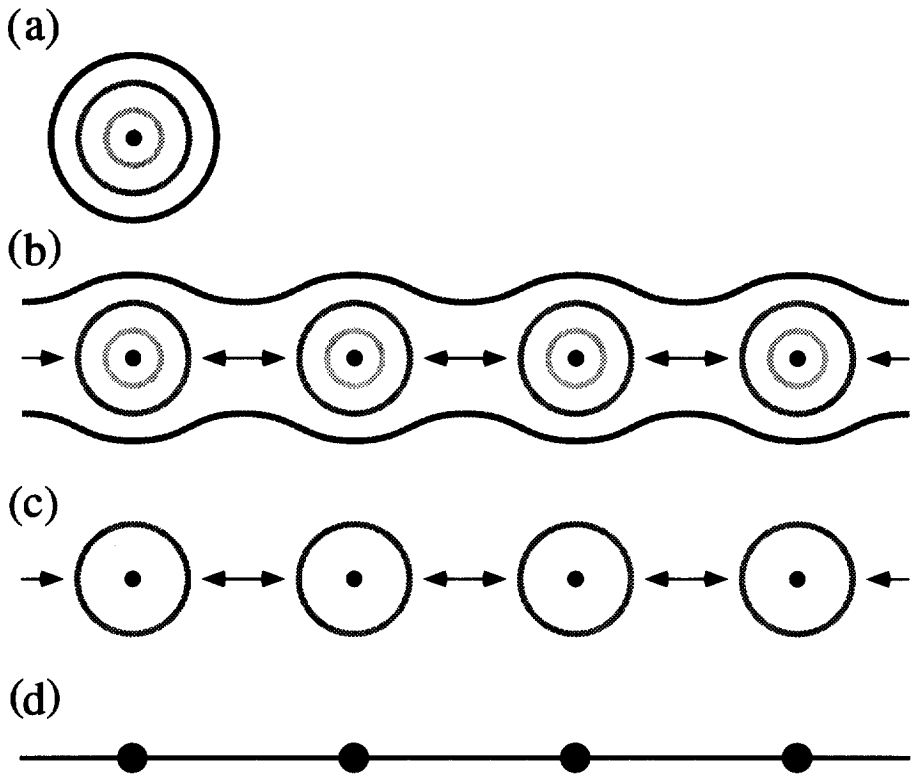

Fig. 1. Highly schematic figures which explain the philosophy of tight-binding descriptions. (a) A single atom which has multiple electrons in different orbits. (b) When atoms come together to form a solid, electrons in the black orbits become itinerant, while those in the light gray orbits are still localized at the original atomic sites. Electrons in the gray orbits are mostly localized around the atomic sites, but tunnel to nearby gray orbits with non-negligible probabilities. (c) We only consider the electrons in the gray orbits, which are expected to play essential roles in determining various aspects of low-energy physics of the system. (d) If the gray orbit is non-degenerate, we get a lattice model in which electrons live on lattice sites and hop from one site to another.

where ε is the energy eigenvalue.*) By introducing the hopping matrix $\mathsf{T} = (t_{x,y})_{x,y\in\Lambda}$, which is a matrix on $\mathfrak{h}$, this can be written in a coordinate free vector form as

$$\varepsilon\boldsymbol{\varphi} = \mathsf{T}\boldsymbol{\varphi}. \tag{2·3}$$

Since T is real symmetric, the eigenvalue equation (2·3) has N_{s} eigenvalues $\varepsilon_1, \ldots, \varepsilon_{N_{\mathrm{s}}}$. The corresponding eigenstate**) $\boldsymbol{\psi}^{(j)} = (\psi_x^{(j)})_{x\in\Lambda}$ satisfies

$$\varepsilon_j\boldsymbol{\psi}^{(j)} = \mathsf{T}\boldsymbol{\psi}^{(j)} \tag{2·4}$$

*) It is also common to put a minus sign in front of $t_{x,y}$ in (2·2). We note that the hopping amplitude $t_{x,y}$ depends on the delicate overlap between orbital wave functions, and there are no simple principles with which we can determine their magnitudes or signs. Also see Appendix A for discussion of the arbitrariness of the sign of $t_{x,y}$.

**) In notation like $\psi_x^{(j)}$, the superscript j is the name of the state and the subscript x is the index for its component.

for each $j = 1, \ldots, N_s$. We can assume that the energy eigenvalues are ordered as $\varepsilon_j \leq \varepsilon_{j+1}$, and eigenstates are orthonormal in the sense that $\left\langle \boldsymbol{\psi}^{(j)}, \boldsymbol{\psi}^{(j')} \right\rangle = \delta_{j,j'}$.

Let us consider a standard example. We take the one-dimensional lattice $\Lambda = \{1, 2, \ldots, N_s\}$, and set $t_{x,x+1} = t_{x+1,x} = -t$ for all $x \in \Lambda$, and $t_{x,y} = 0$ otherwise. We impose a periodic boundary condition and identify N_s+1 with 1. The eigenvalues and eigenstates can be most naturally indexed as $\boldsymbol{\eta}^{(k)} = (\eta_x^{(k)})_{x\in\Lambda}$ and $\varepsilon(k)$, respectively, by the wave number $k = 2\pi n/N_s$ where $n = 0, \pm 1, \pm 2, \ldots, \pm\{(N_s/2) - 1\}, N_s/2$ (assuming N_s is even). Then we have

$$\eta_x^{(k)} = \frac{1}{\sqrt{N_s}} e^{ikx}, \tag{2·5}$$

and $\varepsilon(k) = -2t \cos k$. Note that the eigenstates are described by plane waves.

2.2. *Fermion operators and Hilbert space*

We define the Hilbert space for many-electron problems using the fermion operator formalism.*) For each lattice site $x \in \Lambda$ and spin index $\sigma = \uparrow, \downarrow$, we associate a fermion operator $c_{x,\sigma}$. One can freely take the conjugate,**) products, and linear combinations (with complex coefficients) of these operators (and the identity operator) to get new operators. We require that these operators satisfy the anticommutation relations***)

$$\left\{c_{x,\sigma}^\dagger, c_{y,\tau}\right\} = \delta_{x,y}\delta_{\sigma,\tau}, \tag{2·6}$$

and

$$\left\{c_{x,\sigma}^\dagger, c_{y,\tau}^\dagger\right\} = \{c_{x,\sigma}, c_{y,\tau}\} = 0, \tag{2·7}$$

for any $x, y \in \Lambda$ and $\sigma, \tau = \uparrow, \downarrow$, where $\{A, B\} = AB + BA$. Note that (2·7) implies $(c_{x,\sigma})^2 = (c_{x,\sigma}^\dagger)^2 = 0$.

Physically, $c_{x,\sigma}$ and $c_{x,\sigma}^\dagger$ are interpreted as the operators which respectively annihilate and create an electron at site x with spin σ. The corresponding number operator is defined as

$$n_{x,\sigma} = c_{x,\sigma}^\dagger c_{x,\sigma}. \tag{2·8}$$

From (2·7), we find that number operators with different indices commute with each other. From (2·6) and (2·7), we see that $(n_{x,\sigma})^2 = c_{x,\sigma}^\dagger c_{x,\sigma} c_{x,\sigma}^\dagger c_{x,\sigma} = c_{x,\sigma}^\dagger(1 - c_{x,\sigma}^\dagger c_{x,\sigma})c_{x,\sigma} = c_{x,\sigma}^\dagger c_{x,\sigma} = n_{x,\sigma}$. Thus we obtain $n_{x,\sigma}(1-n_{x,\sigma}) = 0$, which means that $n_{x,\sigma}$ can only have eigenvalues 0 and 1. This is a mathematical realization of the Pauli exclusion principle. The number operator for site x is defined as $n_x = n_{x,\uparrow} + n_{x,\downarrow}$.

We can now construct the Hilbert space for many-electron problems. We start from a single (vector) state Φ_{vac}, which physically corresponds to a (fictitious) state

*) The formalism is also called "second quantization." One should recall, however, that we are working with a many-body problem which is "quantized" only once. The explicit relation to the "first quantization" formalism can be found in Appendix D. Readers with background in fields like functional analysis are suggested to take a look at this appendix.

**) We denote the conjugate of an operator A by $A^\dagger$. We write $c_{x,\sigma}^\dagger$ instead of $(c_{x,\sigma})^\dagger$.

***) The right-hand side of (2·6) means $\delta_{x,y}\delta_{\sigma,\tau}$ times the identity operator. Throughout the present paper, we refrain from writing the identity operator explicitly.

Fig. 2. An allowed configuration in a tight-binding model with a single orbit per site. Each site in the lattice can be either empty, singly occupied by an electron with up or down spin, or doubly occupied by electrons with opposite spins. If we consider the Hubbard type interaction, we get an extra energy $U > 0$ whenever two electrons occupy a single site. (See §2.5.) The interaction energy for the above configuration is therefore $3U$.

with no electrons in the lattice. This property is mathematically represented as

$$c_{x,\sigma}\Phi_{\mathrm{vac}} = 0 \quad \text{for any } x \in \Lambda \text{ and } \sigma = \uparrow, \downarrow. \tag{2·9}$$

We fix a positive integer N_{e} such that $1 \leq N_{\mathrm{e}} \leq 2N_{\mathrm{s}}$, which is the total number of electrons in the system. It is useful to express the electron number in terms of the filling factor $\nu = N_{\mathrm{e}}/(2N_{\mathrm{s}})$, which takes a value in the range $0 < \nu \leq 1$. Take N_{e} arbitrary sites $x_1, x_2, \ldots, x_{N_{\mathrm{e}}} \in \Lambda$ (with possible overlaps) and spin indices $\sigma_1, \sigma_2, \ldots, \sigma_{N_{\mathrm{e}}} = \uparrow, \downarrow$, and define the state

$$\Phi_{x_1,\sigma_1;x_2,\sigma_2;\ldots;x_{N_{\mathrm{e}}},\sigma_{N_{\mathrm{e}}}} = c^{\dagger}_{x_1,\sigma_1} c^{\dagger}_{x_2,\sigma_2} \cdots c^{\dagger}_{x_{N_{\mathrm{e}}},\sigma_{N_{\mathrm{e}}}} \Phi_{\mathrm{vac}}. \tag{2·10}$$

We interpret (2·10) as the state in which there is an electron at site x_i with spin σ_i for $i = 1, \ldots, N_{\mathrm{e}}$. We allow all the possible states of the form (2·10), but make identifications according to the anticommutation relations (2·7). In particular, the state (2·10) is vanishing whenever $(x_i, \sigma_i) = (x_j, \sigma_j)$ for some $i \neq j$. This is nothing but the Pauli exclusion principle.*) In other words, each site in the lattice can be either empty, singly occupied by an electron with up or down spin, or doubly occupied by electrons with opposite spins (Fig. 2). Also note that the anticommutation relation (2·7) leads to relations like

$$\Phi_{x_1,\sigma_1;x_2,\sigma_2} = -\Phi_{x_2,\sigma_2;x_1,\sigma_1}, \tag{2·11}$$

which is the well-known rule that a state changes its sign when one exchanges the *names* of two fermions.

The Hilbert space $\mathcal{H}_{N_{\mathrm{e}}}$ for the given electron number N_{e} is generated by all the basis states of the form (2·10). The inner product,**) which we again denote as $\langle \cdot, \cdot \rangle$, is defined by $\langle \Phi_{\mathrm{vac}}, \Phi_{\mathrm{vac}} \rangle = 1$ and the anticommutation relations. We denote the norm of a state $\Phi \in \mathcal{H}_{N_{\mathrm{e}}}$ as $\|\Phi\| = \langle \Phi, \Phi \rangle^{1/2}$.

We remark that there can be no *physical* situations which are represented by linear combinations of states with different electron numbers. To see this, we take two states $\Phi \in \mathcal{H}_{N_{\mathrm{e}}}$ and $\Phi' \in \mathcal{H}_{N'_{\mathrm{e}}}$ with $N_{\mathrm{e}} \neq N'_{\mathrm{e}}$. Since the total charge in the universe is conserved (as far as we know), the only (physically) possible way to

*) If we set $N_{\mathrm{e}} > 2N_{\mathrm{s}}$, then the state (2·10) always vanishes.

**) We do not use Dirac notation since we encounter many non-hermitian operators. Try rewriting the equation $\langle A\Phi, B\Psi \rangle = \langle \Phi, A^{\dagger}B\Psi \rangle$ in the Dirac notation.

linearly combine Φ and Φ' is to form a state like $\Xi = \Phi \otimes \Gamma_{N_e} + \Phi' \otimes \Gamma_{N'_e}$. Here Γ_{N_e} and $\Gamma_{N'_e}$ are some states of the whole outside world with total charge N_e and N'_e, respectively. Note that the states Γ_{N_e} and $\Gamma_{N'_e}$ are inevitably orthogonal. Therefore if A is any operator of the electron system, its expectation value in Ξ becomes

$$\begin{aligned}\langle A \rangle_\Xi &= \langle \Xi, (A \otimes \mathbf{1}), \Xi \rangle \\ &= \langle \Phi, A\Phi \rangle \langle \Gamma_{N_e}, \Gamma_{N_e} \rangle + \langle \Phi', A\Phi' \rangle \langle \Gamma_{N'_e}, \Gamma_{N'_e} \rangle \\ &= \omega \langle \Phi, A\Phi \rangle + \omega' \langle \Phi', A\Phi' \rangle , \end{aligned} \tag{2·12}$$

where $\mathbf{1}$ is the identity operator for the outside world. This means that the state Ξ must be represented as a mixed state*) if we restrict ourselves to the electron system.**)

2.3. *Coordinate-free notation*

We introduce the standard coordinate-free notation for fermion operators. The systematic use of this notation simplifies some routine calculations. For a single-electron state $\varphi = (\varphi_x)_{x \in \Lambda} \in \mathfrak{h}$, we define

$$C_\sigma^\dagger(\varphi) = \sum_{x \in \Lambda} \varphi_x \, c_{x,\sigma}^\dagger, \quad C_\sigma(\varphi) = \sum_{x \in \Lambda} (\varphi_x)^* \, c_{x,\sigma}. \tag{2·13}$$

These operators satisfy the generalized canonical anticommutation relations

$$\left\{ C_\sigma(\varphi), C_{\sigma'}^\dagger(\psi) \right\} = \delta_{\sigma,\sigma'} \langle \varphi, \psi \rangle \tag{2·14}$$

and

$$\{ C_\sigma(\varphi), C_{\sigma'}(\psi) \} = \left\{ C_\sigma^\dagger(\varphi), C_{\sigma'}^\dagger(\psi) \right\} = 0 \tag{2·15}$$

for any $\varphi, \psi \in \mathfrak{h}$ and $\sigma, \sigma' = \uparrow, \downarrow$.

Again (2·15) implies $(C_\sigma^\dagger(\varphi))^2 = (C_\sigma(\varphi))^2 = 0$. We also have the following property.

Lemma 2.1 (Linear independence and the product of creation operators) *Let $\varphi^{(1)}, \ldots, \varphi^{(n)}$ be n arbitrary states in $\mathfrak{h}$. The state*

$$C_\sigma^\dagger(\varphi^{(1)}) \cdots C_\sigma^\dagger(\varphi^{(n)}) \Phi_{\mathrm{vac}}, \tag{2·16}$$

which is usually called the Slater determinant state (see Appendix D), is nonvanishing if and only if $\varphi^{(1)}, \ldots, \varphi^{(n)}$ are linearly independent.

*) Note that the expectation value in the (unphysical) pure state $\Xi' = \alpha\Phi + \alpha'\Phi'$ becomes $\langle A \rangle_{\Xi'} = |\alpha|^2 \langle \Phi, A\Phi \rangle + |\alpha'|^2 \langle \Phi', A\Phi' \rangle + \{\alpha^* \alpha' \langle \Phi, A\Phi' \rangle + (\text{h.c.})\}$, which has extra cross terms.

**) Although this remark might sound entirely trivial (and it indeed is), many beginners (and even some experts) are confused when they encounter BCS-type states which are linear combinations of states with different N_e. One should always keep in mind that such linear combinations are introduced for purely mathematical (or theoretical) reasons (which are indeed deep and beautiful) and have nothing to do with realistic particle number fluctuations. When one has such a linear combination state, one *always* gets physically meaningful states with fixed electron numbers by taking suitable projections.

Proof: Let $O = C_\sigma^\dagger(\varphi^{(1)}) \cdots C_\sigma^\dagger(\varphi^{(n)})$. Assume that the n states are linearly dependent. Then we can write $\varphi^{(1)} = \sum_{j=2}^n \alpha_j \varphi^{(j)}$ with some coefficients $\alpha_j \in \mathbb{C}$, and hence $C_\sigma^\dagger(\varphi^{(1)}) = \sum_{j=2}^n \alpha_j C_\sigma^\dagger(\varphi^{(j)})$. The product O vanishes because $(C_\sigma^\dagger(\varphi^{(j)}))^2 = 0$.

Next we assume that the n states are linearly independent and show that $O\Phi_{\rm vac}$ is nonvanishing. By repeatedly using (2·14), (2·15) and $C_\sigma(\varphi)\Phi_{\rm vac} = 0$, we get

$$\begin{aligned} \|O\Phi_{\rm vac}\|^2 &= \langle \Phi_{\rm vac}, O^\dagger O \Phi_{\rm vac} \rangle \\ &= \left\langle \Phi_{\rm vac}, C_\sigma(\varphi^{(n)}) \cdots C_\sigma(\varphi^{(1)}) C_\sigma^\dagger(\varphi^{(1)}) \cdots C_\sigma^\dagger(\varphi^{(n)}) \Phi_{\rm vac} \right\rangle \\ &= \sum_{p:(1,\dots,n)\to(p(1),\dots,p(n))} (-1)^p \left\langle \varphi^{(1)}, \varphi^{(p(1))} \right\rangle \cdots \left\langle \varphi^{(n)}, \varphi^{(p(n))} \right\rangle, \end{aligned} \tag{2·17}$$

where p is summed over the $n!$ permutations of $(1, 2, \dots, n)$, and $(-1)^p$ denotes the parity of p. The Gramm matrix G is an $n \times n$ matrix defined by $(G)_{i,j} = \langle \varphi^{(i)}, \varphi^{(j)} \rangle$. Then (2·17) implies

$$\|O\Phi_{\rm vac}\|^2 = \det(G). \tag{2·18}$$

It is a well-known fact in linear algebra that G is regular (and hence $\det(G) \neq 0$) if and only if $\varphi^{(1)}, \dots, \varphi^{(n)}$ are linearly independent. ■

The following lemma gives a basic characterization of the Slater determinant states (2·16). Although we do not use the lemma in the present paper, we state it here since it is enlightening. We encourage interested readers to prove the lemma.

Lemma 2.2 (Slater determinant depends on a subspace) *Suppose that two sets $\{\varphi^{(1)}, \dots, \varphi^{(n)}\}$ and $\{\psi^{(1)}, \dots, \psi^{(n)}\}$ of states in $\mathfrak{h}$ span the same n-dimensional subspace of $\mathfrak{h}$. Then there is a nonvanishing constant $c \in \mathbb{C}$, and we have*

$$C_\sigma^\dagger(\varphi^{(1)}) \cdots C_\sigma^\dagger(\varphi^{(n)}) \Phi_{\rm vac} = c\, C_\sigma^\dagger(\psi^{(1)}) \cdots C_\sigma^\dagger(\psi^{(n)}) \Phi_{\rm vac}. \tag{2·19}$$

The following lemma is elementary, but of fundamental importance.

Lemma 2.3 (General basis of $\mathcal{H}_{N_e}$) *Let $\varphi^{(1)}, \dots, \varphi^{(N_s)}$ be N_s arbitrary states in $\mathfrak{h}$ which are linearly independent (but not necessarily orthogonal with each other). Then the states*

$$\Gamma_{S_\uparrow, S_\downarrow} = \left(\prod_{j \in S_\uparrow} C_\uparrow^\dagger(\varphi^{(j)}) \right) \left(\prod_{j \in S_\downarrow} C_\downarrow^\dagger(\varphi^{(j)}) \right) \Phi_{\rm vac} \tag{2·20}$$

for arbitrary subsets $S_\uparrow, S_\downarrow$ of $\{1, 2, \dots, N_s\}$ such that [*)] $|S_\uparrow| + |S_\downarrow| = N_e$ *span the Hilbert space $\mathcal{H}_{N_e}$.*

Proof: Since the N_s vectors are linearly independent, we have $\delta_{x,y} = \sum_{j=1}^{N_s} a_{x,j} \varphi_y^{(j)}$ with some regular matrix $(a_{x,j})_{x \in \Lambda, j=1,\dots,N_s}$. Thus we have

$$c_{x,\sigma}^\dagger = \sum_{j=1}^{N_s} a_{x,j} C_\sigma^\dagger(\varphi^{(j)}), \tag{2·21}$$

[*)] Throughout the present paper, we denote by $|S|$ the number of elements in the set S.

which means that the basis state (2·10) can be written as a linear combination of the states (2·20). ■

Let $\mathsf{A} = (a_{x,y})_{x,y\in\Lambda}$ be a matrix on $\mathfrak{h}$. We define the corresponding bilinear form of fermion operators

$$B(\mathsf{A}) = \sum_{\substack{x,y\in\Lambda \\ \sigma=\uparrow,\downarrow}} c^\dagger_{x,\sigma}\, a_{x,y}\, c_{y,\sigma}, \tag{2·22}$$

which is usually called the "second quantization" of A. The easily verified commutation relation

$$[B(\mathsf{A}), C^\dagger_\sigma(\varphi)] = C^\dagger_\sigma(\mathsf{A}\varphi), \tag{2·23}$$

where $[A,B] = AB - BA$, sheds light on the relation between the single-particle quantum mechanics and the operator formalism. This will be useful later. A similar commutation relation for two bilinear forms

$$[B(\mathsf{A}), B(\mathsf{B})] = B([\mathsf{A},\mathsf{B}]) \tag{2·24}$$

is also easy to prove.

We have so far treated the spin index σ separately from the coordinate x. It is of course possible to treat the combination (x,σ) as the coordinates of the system and consider the corresponding $2N_{\mathrm{s}}$-dimensional single-electron Hilbert space.*) We can then restate all of the above results in the new language with suitable modifications. Let us only mention the relation corresponding to (2·24), because it will be useful later. Let $\tilde{\mathsf{A}}$ be a $2N_{\mathrm{s}} \times 2N_{\mathrm{s}}$ matrix indexed by (x,σ) with $x \in \Lambda$ and $\sigma = \uparrow, \downarrow$, and define $\tilde{B}(\tilde{\mathsf{A}}) = \sum_{x,y\in\Lambda}\sum_{\sigma,\tau=\uparrow,\downarrow} c^\dagger_{x,\sigma}(\tilde{\mathsf{A}})_{(x,\sigma),(y,\tau)}\, c_{y,\tau}$. Then for two such matrices $\tilde{\mathsf{A}}$ and $\tilde{\mathsf{B}}$, we have

$$[\tilde{B}(\tilde{\mathsf{A}}), \tilde{B}(\tilde{\mathsf{B}})] = \tilde{B}([\tilde{\mathsf{A}}, \tilde{\mathsf{B}}]), \tag{2·25}$$

where $[\tilde{\mathsf{A}}, \tilde{\mathsf{B}}]$ is the commutator as $2N_{\mathrm{s}} \times 2N_{\mathrm{s}}$ matrices.

2.4. *Non-interacting system*

Now that the Hilbert space has been prepared, we can introduce Hamiltonians. The Hamiltonian which describes the quantum mechanical hopping with the hopping matrix $\mathsf{T} = (t_{x,y})_{x,y\in\Lambda}$ is

$$H_{\mathrm{hop}} = B(\mathsf{T}) = \sum_{\substack{x,y\in\Lambda \\ \sigma=\uparrow,\downarrow}} t_{x,y}\, c^\dagger_{x,\sigma} c_{y,\sigma}. \tag{2·26}$$

To see that (2·26) describes the desired hopping, define the single-electron state $\Phi_\varphi = C^\dagger_\sigma(\varphi)\Phi_{\mathrm{vac}}$ for $\varphi \in \mathfrak{h}$. Then from the commutation relation (2·23), we immediately find that the Schrödinger equation $\varepsilon\Phi_\varphi = H_{\mathrm{hop}}\Phi_\varphi$ is equivalent to the single-electron Schrödinger equation (2·2) or (2·3).

When one has diagonalized the single-electron Schrödinger equation (2·2), it is easy to also diagonalize the many-body Hamiltonian (2·26). As in §2.1, we let $\psi^{(j)}$

*) We shall use such a formalism in Appendix D.

Fig. 3. Schematic picture of the ground state of a non-interacting many-electron system. The lowest $N_e/2$ single-electron energy levels are "filled" by both up spin and down spin electrons. The state naturally exhibits paramagnetism known as 'Pauli paramagnetism.'

be the eigenstate satisfying (2·4) with energy ε_j, for $j = 1, 2, \ldots, N_s$. Define the new fermion operator by

$$a^\dagger_{j,\sigma} = C^\dagger_\sigma(\boldsymbol{\psi}^{(j)}) \tag{2·27}$$

for $j = 1, 2, \ldots, N_s$ and $\sigma = \uparrow, \downarrow$.

Let $S_\uparrow$ and $S_\downarrow$ be arbitrary subsets of $\{1, 2, \ldots, N_s\}$ such that $|S_\uparrow| + |S_\downarrow| = N_e$, and define

$$\Psi_{S_\uparrow, S_\downarrow} = \left(\prod_{j\in S_\uparrow} a^\dagger_{j,\uparrow}\right)\left(\prod_{j\in S_\downarrow} a^\dagger_{j,\downarrow}\right)\Phi_{\rm vac}. \tag{2·28}$$

Lemma 2.3 shows that these states form a basis of $\mathcal{H}_{N_e}$. Note that the commutation relation (2·23) and the eigenstate equation (2·4) imply $[H_{\rm hop}, a^\dagger_{j,\sigma}] = [B(\mathsf{T}), C^\dagger_\sigma(\boldsymbol{\psi}^{(j)})] = C^\dagger_\sigma[\mathsf{T}\boldsymbol{\psi}^{(j)}] = \varepsilon_j a^\dagger_{j,\sigma}$. This and $H_{\rm hop}\Phi_{\rm vac} = 0$ immediately imply

$$H_{\rm hop}\Psi_{S_\uparrow, S_\downarrow} = \left(\sum_{j\in S_\uparrow}\varepsilon_j + \sum_{j\in S_\downarrow}\varepsilon_j\right)\Psi_{S_\uparrow, S_\downarrow}. \tag{2·29}$$

We have thus diagonalized $H_{\rm hop}$.

By choosing subsets $S_\uparrow, S_\downarrow$ which minimize the energy eigenvalue $\sum_{j\in S_\uparrow}\varepsilon_j + \sum_{j\in S_\downarrow}\varepsilon_j$, we get ground state(s) of the present non-interacting model. In particular, if the corresponding single-electron energy eigenvalues are nondegenerate, i.e., $\varepsilon_j < \varepsilon_{j+1}$, and if N_e is even, the ground state of $H_{\rm hop}$ is unique and written as

$$\Phi_{\rm GS} = \left(\prod_{j=1}^{N_e/2} a^\dagger_{j,\uparrow}a^\dagger_{j,\downarrow}\right)\Phi_{\rm vac}. \tag{2·30}$$

This is nothing but the state obtained by "filling up" the low energy levels with up and down spin electrons, as one learns in elementary quantum mechanics (Fig. 3).

In a single-electron eigenstate of the one-dimensional example in §2.1, the electron is in a plane wave state (2·5) with a definite wave number k. The same is true for any translation invariant model, as we see in Appendix E. The fact that the Hamiltonian $H_{\rm hop}$ is diagonalized in the basis (2·28) implies that the electrons behave as "waves" in this non-interacting (Hubbard) model.

2.5. *Interaction*

It is believed that interactions between electrons in a solid mainly come from the electrostatic Coulomb force. Although the Coulomb force in vacuum is long-ranged, we consider *an extremely short-range interaction which acts only when two*

electrons occupy the same site (i.e., the same atomic orbit). A crude justification of such a short-range (Coulomb) interaction comes from the observation that the Coulomb force should be most dominant when two electrons approach within the minimum possible distance. In a slightly more sophisticated justification, one argues that the long range Coulomb force is screened by electrons in different orbital states which we have decided to forget. Our point of view, however, is that models with artificial short-range interactions are worth studying because they are among *the minimum models which can be studied to elicit universal properties of strongly interacting electron systems.*

The Hamiltonian for the short-range Coulomb repulsion is

$$H_{\text{int}} = U \sum_{x \in \Lambda} n_{x,\uparrow} n_{x,\downarrow}, \tag{2·31}$$

where $U \geq 0$ is the energy from the repulsive interaction. (See Fig. 2.)

The expression (2·31) is already diagonalized, and it is trivial to write down eigenstates of H_{int}. Let $L_\uparrow, L_\downarrow$ be arbitrary subsets of the lattice Λ such that $|L_\uparrow| + |L_\downarrow| = N_{\text{e}}$, and define

$$\Psi_{L_\uparrow, L_\downarrow} = \left(\prod_{x \in L_\uparrow} c^\dagger_{x,\uparrow} \right) \left(\prod_{x \in L_\downarrow} c^\dagger_{x,\downarrow} \right) \Phi_{\text{vac}}. \tag{2·32}$$

Then by using the commutation relation $[n_{x,\sigma}, c^\dagger_{x',\sigma'}] = \delta_{x,x'} \delta_{\sigma,\sigma'} c^\dagger_{x,\sigma}$, we find

$$H_{\text{int}} \Psi_{L_\uparrow, L_\downarrow} = U |L_\uparrow \cap L_\downarrow| \Psi_{L_\uparrow, L_\downarrow}. \tag{2·33}$$

The ground state for a given electron number N_{e} can be constructed by choosing subsets $L_\uparrow, L_\downarrow$ that minimize the energy eigenvalue $U|L_\uparrow \cap L_\downarrow|$. When $N_{\text{e}} \leq N_{\text{s}}$, one can always choose $L_\uparrow$ and $L_\downarrow$ so that $L_\uparrow \cap L_\downarrow = \emptyset$ holds. In this case, the ground states are highly degenerate and have energy equal to 0.

It is clear (from the beginning) that the interaction Hamiltonian H_{int} is most naturally treated if we regard electrons as (classical) "particles" which live on lattice sites.

2.6. *Hubbard model*

The Hubbard model describes a tight-binding electron model in which *electrons hop around the lattice and interact with each other through short-range repulsive interactions.* The full Hamiltonian of the single-orbital Hubbard model*) is simply

$$H = H_{\text{hop}} + H_{\text{int}}. \tag{2·34}$$

We have already seen that both H_{hop} and H_{int} can be easily diagonalized. We have observed, however, that electrons behave as "waves" in H_{hop}, while they behave as "particles" in H_{int}. How do they behave in a system whose Hamiltonian is a sum

*) This model is often called the single-band Hubbard model. We find this terminology confusing since a single-orbital model can have multiple bands depending on the structure of the hopping matrix T. See Appendix E.

of these totally different Hamiltonians? This is indeed a fascinating problem which is deeply related to the wave-particle dualism in quantum physics. We might say that many of the important models in many-body problems, including the φ^4 quantum field theory and the Kondo problem, are minimum models which take into account both the wave-like nature and the particle-like nature (through point-like nonlinear interactions) of matter.

From a technical point of view, the wave-particle dualism implies that the Hamiltonians $H_{\rm int}$ and $H_{\rm hop}$ do not commute with each other. Even when each Hamiltonian is diagonalized, it is still highly nontrivial (or impossible) to find the properties of their sum. Of course, mathematical difficulty does not automatically guarantee that the model is worth studying. A truly exciting characteristic of the Hubbard model is that, though the Hamiltonians $H_{\rm hop}$ and $H_{\rm int}$ do not favor any nontrivial order, their sum $H = H_{\rm hop} + H_{\rm int}$ is believed to generate various types of nontrivial order including antiferromagnetism, ferromagnetism, and superconductivity. When we sum up the two innocent Hamiltonians $H_{\rm hop}$ and $H_{\rm int}$, competition between their wave-like and particle-like characters (or between linearity and nonlinearity) takes place, and one gets various interesting "physics". To confirm this fascinating scenario is a challenging problem in theoretical and mathematical physics.

§3. Magnetism in the Hubbard model

3.1. *Spin operators and $SU(2)$ invariance*

We introduce the total spin operators*) $\hat{\mathbf{S}}_{\rm tot} = (\hat{S}^{(1)}_{\rm tot}, \hat{S}^{(2)}_{\rm tot}, \hat{S}^{(3)}_{\rm tot})$ of the system by

$$\hat{S}^{(\alpha)}_{\rm tot} = \frac{1}{2} \sum_{x \in \Lambda} \sum_{\sigma,\tau=\uparrow,\downarrow} c^{\dagger}_{x,\sigma} (p^{(\alpha)})_{\sigma,\tau} \, c_{x,\sigma} \tag{3·1}$$

for $\alpha = 1, 2$ and 3, where $p^{(\alpha)}$ are the Pauli matrices. It is clear from the general commutation relation (2·25) that**) $\hat{S}^{(1)}_{\rm tot}, \hat{S}^{(2)}_{\rm tot}$ and $\hat{S}^{(3)}_{\rm tot}$ satisfy the standard commutation relation for quantum mechanical angular momentum operators. We define the raising and lowering operators by $S^{\pm}_{\rm tot} = \hat{S}^{(1)}_{\rm tot} \pm i \hat{S}^{(2)}_{\rm tot}$.

The operators $\hat{\mathbf{S}}_{\rm tot}$ are the generators of the global $SU(2)$ rotations in the spin space. We say an operator A is $SU(2)$ invariant if it commutes with $\hat{S}^{(\alpha)}_{\rm tot}$ for $\alpha = 1, 2$ and 3. Intuitively speaking, an $SU(2)$ invariant operator does not change if we change the "quantization axis" of spins in an arbitrary manner.

A typical $SU(2)$ invariant operator is the number operator $n_x = n_{x,\uparrow} + n_{x,\downarrow}$. The hopping Hamiltonian $H_{\rm hop}$ of (2·26) is also $SU(2)$ invariant. These facts can be checked easily by using the general commutation relations (2·25). The interaction Hamiltonian $H_{\rm int}$ of (2·31) is also $SU(2)$ invariant. This fact becomes evident if we note $n_{x,\uparrow} n_{x,\downarrow} = \{(n_x)^2 - n_x\}/2$.

Knowing that the Hamiltonian $H = H_{\rm hop} + H_{\rm int}$ is $SU(2)$ invariant, we can make use of the standard representation theory of quantum mechanical angular momenta.

*) We use the index $\alpha = 1, 2, 3$ to indicate the three axes, because the symbols x, y, z are already used as lattice sites.

**) Note that $\hat{S}^{(\alpha)}_{\rm tot} = \tilde{B}(\tilde{p}^{(\alpha)})$ with $(\tilde{p}^{(\alpha)})_{(x,\sigma),(y,\tau)} = \delta_{x,y} (p^{(\alpha)})_{\sigma,\tau}$.

We note that the three operators H, $\hat{S}^{(3)}_{\rm tot}$, and $(\hat{\mathbf{S}}_{\rm tot})^2 = \sum_{\alpha=1,2,3}(\hat{S}^{(\alpha)}_{\rm tot})^2$ commute with each other. We will always consider simultaneous eigenstates of these operators. We denote by $S^{(3)}_{\rm tot}$ the eigenvalue of $\hat{S}^{(3)}_{\rm tot}$, and by $S_{\rm tot}(S_{\rm tot}+1)$ the eigenvalue of $(\hat{\mathbf{S}}_{\rm tot})^2$. We call $S_{\rm tot}$ the total spin of the state. Let

$$S_{\max} = \begin{cases} N_{\rm e}/2 & \text{if } N_{\rm e} \le N_{\rm s}; \\ (2N_{\rm s} - N_{\rm e})/2 & \text{if } N_{\rm e} \ge N_{\rm s}. \end{cases} \tag{3·2}$$

Then the allowed values of $S_{\rm tot}$ are $S_{\rm tot} = 0, 1, \ldots, S_{\max}$ if $N_{\rm e}$ is even, and $S_{\rm tot} = 1/2, 3/2, \ldots, S_{\max}$ if $N_{\rm e}$ is odd.

3.2. *Ferromagnetism*

Ferromagnetism is probably the most intuitive among various magnetic phenomena exhibited by solids. Here we shall be rather restrictive and only consider the strongest form of ferromagnetism, namely, saturated ferromagnetism in ground states.

Definition 3.1 *A Hubbard model is said to exhibit ferromagnetism if any ground state of H has the total spin $S_{\rm tot} = S_{\max}$.*

Recall that any state with $S_{\rm tot} = S_{\max}$ has its copies in the subspaces with $S^{(3)}_{\rm tot} = -S_{\max}, -S_{\max}+1, \ldots, S_{\max}$. Therefore the ground states are at least $(2S_{\max}+1)$-fold degenerate when there is ferromagnetism (in the above strong sense). Let $\Phi_{\rm GS}$ be a ground state with $S^{(3)}_{\rm tot} = S_{\max}$. Since $\Phi_{\rm GS}$ contains only up spin electrons, we must have $H_{\rm int}\Phi_{\rm GS} = 0$. This means that $\Phi_{\rm GS}$ is the lowest energy state of $H_{\rm hop}$ within the subspace of $N_{\rm e}$ up spin electrons. Recalling the general eigenstates (2·28) of $H_{\rm hop}$, we find that the desired ferromagnetic ground state is

$$\Phi_{\rm GS} = \left(\prod_{j=1}^{N_{\rm e}} a^{\dagger}_{j,\uparrow}\right)\Phi_{\rm vac}, \tag{3·3}$$

with $a^{\dagger}_{j,\uparrow}$ defined in (2·27), which has the ground state energy

$$E_{\rm ferro} = \sum_{j=1}^{N_{\rm e}} \varepsilon_j. \tag{3·4}$$

When we have $\varepsilon_{N_{\rm e}} < \varepsilon_{N_{\rm e}+1}$, (3·3) is the unique ground state*) in the subspace with $S^{(3)}_{\rm tot} = S_{\max}$. The ground state Φ_M with $S^{(3)}_{\rm tot} = M$ can be obtained from this ground state by the standard relation

$$\Phi_M = \frac{(S^{-}_{\rm tot})^{S_{\max}-M}\Phi_{\rm GS}}{\left\|(S^{-}_{\rm tot})^{S_{\max}-M}\Phi_{\rm GS}\right\|}. \tag{3·5}$$

The above elementary construction of the ground states (provided that the model exhibits ferromagnetism) is based on the fact that any state with $S_{\rm tot} = S_{\max}$ *does*

*) When $\varepsilon_{N_{\rm e}}$ is degenerate with $\varepsilon_n, \ldots, \varepsilon_m$ (where $n \le N_{\rm e} < m$), we can replace the states $j = n, \ldots, N_{\rm e}$ with arbitrary states from $j = n \ldots, m$ to get other ground states. The ground states are degenerate even in the subspace with $S^{(3)}_{\rm tot} = S_{\max}$.

not feel the on-site Coulomb repulsion. This reduces the problem to that of non-interacting spinless fermions. We stress that this is a very special feature of the Hubbard model, which has only on-site interactions.

3.3. *Instability of ferromagnetism*

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

We first look at the non-interacting model with the Hamiltonian $H = H_{\text{hop}}$ that we studied in §2.4. Assuming that the single-electron energy eigenvalues are non-degenerate, we found that the ground state is uniquely given by (2·30). By noting that the operator $a^\dagger_{j,\uparrow}a^\dagger_{j,\downarrow}$ is $SU(2)$ invariant and $\hat{S}^{(\alpha)}_{\text{tot}}\Phi_{\text{vac}} = 0$, we immediately find $\hat{S}^{(\alpha)}_{\text{tot}}\Phi_{\text{GS}} = 0$. Thus the ground state has the total spin*) $S_{\text{tot}} = 0$, and there is no ferromagnetism. This is nothing but the well-known Pauli paramagnetism. (See Fig. 3.)

It is also trivial that the non-hopping model with $H = H_{\text{int}}$ we studied in §2.5 does not exhibit ferromagnetism. In this case any state (2·32) for $L_\uparrow, L_\downarrow$ with minimum $|L_\uparrow \cap L_\downarrow|$ is a ground state. Thus the ground states are highly degenerate and exhibit a kind of paramagnetism.

Therefore neither H_{hop} nor H_{int} alone favor ferromagnetism. As we have stressed in §2.6, our hope is that, when these two Hamiltonians are added into a single Hubbard Hamiltonian $H = H_{\text{hop}} + H_{\text{int}}$, their "competition" generates totally new phenomena, including ferromagnetism.

Next we consider the situation in which the Coulomb interaction U is finite but small. We find here that there cannot be (saturated) ferromagnetism.

Theorem 3.2 (Impossibility of ferromagnetism for small U) *Suppose* $0 \le U < \varepsilon_{N_e} - \varepsilon_1$. *Then the ground state of the Hubbard model does not have* $S_{\text{tot}} = S_{\max}$, *i.e., the model does not exhibit ferromagnetism. Note that the fermi energy* $\varepsilon_{N_e} - \varepsilon_1$ *is usually independent of the system size for a fixed filling factor* ν.

Proof: One of the lowest energy states with $S_{\text{tot}} = S_{\max}$ is given by (3·3) and has the energy (3·4). Consider a normalized trial state

$$\Psi = a^\dagger_{1,\downarrow}\left(\prod_{j=1}^{N_e-1} a^\dagger_{j,\uparrow}\right)\Phi_{\text{vac}}, \tag{3·6}$$

which is obtained from (3·3) by removing the up spin electron with the highest energy and then adding a down spin electron with the lowest energy. Noting the $SU(2)$ invariance of $a^\dagger_{1,\downarrow}a^\dagger_{1,\uparrow}$, one finds that Ψ has $S_{\text{tot}} = S_{\max} - 1$. We want to evaluate the energy expectation value $\langle\Psi, H\Psi\rangle$. For the kinetic energy, we have $\langle\Psi, H_{\text{hop}}\Psi\rangle = \varepsilon_1 + \sum_{j=1}^{N_e-1}\varepsilon_j$. As for H_{int}, we note that the inequality**) $n_{x,\uparrow} \le 1$ implies $H_{\text{int}} \le U\sum_{x\in\Lambda} n_{x,\downarrow}$ to get $\langle\Psi, H_{\text{int}}\Psi\rangle \le \langle\Psi, U\sum_{x\in\Lambda} n_{x,\downarrow}\Psi\rangle = U$. Therefore

*) That $S_{\text{tot}} = 0$ also follows from the uniqueness of the ground state.

**) See Definition C.1 for the definition of inequalities for operators.

we have

$$\langle \Psi, H\Psi \rangle - E_{\text{ferro}} \leq \varepsilon_1 - \varepsilon_{N_e} + U < 0, \tag{3·7}$$

where E_{ferro} is defined in (3·4), and the final bound follows from the condition of the theorem. From the variational principle, we see that E_{ferro} is not the ground state energy of 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 which (for the moment) is possible only in the simplest one-dimensional model.

Finally, we 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 easily 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*) c, n_0, ρ_0 and d, and the single electron energy eigenvalues satisfy

$$\varepsilon_n - \varepsilon_1 \geq c \left(\frac{n - n_0}{N_s} \right)^{2/d} \tag{3·8}$$

for any n such that $n/N_s \leq \rho_0$. Note that the right-hand side represents the n dependence of energy levels in a usual d-dimensional quantum mechanical system. Then we have the following theorem due to Pieri, Daul, Baeriswyl, Dzierzawa and Fazekas.[26]

Theorem 3.3 (Impossibility of ferromagnetism at low densities) *Take a H_{hop} which has translation invariance (as in Appendix E) and satisfies (3·8) 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 ferromagnetism for any $U \geq 0$ if $N_e/N_s \leq \rho_1$ holds.*

Outline of proof: The naive trial state (3·6) does not work for large U. We follow Ref. 27), and consider the Roth state[28]

$$\tilde{\Psi} = P_0 \Psi, \tag{3·9}$$

where Ψ is defined in (3·6), and

$$P_0 = \prod_{x \in \Lambda} (1 - n_{x,\uparrow} n_{x,\downarrow}) \tag{3·10}$$

is the orthogonal projection (called the 'Gutzwiller projection') onto the space with no doubly occupied sites. Because of the projection, the state (3·9) minimizes the Coulomb interaction as $H_{\text{int}}\Psi = 0$. Thus we only need to evaluate the expectation

*) n_0 and d are the degeneracy of the single-electron ground states and the dimension of the system, respectively.

value of H_{hop}. After a tedious but straightforward calculation whose details can be found in Appendix F, we find

$$\frac{\left\langle \tilde{\Psi}, H\tilde{\Psi} \right\rangle}{\left\langle \tilde{\Psi}, \tilde{\Psi} \right\rangle} - E_{\text{ferro}} \leq \varepsilon_1 - \varepsilon_{N_e} + c'\rho, \tag{3·11}$$

where $\rho = N_e/N_s$ is the electron density and $c' > 0$ is a constant. From the assumption (3·8), 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 3.3 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 ideal 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.

3.4. *Two more theorems for the absence of ferromagnetism*

We briefly discuss (without proofs) two strong theorems which also rule out ferromagnetism.

The classical Lieb-Mattis theorem [29] states (among other things) that one can never have ferromagnetism in the one-dimensional Hubbard model with only nearest-neighbor hoppings.*) One-dimensional Hubbard models with next-nearest-neighbor hoppings may exhibit ferromagnetism as we explicitly see in §§6 and 8.

Theorem 3.4 (Lieb-Mattis theorem) *Consider a Hubbard model with even N_e on a one-dimensional lattice $\Lambda = \{1, 2, \ldots, N_s\}$ with open boundary conditions. We assume that the hopping matrix elements satisfy $|t_{x,y}| < \infty$ when $x = y$, $0 < |t_{x,y}| < \infty$ when $|x-y| = 1$, and are vanishing otherwise. Then for any real U, the ground state of the model is unique and has $S_{\text{tot}} = 0$.*

The next important theorem is due to Lieb. [11]

Theorem 3.5 (Lieb's theorem, special case) *Suppose that the lattice Λ is decomposed into two sublattices as $\Lambda = A \cup B$ with $|A| = |B|$, and we have $t_{x,y} = 0$ when $x, y \in A$ or $x, y \in B$. We also assume that the entire lattice is connected by nonvanishing $t_{x,y}$. When $N_e = N_s$, the ground state of the model is unique and has $S_{\text{tot}} = 0$ for any $U \geq 0$.*

The electron number $N_e = N_s$ is usually referred to as "half-filling", since $2N_s$ is the maximum possible number for N_e. The low energy properties of a Hubbard model at half-filling is believed to be described by the antiferromagnetic Heisenberg model. Lieb's theorem stated above gives a partial justification to this belief. This theorem applies to models on lattices with $|A| \neq |B|$ as well. In this case, it implies the existence of *ferrimagnetism*, as is explicitly stated in Ref. 12).

*) The present theorem appears in the Appendix of Ref. 29). The main body of Ref. 29) treats interacting electron systems in continuous spaces.

§4. Nagaoka's ferromagnetism

4.1. *Weak version of Nagaoka's theorem*

We are now ready to discuss Nagaoka's ferromagnetism.*), [10] Briefly speaking, Nagaoka's theorem establishes that some Hubbard models exhibit saturated ferromagnetism when the number of electrons is one less than the half-filling (i.e., $N_e = N_s - 1$) and the Coulomb repulsion U is infinitely large. Given the general fact that a half-filled system never exhibits ferromagnetism, this is a rather striking result, which demonstrates that strongly interacting electron systems can produce very rich and sometimes surprising phenomena.

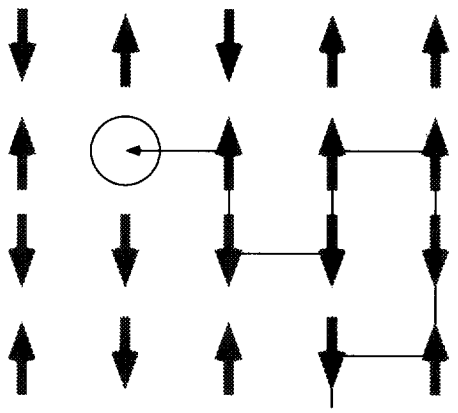

Fig. 4. Schematic picture of the origin of Nagaoka's ferromagnetism. When the hole hops around the lattice, the spin configuration is changed. For a model with $t_{x,y} \geq 0$, the hole motion produces a precise linear combination of various spin configurations which leads to a ferromagnetic state.

When $U = \infty$ and $N_e = N_s - 1$, states with finite energies have no doubly occupied sites, and there is exactly one empty site which we call "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. (See Fig. 4.) Thouless[9] also discussed the same mechanism of ferromagnetism in slightly more restricted situations. (Also see Ref. 31).)

We start from the following weaker result which is easy to state and prove.

Theorem 4.1 (Weak version of Nagaoka's theorem) *Consider an arbitrary Hubbard model with $t_{x,y} \geq 0$ for any $x, y \in \Lambda$, $N_e = N_s - 1$, and $U = \infty$. Then among the ground states there are $(2S_{tot} + 1)$ states with total spin $S_{tot} = S_{max} (= N_e/2)$.*

Note that the theorem does not establish the existence of ferromagnetism since it does not state ferromagnetic states are the only ground states.**) Stronger statement will be proved in the next section as Theorem 4.5.

*) As for the presentation of the results and the proofs, we follow Ref. 30), where a generalization of Nagaoka's theorem was discussed. The proof briefly described in Ref. 30) is now presented in its full detail.

**) Note that the statement of the theorem is valid in the trivial model with $t_{x,y} = 0$ for all x, y, where all the possible spin states are degenerate. We must remark that some of the published "proofs" of Nagaoka's theorem and its extensions only prove such weak statements. (See also footnote *) on p. 516.)

Let us prove Theorem 4.1. We first consider the treatment of the $U \to \infty$ limit. Let us decompose the Hilbert space $\mathcal{H}_{N_e}$ as

$$\mathcal{H}_{N_e} = \mathcal{H}_{N_e}^{(0)} \oplus \mathcal{H}'_{N_e}, \tag{4·1}$$

where $\mathcal{H}_{N_e}^{(0)}$ consists of the states*) satisfying $H_{\rm int}\Phi = 0$. We denote by P_0 (see (3·10)) the orthogonal projection onto $\mathcal{H}_{N_e}^{(0)}$. Then we have the following.

Lemma 4.2 (Characterization of the $U \to \infty$ limit) *The $U \to \infty$ limit of the Hubbard model is equivalent to studying the Hamiltonian**) $\tilde{H} = P_0 H_{\rm hop}$ on the Hilbert space $\mathcal{H}_{N_e}^{(0)}$.*

Proof: By continuity, the eigenstates of $H = H_{\rm hop} + H_{\rm int}$ can be classified into those with energies diverging as $U \to \infty$ and those with finite energies in the $U \to \infty$ limit. We are only interested in the latter. Let Φ be an eigenstate with energy E which has a finite limit. We can assume both Φ and E are continuously parameterized by U. Note that we have $P_0\Phi \to \Phi$ in the $U \to \infty$ limit, because otherwise E diverges in this limit. By applying the projection P_0 onto the Schrödinger equation $E\Phi = (H_{\rm hop} + H_{\rm int})\Phi$, we get $EP_0\Phi = P_0 H_{\rm hop}\Phi$ because $P_0 H_{\rm int}\Phi = 0$. In the $U \to \infty$ limit, this becomes $E\Phi = \tilde{H}\Phi$ for $\Phi \in \mathcal{H}_{N_e}^{(0)}$. ■

We now prepare a basis for the Hilbert space $\mathcal{H}_{N_e}^{(0)}$. We use the basis states characterized by the position x of the hole and the spin configuration***) $\boldsymbol{\sigma} = (\sigma_y)_{y\in\Lambda\setminus x} \in \mathcal{S}_{\Lambda\setminus x}$, defined as

$$\Phi_{x,\boldsymbol{\sigma}} = c_{x,\uparrow}\left(\prod_{y\in\Lambda} c^\dagger_{y,\sigma'_y}\right)\Phi_{\rm vac} = c_{x,\downarrow}\left(\prod_{y\in\Lambda} c^\dagger_{y,\sigma''_y}\right)\Phi_{\rm vac}. \tag{4·2}$$

Here the product is taken over all the sites in Λ with an arbitrary but fixed order. We gave two equivalent expressions for $\Phi_{x,\boldsymbol{\sigma}}$. The spin configurations $(\sigma'_y)_{y\in\Lambda}$ and $(\sigma''_y)_{y\in\Lambda}$ are essentially 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 $\sigma''_x = \downarrow$. In the definition (4·2), we are simply supplying an electron at the hole site x, and then annihilating the electron by $c_{x,\uparrow}$ or $c_{x,\downarrow}$. This may sound meaningless, but we get fermion signs appropriate for our purpose in this way.

We wish to examine the action of $\tilde{H} = P_0 H_{\rm hop}$ on the states (4·2). In order to get a finite contribution, an electron must hop into the hole site x from other sites. So we examine the action of $\sum_{\sigma=\uparrow,\downarrow} c^\dagger_{x,\sigma}c_{z,\sigma}$ on $\Phi_{x,\boldsymbol{\sigma}}$. Using the two equivalent

*) We are assuming $N_e \le N_s$. If $N_e > N_s$, the relevant condition is replaced by $H_{\rm int}\Phi = U(N_e - N_s)\Phi$, and Lemma 4.2 is still valid.

**) In the present case, we will eventually find that the ground states in the $U \to \infty$ limit are eigenstates of $H_{\rm hop}$. This is of course an accidental situation for the ferromagnetic states. Examples of exact ground states in the $U \to \infty$ limit which are not eigenstates of $H_{\rm hop}$ can be found in Refs. 32) and 33).

***) By $\Lambda\setminus x$ we mean the lattice obtained by removing x from Λ.

expressions (4·2) for $\Phi_{x,\boldsymbol{\sigma}}$, we get

$$\begin{aligned}\sum_{\sigma=\uparrow,\downarrow} c^{\dagger}_{x,\sigma}c_{z,\sigma}\Phi_{x,\boldsymbol{\sigma}} &= -c_{z,\uparrow}n_{x,\uparrow}\left(\prod_{y\in\Lambda} c^{\dagger}_{y,\sigma'_y}\right)\Phi_{\mathrm{vac}} - c_{z,\downarrow}n_{x,\downarrow}\left(\prod_{y\in\Lambda} c^{\dagger}_{y,\sigma''_y}\right)\Phi_{\mathrm{vac}} \\ &= -c_{z,\uparrow}\left(\prod_{y\in\Lambda} c^{\dagger}_{y,\sigma'_y}\right)\Phi_{\mathrm{vac}} - c_{z,\downarrow}\left(\prod_{y\in\Lambda} c^{\dagger}_{y,\sigma''_y}\right)\Phi_{\mathrm{vac}} \\ &= -\Phi_{z,\boldsymbol{\sigma}_{z\to x}}, \end{aligned} \tag{4·3}$$

where $\boldsymbol{\sigma}_{z\to x}\in\mathcal{S}_{\Lambda\backslash z}$ is the new spin configuration on $\Lambda\backslash z$ obtained from $\boldsymbol{\sigma}$ by moving σ_z to x. Note that in the second line of (4·3), only one of the two terms survive depending on the value of σ_z. Therefore the matrix elements of the effective Hamiltonian $\tilde{H}$ are given by

$$\left\langle \Phi_{y,\boldsymbol{\tau}}, \tilde{H}\Phi_{x,\boldsymbol{\sigma}}\right\rangle = \begin{cases} -t_{x,y} & \text{if } \boldsymbol{\tau}=\boldsymbol{\sigma}_{y\to x}; \\ 0 & \text{otherwise.}\end{cases} \tag{4·4}$$

Let Φ_{GS} be a ground state of H. Since it has a finite energy, it is expanded as

$$\Phi_{\mathrm{GS}} = \sum_{x\in\Lambda}\sum_{\boldsymbol{\sigma}\in\mathcal{S}_{\Lambda\backslash x}} \varphi(x,\boldsymbol{\sigma})\Phi_{x,\boldsymbol{\sigma}}. \tag{4·5}$$

Since the matrix elements (4·4) of $\tilde{H}$ are real, we can assume that the coefficients $\varphi(x,\boldsymbol{\sigma})$ are real.*) We define

$$\xi_x = \left(\sum_{\boldsymbol{\sigma}\in\mathcal{S}_{\Lambda\backslash x}} (\varphi(x,\boldsymbol{\sigma}))^2\right)^{1/2}, \tag{4·6}$$

and a ferromagnetic state

$$\Phi_{\uparrow} = \sum_{x\in\Lambda}\xi_x\Phi_{x,(\uparrow)}, \tag{4·7}$$

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

By using (4·5) and (4·4), we find

$$\begin{aligned}\left\langle \Phi_{\mathrm{GS}}, \tilde{H}\Phi_{\mathrm{GS}}\right\rangle &= \sum_{x,y\in\Lambda}\sum_{\substack{\boldsymbol{\sigma}\in\mathcal{S}_{\Lambda\backslash x}\\ \boldsymbol{\tau}\in\mathcal{S}_{\Lambda\backslash y}}} \varphi(y,\boldsymbol{\tau})\varphi(x,\boldsymbol{\sigma})\left\langle \Phi_{y,\boldsymbol{\tau}}, \tilde{H}\Phi_{x,\boldsymbol{\sigma}}\right\rangle \\ &= -\sum_{x,y\in\Lambda} t_{x,y}\sum_{\boldsymbol{\sigma}\in\mathcal{S}_{\Lambda\backslash x}} \varphi(y,\boldsymbol{\sigma}_{y\to x})\varphi(x,\boldsymbol{\sigma}) \\ &\geq -\sum_{x,y\in\Lambda} t_{x,y}\left(\sum_{\boldsymbol{\sigma}\in\mathcal{S}_{\Lambda\backslash x}}\{\varphi(y,\boldsymbol{\sigma}_{y\to x})\}^2\right)^{1/2}\left(\sum_{\boldsymbol{\sigma}\in\mathcal{S}_{\Lambda\backslash x}}\{\varphi(x,\boldsymbol{\sigma})\}^2\right)^{1/2} \\ &= -\sum_{x,y\in\Lambda} t_{x,y}\xi_y\xi_x \\ &= \langle\Phi_{\uparrow}, H\Phi_{\uparrow}\rangle, \end{aligned} \tag{4·8}$$

*) If this is not the case, we redefine $\{\varphi(x,\boldsymbol{\sigma})+\varphi(x,\boldsymbol{\sigma})^*\}/2$ as $\varphi(x,\boldsymbol{\sigma})$. The corresponding Φ_{GS} is also a ground state.

where we have used the Schwartz inequality (with the assumption $t_{x,y} \geq 0$) to get the third line. This bound shows that $\Phi_\uparrow$ is also a ground state. This completes the proof of Theorem 4.1.

4.2. *Nagaoka's theorem*

We now state a stronger and the most general version of Nagaoka's theorem. Under an additional condition (which can be easily verified in some typical cases), we will prove that the ferromagnetic states are the only possible ground states. To determine the additional conditions, it is better to start from mathematics.

Let us recall the Perron-Frobenius theorem, which is standard in linear algebra. The following is the simplest version of the theorem.*)

Theorem 4.3 (Perron-Frobenius theorem for a real symmetric matrix) *Let $M = (m_{i,j})_{i,j=1,\dots,N}$ 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 $i \neq j$.
*ii) All $i \neq j$ are connected via nonvanishing matrix elements of M. More precisely,**) for any $i \neq j$, we can take a sequence $(i_1, \dots, i_K)$ such that $i_1 = i$, $i_K = j$, and $m_{i_k,i_{k+1}} \neq 0$ for all $k < K$.*

Then the lowest eigenvalue of M is nondegenerate and the corresponding eigenvector $\mathbf{v} = (v_i)_{i=1,\dots,N}$ 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. This idea is familiar in quantum mechanics.***)

1) We first prove that if an eigenvector $\mathbf{u} = (u_i)_{i=1,\dots,N}$ of M satisfies $u_i \geq 0$ for any i, then it inevitably satisfies $u_i > 0$ for any i. To do this, we assume the converse, i.e., $u_i \geq 0$ for all i, and $u_j = 0$ for some j. Then from the eigenvalue equation, we see that $\sum_i m_{j,i} u_i = \mu u_j = 0$. Since $m_{j,i} u_i \leq 0$, this means $u_i = 0$ for all i with $m_{j,i} \neq 0$. Because we have the connectivity ii), we can repeat this argument until we see $u_i = 0$ for all i, which is a contradiction.

2) We then prove that a normalized eigenvector $\mathbf{v} = (v_i)_{i=1,\dots,N}$ for the lowest eigenvalue μ_0 can be chosen to satisfy $v_i > 0$ for all i. Since all $m_{i,j}$ and μ_0 are real, we can assume that the v_i are all real. With 1) in mind, we assume the converse, i.e., $v_j > 0$ and $v_k < 0$ hold for some j and k. Define $\mathbf{u} = (u_i)_{i=1,\dots,N}$ by $u_i = |v_i|$. Then from i), we see

$$\mu_0 = \sum_{i,j=1}^{N} v_i m_{i,j} v_j \geq \sum_{i,j=1}^{N} u_i m_{i,j} u_j. \tag{4·9}$$

Since μ_0 is the lowest eigenvalue, the right-hand side must also be equal to μ_0, which means that $\mathbf{u}$ is an eigenvector of M. Then the above 1) implies $u_i > 0$, and hence

*) The full version of the theorem applies to non-symmetric matrices as well. See, for example, p. 130 of Ref. 34).

**) Another way of stating the condition is that, for any $i \neq j$, there is K such that $(M^K)_{i,j} \neq 0$.

***) See, for example, Section 20 of Ref. 35).

$v_i \neq 0$ for all i. Recalling the connectivity ii), the latter property implies we can find i and j such that $v_i m_{i,j} v_j > 0$. Then we have $u_i m_{i,j} u_j < 0$ for the same i and j, which means (4·9) is valid with $\geq$ replaced by $>$. This contradicts with the assumption that μ_0 is the lowest eigenvalue.

3) Finally suppose that the lowest eigenvalue of M is degenerate. Then we can find two mutually orthogonal eigenvectors $\mathbf{u}$ and $\mathbf{v}$. But from 2), we must have $\mathbf{u} \cdot \mathbf{v} \neq 0$, which is a contradiction. ■

We wish to apply this theorem to the present problem of the $U = \infty$ Hubbard model with a single hole. As for the matrix M, we take the matrix representation (4·4) of the Hamiltonian for the basis states (4·2) with a fixed $S_{\rm tot}^{(3)} = \sum_{y \in \Lambda \setminus x} \sigma_y$. Because of (4·4) and the assumption $t_{x,y} \geq 0$, the condition i) of Theorem 4.3 is satisfied. The condition ii), on the other hand, is not always valid. This motivates us to consider the following *connectivity condition.*

Definition 4.4 (Connectivity condition) *A Hubbard model with $U = \infty$ and $N_{\rm e} = N_{\rm s} - 1$ (or more precisely the hopping matrix T) is said to satisfy the* connectivity condition *if all the basis states $\Phi_{x,\sigma}$ with common $S_{\rm tot}^{(3)} = \sum_{y \in \Lambda \setminus x} \sigma_y$ are connected with each other through nonvanishing matrix elements of H.*

As we shall see in the next section, the connectivity condition can be easily verified in the Hubbard model with nearest neighbor hoppings on most standard lattices including triangular, square, simple cubic, fcc and bcc.

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 $S_{\rm tot}^{(3)}$ is unique. Then Theorem 4.1 implies that this ground state must be ferromagnetic. So we have proved the following, which is the full (and most generalized) version of Nagaoka's famous theorem.

Theorem 4.5 (Generalized Nagaoka theorem) *Consider an arbitrary Hubbard model with $t_{x,y} \geq 0$ for any $x, y \in \Lambda$, $N_{\rm e} = N_{\rm s} - 1$, and $U = \infty$, and further assume that the model satisfies the connectivity condition. Then the ground states have total spin $S_{\rm tot} = S_{\max} (= N_{\rm e}/2)$, and are non-degenerate apart from the trivial $(2S_{\max} + 1)$-fold degeneracy.*

As stressed earlier, the knowledge that all the ground states are ferromagnetic is of fundamental importance. The theorem is of course no longer valid for the trivial model with $t_{x,y} = 0$ for all x and y. Since the theorem asserts the nondegeneracy of the ferromagnetic ground state 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 of how large U should be.

4.3. *Connectivity condition*

We still have to verify the connectivity condition for some systems to make Theorem 4.5 meaningful. It seems, however, that to write down a simple necessary and sufficient condition for the connectivity condition is a nontrivial problem. We here follow Nagaoka's original spirit, and provide a constructive criterion (i.e., a

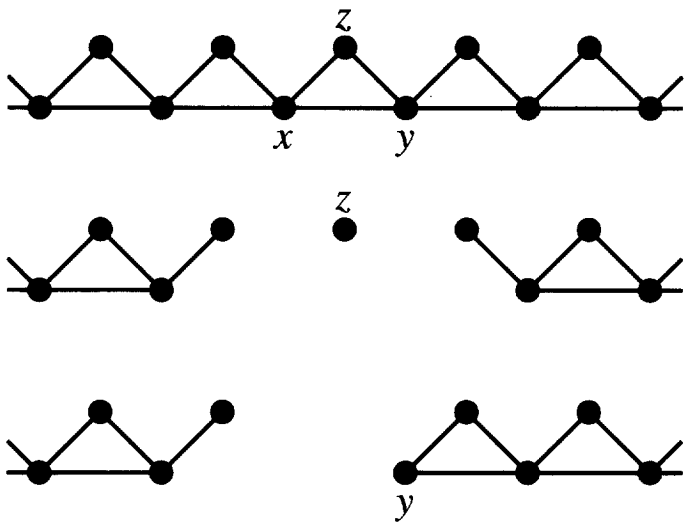

Fig. 5. *Exchange bonds* in the "delta-chain." The horizontal bond $\{x, y\}$ is not an exchange bond since the site z is disconnected from the rest when x and y are removed. The bond $\{x, z\}$ is an exchange bond since the lattice remains connected after the removal of x and y provided that we use periodic boundary conditions.

sufficient condition) for the connectivity condition.

Let us introduce some terminology. By a *loop* of length m, we mean an ordered set $(x_1, \ldots, x_m)$ of sites such that $t_{x_i,x_{i+1}} \neq 0$ for all $i = 1, \ldots, m-1$, and $t_{x_m,x_1} \neq 0$. We say that a pair $\{x, y\}$ of lattice sites is an *exchange bond* if they belong to a loop of length three or four, and the whole lattice remains connected via nonvanishing $t_{x,y}$ when the sites x and y are removed. (See Fig. 5.)

Then we have the following sufficient condition for the connectivity.

Lemma 4.6 (A sufficient condition for the connectivity) *If the whole lattice is connected by exchange bonds, then the model satisfies the connectivity condition.*

This sufficient condition can be easily verified in various systems. In models defined on regular lattices like triangular, square, simple cubic, fcc or bcc lattices with nonvanishing hopping amplitudes between nearest neighbor sites, it is obvious that all the nearest neighbor bonds are exchange bonds. Thus they trivially satisfy the condition. A less trivial example is the delta chain with periodic boundary conditions in Fig. 5. Although the horizontal bonds are not exchange bonds, the whole lattice is connected via non-horizontal bonds, which are exchange bonds.

Proof of Lemma 4.6: Suppose that we are given an arbitrary configuration of $N_e = N_s - 1$ electrons on Λ. Our goal is to show that we can get an arbitrary configuration with the same $S^{(3)}_{tot}$ by moving the single hole along nonvanishing $t_{x,y}$.

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

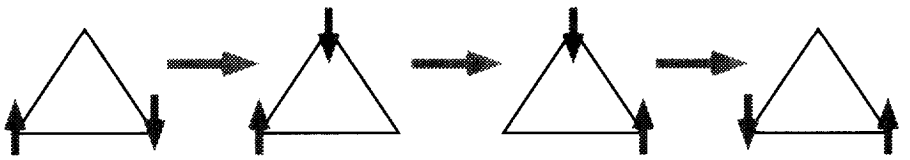

Fig. 6. The two spins are exchanged when the hole hops around the loop once. Such an "exchange process along a triangle" appears repeatedly in various examples of ferromagnetism, and is regarded as a universal and fundamental mechanism leading to ferromagnetism.[21]

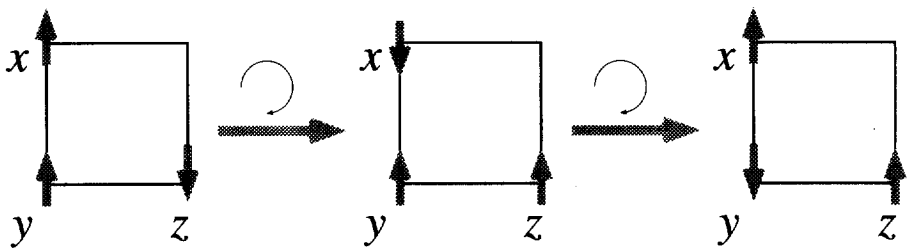

Fig. 7. The spins at x and z are exchanged when the hole hops around the loop once. The spins at y and z are exchanged when the hole hops around the loop twice (or once in the opposite orientation).

of spin configurations by successive exchanges on the exchange bonds. 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 $\{x, y\}$. Next we let the hole move 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. 6. 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. 7. Finally, we bring the hole back to the original location. By following the same path as in the first step backwards, we recover exactly the same configuration, except on sites x and y. ■

4.4. *Stability of Nagaoka's ferromagnetism*

It is desirable to extend Nagaoka's ferromagnetism to systems with finite U and with finite densities of holes. Unfortunately, the Perron-Frobenius argument which works for the one-hole case fails even for models with two holes. There is a considerable number of rigorous works (including that in Nagaoka's original work[10]) which establish that saturated ferromagnetism *does not* take place in certain situations. See, for example, Refs. 36), 27), 37) ~ 39) and 24). Most of these works are essentially based on variational arguments where one constructs sophisticated

[*] The exchange on a length four loop is possible because electronic spins take (only) two values.

variational states which have lower energies than the ferromagnetic state. (We have seen the most elementary versions of the argument in §3.3.) As far as we know, there are no rigorous results about the *stability* of Nagaoka's ferromagnetism*) in the Hubbard model.

There is also a considerable number of numerical and theoretical works which indicate stability or instability of Nagaoka's ferromagnetism in various situations.[42)-45)]

In spite of all these efforts, it is still not known if straightforward extensions of Nagaoka's ferromagnetism to finite U and finite hole density are possible. It seems that a recent dominant opinion is that the possibility of extension depends strongly on lattice structures, where the triangular lattice is regarded as one of the most promising candidates. The importance of lattice structures is closely related to the approach from flat-band models that we discuss in §6.

§5. Ferromagnetism in the Hubbard model with long-range hopping

5.1. *Main statement and preliminary results*

There is at least one situation in which the extension of Nagaoka's ferromagnetism to finite U is possible. This is an artificial model with long range hopping that we shall now define.

We associate with each site x a constant $\lambda_x > 0$, and define the hopping matrix $\mathsf{T} = (t_{x,y})_{x,y\in\Lambda}$ with long range hopping amplitudes by**)

$$t_{x,y} = t\lambda_x\lambda_y, \tag{5·1}$$

where $t > 0$ is a constant (which does not play any essential role). Note that an electron can hop from any site in the lattice to any other site (Fig. 8). Then we have the following extension of Nagaoka's theorem.

Theorem 5.1 (Ferromagnetism in the long-range hopping model) *Consider the Hubbard model with the hopping (5·1) with electron number $N_e = N_s - 1$. For any $U > 0$, the ground states have total spin $S_{tot} = S_{max} (= N_e/2)$, and are non-degenerate apart from the trivial $(2S_{max} + 1)$-fold degeneracy.*

At first glance, the theorem looks surprising and attractive since the precise statement of Nagaoka's theorem is extended to an arbitrary positive value of U. As we shall see below, this is indeed a consequence of a very special property of the present model.

With the hopping (5·1), the action of T onto any $\boldsymbol{\varphi} \in \mathfrak{h}$ becomes $\mathsf{T}\boldsymbol{\varphi} = t\boldsymbol{\lambda}\langle\boldsymbol{\lambda}, \boldsymbol{\varphi}\rangle$, where $\boldsymbol{\lambda} = (\lambda_x)_{x\in\Lambda} \in \mathfrak{h}$. Thus we find $\langle\boldsymbol{\varphi}, \mathsf{T}\boldsymbol{\varphi}\rangle = t\langle\boldsymbol{\varphi}, \boldsymbol{\lambda}\rangle\langle\boldsymbol{\lambda}, \boldsymbol{\varphi}\rangle = |\langle\boldsymbol{\lambda}, \boldsymbol{\varphi}\rangle|^2 \geq 0$,

*) Interesting lower bounds for the ground state energy of the $U = \infty$ model with multiple holes are proved in Refs. 40) and 41). We do not, however, interpret these bounds as "proofs of stability of Nagaoka's ferromagnetism" since the bounds do not rule out paramagnetism (e.g., in the trivial model with $t_{x,y} = 0$ for any x, y). (See also footnote **) on p. 509.)

**) In coordinate-free notation, this becomes $\mathsf{T} = t\boldsymbol{\lambda} \otimes \boldsymbol{\lambda}$, where $\otimes$ is understood as a Kronecker product, and $\boldsymbol{\lambda} = (\lambda_x)_{x\in\Lambda}$. As for this construction, the Dirac notation $\mathsf{T} = t|\boldsymbol{\lambda}\rangle\langle\boldsymbol{\lambda}|$ may be more informative.

which means that $\mathsf{T} \geq 0$. On the other hand, the single-electron Schrödinger equation (2·2) becomes

$$\varepsilon \boldsymbol{\varphi} = t \boldsymbol{\lambda} \langle \boldsymbol{\lambda}, \boldsymbol{\varphi} \rangle . \qquad (5\cdot2)$$

This means that any $\boldsymbol{\varphi}$ orthogonal to $\boldsymbol{\lambda}$ is an eigenstate of (5·2) with $\varepsilon = 0$, which is the minimum possible eigenvalue. Clearly, there are $(N_\mathrm{s} - 1)$-fold degenerate eigenstates with $\varepsilon = 0$. The remaining eigenstate is $\boldsymbol{\lambda}$ itself, and it has the eigenvalue $\varepsilon = t \sum_{x \in \Lambda} (\lambda_x)^2 > 0$.

It is crucial for the electron number N_e to be set equal to the dimension $N_\mathrm{s} - 1$ of the above degeneracy. We see from (3·4) that the lowest energy among ferromagnetic states is $E_\mathrm{ferro} = \sum_{j=1}^{N_\mathrm{s}-1} \varepsilon_j = 0$.

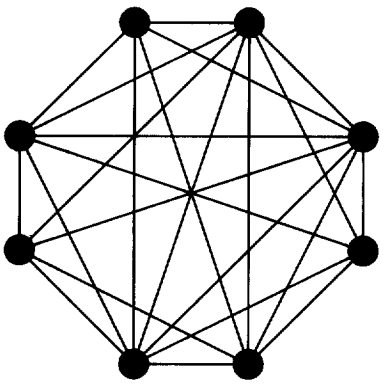

Fig. 8. In the long-range hopping model, hopping between two arbitrary sites in the lattice is possible. The model serves as an intermediate step in our attempt to relate Nagaoka's ferromagnetism and flat-band ferromagnetism.

On the other hand, it is clear from (2·29) that the lowest eigenvalue of H_hop is 0 if $N_\mathrm{e} \leq 2(N_\mathrm{s} - 1)$. Hence we can write $H_\mathrm{hop} \geq 0$ for $N_\mathrm{e} = N_\mathrm{s} - 1$. (See Definition C.1 and Lemma C.2.) We also have $H_\mathrm{int} \geq 0$ in general. Thus (by using Lemma C.4) we get $H = H_\mathrm{hop} + H_\mathrm{int} \geq 0$. This, along with the fact that there is a ferromagnetic state with energy zero, implies that the ground state energy of H is 0. We have thus found that there are ferromagnetic states among the ground states.

Let $U > 0$, and let Φ_GS be an arbitrary ground state. Then (from Lemma C.6) $H_\mathrm{hop} \geq 0$, $H_\mathrm{int} \geq 0$, and $H\Phi_\mathrm{GS} = (H_\mathrm{hop} + H_\mathrm{int})\Phi_\mathrm{GS} = 0$ imply

$$H_\mathrm{hop}\Phi_\mathrm{GS} = 0, \quad H_\mathrm{int}\Phi_\mathrm{GS} = 0. \qquad (5\cdot3)$$

In other words, the ground state happens to be a simultaneous ground state *) of H_hop and H_int. This is of course a very special property of the present model with singular degeneracy in the single-electron eigenstates. Since $U \neq 0$, the second relation in (5·3) implies

$$\sum_{x \in \Lambda} n_{x,\uparrow} n_{x,\downarrow} = 0. \qquad (5\cdot4)$$

5.2. *First proof*

We give a proof of Theorem 5.1 which makes explicit use of Nagaoka's theorem. Since we have seen that there are ferromagnetic states among the ground states for $U \geq 0$, we only have to show that they are the only ground states for $U > 0$.

The ground states for any $U > 0$ are fully characterized by $H_\mathrm{hop}\Phi_\mathrm{GS} = 0$ and (5·4). Noting that (5·4) implies $H_\mathrm{int}\Phi_\mathrm{GS} = 0$ for any $U > 0$, we see that the ground

*) Of course the existence of one simultaneous eigenstate does not imply H_hop and H_int are simultaneously diagonalizable. Recall that quantum mechanical angular momenta have simultaneous eigenstates with vanishing eigenvalue.

states of a given $U > 0$ remain as ground states for any values of $U > 0$, and hence in the limit $U \to \infty$. Since the ground states for $U \to \infty$ are completely characterized by Nagaoka's theorem (Theorem 4.5), we have proved Theorem 5.1.

5.3. *Second proof*

We describe another proof of Theorem 5.1. This proof is certainly more involved than the first one, but provides us with an entirely different physical picture of the problem. In the new picture, ferromagnetism in this model is generated by an "exchange interaction" among the spins of electrons which are "frozen" in certain single-electron states. We recall that the first proof is based on Nagaoka's theorem, which suggests a dynamical picture that ferromagnetism is generated by the motion of the hole. It is interesting that the two totally different pictures apply equally to the present model. As we shall investigate in the next sections, the new picture will lead us to a new class of ferromagnetism now known as 'flat-band ferromagnetism.'

We start by constructing a (non-orthonormal) basis for the space of degenerate single-electron ground states. Fix an arbitrary site $x_0 \in \Lambda$, and denote by $\Lambda' = \Lambda \backslash x_0$ the lattice obtained by removing x_0 from Λ. For each $y \in \Lambda'$, we define a single-electron state $\boldsymbol{\varphi}^{(y)} = (\varphi_x^{(y)})_{x\in\Lambda} \in \mathfrak{h}$ by

$$\varphi_x^{(y)} = \begin{cases} \lambda_{x_0} & \text{if } x = y; \\ -\lambda_y & \text{if } x = x_0; \\ 0 & \text{otherwise.} \end{cases} \tag{5·5}$$

This state satisfies $\langle \boldsymbol{\lambda}, \boldsymbol{\varphi}^{(y)} \rangle = 0$, and hence it is a single-electron ground state. Since the states $\boldsymbol{\varphi}^{(y)}$ with $y \in \Lambda'$ are linearly independent, they span the entire space of the single-electron ground states. We define the corresponding fermion operators by $b_{y,\sigma}^\dagger = C_\sigma^\dagger(\boldsymbol{\varphi}^{(y)})$ for $y \in \Lambda'$ and $\sigma = \uparrow, \downarrow$, which satisfies $[H_{\text{hop}}, b_{y,\sigma}^\dagger] = 0$ because of the general commutation rule (2·23) and the definition (2·26) of H_{hop}.

Let us characterize an arbitrary ground state Φ_{GS} for $U > 0$ in a constructive manner. Because $H_{\text{hop}}\Phi_{\text{GS}} = 0$, the ground state Φ_{GS} should consist only of the (single-electron) zero energy states. Therefore it is written as*)

$$\Phi_{\text{GS}} = \sum_{\substack{L_\uparrow, L_\downarrow \subset \Lambda' \\ \text{s.t. } |L_\uparrow|+|L_\downarrow|=N_{\text{e}}}} f(L_\uparrow, L_\downarrow) \left(\prod_{y\in L_\uparrow} b_{y,\uparrow}^\dagger \right) \left(\prod_{y\in L_\downarrow} b_{y,\downarrow}^\dagger \right) \Phi_{\text{vac}}, \tag{5·6}$$

where the $f(L_\uparrow, L_\downarrow)$ are coefficients, and $L_\uparrow$, $L_\downarrow$ are summed over all the subsets of Λ' such that $|L_\uparrow| + |L_\downarrow| = N_{\text{e}} = N_{\text{s}} - 1$. Each state in the sum of (5·6) is nonvanishing because of Lemma 2.1.

Since $n_{x,\uparrow} n_{x,\downarrow} \geq 0$, the condition (5·4) (and Lemma C.6) indeed implies a stronger statement that $n_{x,\uparrow} n_{x,\downarrow} \Phi_{\text{GS}} = 0$ for any $x \in \Lambda$. By further rewriting this relation as $(c_{x,\downarrow} c_{x,\uparrow})^\dagger (c_{x,\downarrow} c_{x,\uparrow}) \Phi_{\text{GS}} = 0$ (and using Lemma C.7), we find that the ground

*) In a more careful proof, one uses Lemma 2.3 with N_{s} linearly independent states $\boldsymbol{\varphi}^{(y)}$ ($y \in \Lambda'$) and $\boldsymbol{\lambda}$ to construct a basis of the entire Hilbert space $\mathcal{H}_{N_{\text{e}}}$, formally writes Φ_{GS} as a linear combination of all the basis states, and finally uses the condition $H_{\text{hop}}\Phi_{\text{GS}} = 0$ to see that the terms including $C_\sigma^\dagger(\boldsymbol{\lambda})$ must be vanishing.

state must satisfy

$$c_{x,\downarrow}c_{x,\uparrow}\Phi_{\rm GS}=0 \tag{5·7}$$

for each $x\in\Lambda$.

We take $x\in\Lambda'$ and examine what (5·7) implies about (5·6). Using the anticommutation relation $\{c_{x,\sigma},b^\dagger_{y,\sigma'}\}=\lambda_{x_0}\delta_{x,y}\delta_{\sigma,\sigma'}$, we obtain

$$c_{x,\downarrow}c_{x,\uparrow}\Phi_{\rm GS}=\sum_{L_\uparrow,L_\downarrow}\chi[x\in L_\uparrow\cap L_\downarrow]\,f(L_\uparrow,L_\downarrow)\,{\rm sgn}[x,L_\uparrow,L_\downarrow]\times\left(\prod_{y\in L_\uparrow\setminus x}b^\dagger_{y,\uparrow}\right)\left(\prod_{y\in L_\downarrow\setminus x}b^\dagger_{y,\downarrow}\right)\Phi_{\rm vac}, \tag{5·8}$$

where $\chi[\text{true}]=1$, $\chi[\text{false}]=0$, and the factor ${\rm sgn}[x,L_\uparrow,L_\downarrow]=\pm1$ comes from the exchange of fermion operators. Since all the terms in the sum of (5·8) are linearly independent, the condition (5·7) implies $f(L_\uparrow,L_\downarrow)=0$ for any $L_\uparrow,L_\downarrow$ such that $x\in L_\uparrow\cap L_\downarrow$. Using this for all $x\in\Lambda'$, we finally see that $f(L_\uparrow,L_\downarrow)=0$ unless $L_\uparrow\cap L_\downarrow=\emptyset$. Since $|L_\uparrow|+|L_\downarrow|=|\Lambda'|$, the condition $L_\uparrow\cap L_\downarrow=\emptyset$ implies $L_\uparrow\cup L_\downarrow=\Lambda'$. This means that we can reorganize the sum (5·6) as

$$\Phi_{\rm GS}=\sum_{\boldsymbol{\sigma}\in\mathcal{S}_{\Lambda'}}g[\boldsymbol{\sigma}]\left(\prod_{y\in\Lambda'}b^\dagger_{y,\sigma_y}\right)\Phi_{\rm vac}, \tag{5·9}$$

where the sum is over all the spin configurations $\boldsymbol{\sigma}=(\sigma_y)_{y\in\Lambda}$ on Λ', and $g[\boldsymbol{\sigma}]$ is a new coefficient. The representation (5·9) suggests a new physical picture that the motion of the electrons is "frozen", and only spin degrees of freedom are left. Note, however, that this interpretation is somewhat arbitrary since the site x_0 is chosen arbitrarily.

Now we consider the condition (5·7) with $x=x_0$. By using (5·9) and the anticommutation relation $\{c_{x_0,\sigma},b^\dagger_{y,\sigma'}\}=-\lambda_y\delta_{\sigma,\sigma'}$ for any $y\in\Lambda'$, we get

$$c_{x_0,\downarrow}c_{x_0,\uparrow}\Phi_{\rm GS}=\sum_{\substack{x,y\in\Lambda'\\ \text{s.t. } x>y}}\sum_{\substack{\boldsymbol{\sigma}\in\mathcal{S}_{\Lambda'}\\ \text{s.t. }\sigma_x=\uparrow,\sigma_y=\downarrow}}{\rm sgn}[x,y]\,t\lambda_x\lambda_y\,(g[\boldsymbol{\sigma}]-g[\boldsymbol{\sigma}_{x\leftrightarrow y}])\left(\prod_{z\in\Lambda'\setminus\{x,y\}}b^\dagger_{z,\sigma_z}\right)\Phi_{\rm vac}, \tag{5·10}$$

where we have introduced arbitrary ordering in Λ', and ${\rm sgn}[x,y]=\pm1$ is again the fermion sign.*) The spin configuration $\boldsymbol{\sigma}_{x\leftrightarrow y}$ is obtained by switching σ_x and σ_y in the original configuration $\boldsymbol{\sigma}$.

Since all the states in the sum (5·10) are linearly independent, the condition (5·7) is satisfied only when

$$g[\boldsymbol{\sigma}]=g[\boldsymbol{\sigma}_{x\leftrightarrow y}] \tag{5·11}$$

*) $\Lambda\setminus\{y,z\}$ is the set obtained by removing y and z from Λ.

holds for all $\boldsymbol{\sigma}$ and all $x, y \in \Lambda'$. Note that we have deduced a kind of "exchange interaction" (5·11) among "localized spins" from the no-double-occupancy condition (5·7).

The exchange relation (5·11) implies that all the $g[\boldsymbol{\sigma}]$ with common $S_{\rm tot}^{(3)} = \sum_{y\in\Lambda'} \sigma_y$ assume exactly the same values.*) This means that the lowest energy state in the space with a fixed $S_{\rm tot}^{(3)}$ is unique. Since we already know that there are ferromagnetic ground states, this completes the second proof of Theorem 5.1.

§6. Flat-band ferromagnetism

6.1. *Definition*

We have seen that the Hubbard model with artificial long-range hopping exhibits ferromagnetism for arbitrary $U > 0$. As we shall see in the present section, it is possible to assemble many (identical) copies of the long-range model to get Hubbard models with only short range hoppings which still exhibit ferromagnetism.[7),8)] Unlike Nagaoka's ferromagnetism, the electron density is away from half-filling, and U need only to be nonvanishing. On the other hand, these models have very singular band structure which is expressed by the name "flat-band models."

Let us define our model by means of a "cell construction".**) Our lattice Λ can be written as

$$\Lambda = C_1 \cup \cdots \cup C_M, \tag{6·1}$$

where each C_j is called a cell. Each cell consists of a single *internal site* and n *external sites*, where $n \geq 2$ is a constant. The simplest cell is a triangle with $n = 2$. The models to be constructed will again involve "exchange processes along a triangle." This seems to be a universal and fundamental mechanism of ferromagnetism.[21)] (See Fig. 6.)

When assembling M cells to form Λ in (6·1), we identify some external sites from different cells***) to regard them as a single site in Λ. (See Fig. 9.) The lattice Λ is naturally decomposed as $\Lambda = \mathcal{I} \cup \mathcal{E}$, where $\mathcal{I}$ is the set of internal sites, and $\mathcal{E}$ is the set of external sites.

We define the hopping amplitudes for the j-th cell by

$$t_{x,y}^{(j)} = t\lambda_x^{(j)}\lambda_y^{(j)}, \tag{6·2}$$

where

$$\lambda_x^{(j)} = \begin{cases} \lambda & \text{if } x \text{ is the internal site of } C_j; \\ 1 & \text{if } x \text{ is one of the external sites of } C_j; \\ 0 & \text{otherwise.} \end{cases} \tag{6·3}$$

*) Although it is not necessary in the present proof, one can show directly that such a state has $S_{\rm tot} = S_{\rm max}$. (See proof of Theorem 8.1.)

**) A class of exactly solvable Hubbard models with very similar cell structures (with paramagnetic ground states) was discovered by Brandt and Giesekus[32)] before the present model for flat-band ferromagnetism was introduced. See also Refs. 33) and 46) and references therein for further results concerning this model.

***) There can be external sites left unidentified.

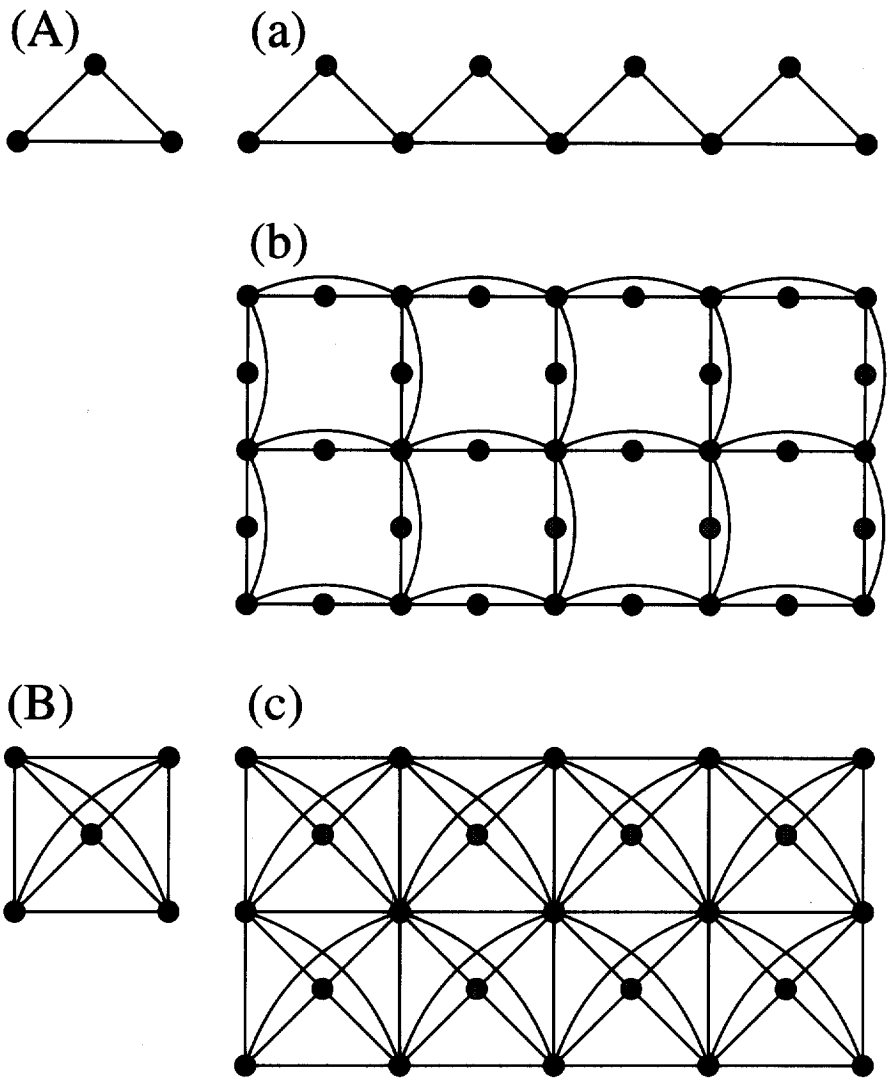

Fig. 9. Examples of cells and lattices. Gray dots represent internal sites. From the triangular cell with three sites (A), one can form (a) the delta-chain by identifying two external sites, or (b) a decorated square lattice by identifying four. From the cell with five sites (B), one can form (c) another decorated square lattice. There are many similar examples in higher dimensions. The flat-band Hubbard model on these lattices exhibits ferromagnetism for any $U > 0$ when the filling factor $\nu = N_e/(2N_s)$ is equal to (a) 1/4, (b) 1/6, or (c) 1/4.

Here $t > 0$ and $\lambda > 0$ are constants. Note that this is the same as the hopping amplitudes (5·1) of the long-range model. An essential difference, which makes the present model less artificial, is that we have this type of hopping only within each cell. The total hopping is defined as

$$t_{x,y} = \sum_{j=1}^{M} t_{x,y}^{(j)}. \tag{6·4}$$

We finally assume that the whole lattice is connected via nonvanishing $t_{x,y}$. We then define the Hubbard model on Λ with the hopping matrix given by (6·4).

Theorem 6.1 (Flat-band ferromagnetism) *Consider the above Hubbard model with the electron number $N_e = |\mathcal{E}|$. For any $U > 0$, the ground states have total spin $S_{tot} = S_{max} (= N_e/2)$, and are non-degenerate apart from the trivial $(2S_{max} + 1)$-fold degeneracy.*

Note that the existence of ferromagnetism has been established in models with finite U, finite-range hoppings, and electron densities away from half-filling. As one might guess, the straightforward (and general) methods using the Perron-Frobenius theorem (as in the proof of Nagaoka's theorem) do not work for this problem. The proof will make use of very special properties of the model. This ferromagnetism is closely related to Nagaoka's ferromagnetism (at least) via the ferromagnetism in the long-range hopping model, but it certainly belongs to a new class of ferromagnetism. This new class is now known as "flat-band ferromagnetism" for a reason which we shall explain in §6.3.

6.2. *Examples*

Clearly the cell construction leads to a wide variety of models.*) Let us discuss a class of examples which is constructed from the most elementary triangular cell with $n = 2$.

We construct the d-dimensional $L \times \ldots \times L$ hypercubic lattice with periodic boundary conditions by assembling together the triangular cell (A) of Fig. 9 regarding it as a basic bond (with length 1). The resulting lattice Λ is the decorated hypercubic lattice with $(d+1)L^d$ sites. The set $\mathcal{E}$ of external sites can be identified with the d-dimensional $L \times \ldots \times L$ hypercubic lattice with L^d sites. The internal sites in $\mathcal{I}$ are the decorating sites at the center of every bond. The lattices (a) and (b) in Fig. 9 represent parts of Λ for $d = 1$ and 2, respectively.

Then the hopping amplitude of (6·4) becomes

$$t_{x,y} = \begin{cases} \lambda t & \text{if } |x-y| = 1/2; \\ t & \text{if } x, y \in \mathcal{E} \text{ and } |x-y| = 1; \\ \lambda^2 t & \text{if } x = y \in \mathcal{I}; \\ 2dt & \text{if } x = y \in \mathcal{E}; \\ 0 & \text{otherwise.} \end{cases} \tag{6·5}$$

Note that there are next-nearest-neighbor hoppings between nearby external sites.

The electron number specified in Theorem 6.1 is $N_e = L^d$. In terms of the filling factor, this corresponds to $\nu = N_e/(2N_s) = \{2(d+1)\}^{-1}$.

6.3. *Single-electron problem*

The present models have peculiar degeneracy in their single-electron ground states which are quite similar to that in the long-range hopping model of the previous section.

We first note that the hopping matrix T defined by (6·4) satisfies $\mathsf{T} \geq 0$. This

*) It is not necessary to have the same n or λ for all the cells. This further extends the possibility of models.

is because each $(t^{(j)}_{x,y})_{x,y\in\Lambda}$ determined by (6·2) is positive semidefinite (which fact is clear from the discussion in §5.1), and the sum of positive semidefinite matrices is positive semidefinite (as in Lemma C.4).

We define for each $y \in \mathcal{E}$ the single-electron state $\boldsymbol{\varphi}^{(y)} = (\varphi^{(y)}_x)_{x\in\Lambda}$ by

$$\varphi^{(y)}_x = \begin{cases} \lambda & \text{if } x = y; \\ -1 & \text{if } x \text{ is the internal site of one of the cells containing } y; \\ 0 & \text{otherwise.} \end{cases} \tag{6·6}$$

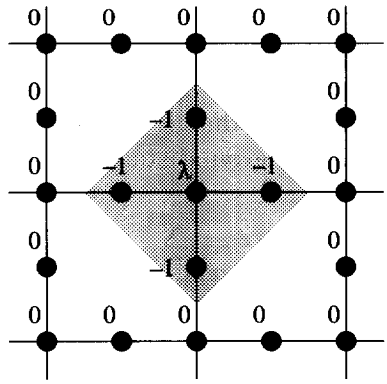

Fig. 10. The components of the single-electron ground state $\boldsymbol{\varphi}^{(y)}$ in the model b) of Fig. 9. The state is localized around the site y, which is at the center of the figure.

(See Fig. 10.) Observe that we have $\langle \boldsymbol{\lambda}^{(j)}, \boldsymbol{\varphi}^{(y)} \rangle = 0$ for any $j = 1, \ldots, M$ and $y \in \mathcal{E}$, where $\boldsymbol{\lambda}^{(j)} = (\lambda^{(j)}_x)_{x\in\Lambda} \in \mathfrak{h}$, and hence

$$\mathsf{T}\boldsymbol{\varphi}^{(y)} = t\sum_{j=1}^{M} \boldsymbol{\lambda}^{(j)} \left\langle \boldsymbol{\lambda}^{(j)}, \boldsymbol{\varphi}^{(y)} \right\rangle = 0. \tag{6·7}$$

Since $\boldsymbol{\varphi}^{(y)}$ with $y \in \mathcal{E}$ are linearly independent, the single-electron Schrödinger equation (2·2) has $|\mathcal{E}|$-fold degenerate ground states*) with $\varepsilon = 0$. It is needless to say that such a huge degeneracy is accidental, and makes the present models very special. We also stress that such a degeneracy is lifted by an arbitrarily small generic perturbation applied to the hopping matrix.

In models with translational invariance, the degeneracy in the single-electron ground states corresponds to the lowest band being completely dispersionless, or "flat." For example, in the models on the d-dimensional hypercubic lattice of §6.2, we find that there are $d+1$ bands with dispersion relations

$$\varepsilon_j(k) = \begin{cases} 0 & \text{if } j = 1; \\ \lambda^2 t & \text{if } j = 2, \ldots, d; \\ (\lambda^2 + 2d)t + t\displaystyle\sum_{\mu=1}^{d} \cos k_\mu & \text{if } j = d+1. \end{cases} \tag{6·8}$$

Note that the lowest band and the $(d-1)$ middle bands are completely flat, while the upper band is dispersive. For definitions of bands and dispersion relations as well as an explicit calculation for the $d = 1$ case, see Appendix E.

6.4. *Proof*

We now prove Theorem 6.1. Interestingly, the proof is completely analogous to and not more difficult than the second proof of the (less attractive) Theorem 5.1 for the long-range hopping model.

*) It is not hard to prove that $\boldsymbol{\lambda}^{(j)}$ with $j = 1, \ldots, M$ span the remaining space with $\varepsilon > 0$.

Since the single-electron ground states of the model are $|\mathcal{E}|$-fold degenerate, and the electron number is set to $N_e = |\mathcal{E}|$, all the preliminary considerations in §§5.1 and 5.3 apply to the present model as well. Any ground state Φ_{GS} satisfies the conditions (5·3), and (5·7) for any $x \in \Lambda$.

Again, introducing $b^\dagger_{y,\sigma} = C^\dagger_\sigma(\varphi^{(y)})$ for $y \in \mathcal{E}$, and using $H_{hop}\Phi_{GS} = 0$, we can represent any ground state as

$$\Phi_{GS} = \sum_{\substack{L_\uparrow, L_\downarrow \subset \mathcal{E} \\ \text{s.t. } |L_\uparrow|+|L_\downarrow|=N_e}} f(L_\uparrow, L_\downarrow) \left(\prod_{y \in L_\uparrow} b^\dagger_{y,\uparrow} \right) \left(\prod_{y \in L_\downarrow} b^\dagger_{y,\downarrow} \right) \Phi_{vac}, \tag{6·9}$$

where $f(L_\uparrow, L_\downarrow)$ are coefficients, and $L_\uparrow$, $L_\downarrow$ are summed over all the subsets of $\mathcal{E}$ such that $|L_\uparrow| + |L_\downarrow| = N_e = |\mathcal{E}|$.

Exactly as before, the condition (5·7) for $x \in \mathcal{E}$ shows that there can be no "double occupancies" in $b^\dagger$, i.e., $f(L_\uparrow, L_\downarrow) = 0$ whenever $L_\uparrow \cup L_\downarrow \neq \emptyset$. We again reorganize the sum to get a spin system representation

$$\Phi_{GS} = \sum_{\boldsymbol{\sigma} \in \mathcal{S}_\mathcal{E}} g[\boldsymbol{\sigma}] \left(\prod_{y \in \mathcal{E}} b^\dagger_{y,\sigma(y)} \right) \Phi_{vac}, \tag{6·10}$$

where the sum is over all the spin configuration $\boldsymbol{\sigma} = (\sigma_y)_{y \in \mathcal{E}}$ on $\mathcal{E}$, and $g[\boldsymbol{\sigma}]$ is a new coefficient.

Next we examine the implication of the condition (5·7) for $x \in \mathcal{I}$ on the ground state (6·10). Unlike in the long-range hopping model, there are still many relations to use. Let $\mathcal{E}_x$ be the set of external sites contained in the cell which contains an internal site x. By using (6·10) and the anticommutation relation $\{c_{x,\sigma}, b^\dagger_{y,\sigma'}\} = -\delta_{\sigma,\sigma'}\chi[y \in \mathcal{E}_x]$ for any $x \in \mathcal{I}$ and $y \in \mathcal{E}$, we get

$$c_{x,\downarrow}c_{x,\uparrow}\Phi_{GS} = \sum_{\substack{y,z \in \mathcal{E}_x \\ \text{s.t. } y>z}} \sum_{\substack{\boldsymbol{\sigma} \in \mathcal{S}_\mathcal{E} \\ \text{s.t. } \sigma_y=\uparrow, \sigma_z=\downarrow}} \mathrm{sgn}[x,y](g[\boldsymbol{\sigma}] - g[\boldsymbol{\sigma}_{y \leftrightarrow z}]) \left(\prod_{u \in \mathcal{E} \setminus \{y,z\}} b^\dagger_{u,\sigma_u} \right) \Phi_{vac}. \tag{6·11}$$

Since this quantity vanishes for all $x \in \mathcal{I}$, we finally find that

$$g[\boldsymbol{\sigma}] = g[\boldsymbol{\sigma}_{y \leftrightarrow z}] \tag{6·12}$$

for any $y, z \in \mathcal{E}$ which belong to a common cell. Note that the "exchange interaction" is short range because we are treating models with short range hoppings. Since the entire lattice is connected, (6·12) ensures that the lowest energy state is unique in each sector with a fixed $S^{(3)}_{tot}$. This completes the proof of Theorem 6.1.

6.5. *Mielke's flat-band ferromagnetism*

A slightly different class of Hubbard models which have highly degenerate single-electron ground states and exhibit ferromagnetism was discovered by Mielke[14),15)] *before* the above models were introduced. Here we briefly summarize Mielke's beautiful construction based on graph theoretic notion. For a general theory of flat-band ferromagnetism obtained by Mielke, see Ref. 47).

We start from abstract notation. Let $G = (V, E)$ be an abstract graph, where V is the set of vertices (sites) $\alpha, \beta, \ldots \in V$, and E is the set of edges (bonds) which are nothing but pairs of vertices like $\{\alpha, \beta\}$. Given a graph G, one can construct the corresponding line graph $L(G) = (V_{\rm L}, E_{\rm L})$ by the following procedure. The set of vertices (sites) $V_{\rm L}$ (whose elements are denoted as $x, y, \ldots \in V_{\rm L}$) is taken to be identical to the set E. This means that we identify edges in G with the vertices (sites) in $L(G)$ as, for example, $x = \{\alpha, \beta\}$, $y = \{\alpha, \gamma\}$, etc. Next we declare that two vertices $x, y \in V_{\rm L}$ are adjacent to each other if the corresponding two edges in E share a common vertex in V. The vertices x and y in the above example are adjacent to each other since the corresponding edges in E have a common vertex α. $E_{\rm L}$ is the set of edges (bonds) in $L(G)$, which consists of all the adjacent pairs (like $\{x, y\}$) of vertices (sites) in $V_{\rm L}$. Finally we set $M(G) = |E| - |V| + 1$ if G is bipartite,*) and $M(G) = |E| - |V|$ if G is non-bipartite.

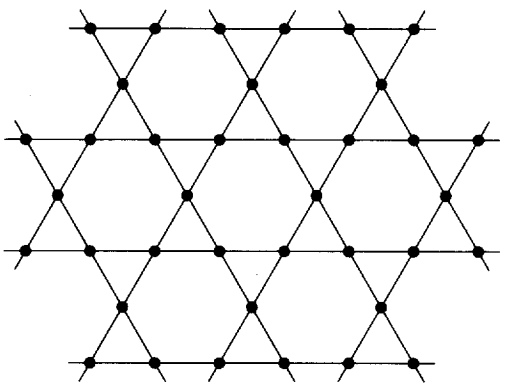

Fig. 11. The kagomé lattice is the line graph of the hexagonal lattice. Mielke showed that the Hubbard model on the kagomé lattice exhibits ferromagnetism when the filling factor is $\nu = 1/6$ for any $U > 0$. This is the most beautiful example of flat-band ferromagnetism.

We define the Hubbard model on the line graph $L(G)$. With each site $x \in V_{\rm L}$, we associate the fermion operator $c_{x,\sigma}$, and consider the Hamiltonian

$$H = t \sum_{\substack{\{x,y\} \in E_{\rm L} \\ \sigma = \uparrow, \downarrow}} (c^{\dagger}_{x,\sigma} c_{y,\sigma} + c^{\dagger}_{y,\sigma} c_{x,\sigma}) + U \sum_{x \in V_{\rm L}} n_{x,\uparrow} n_{x,\downarrow}, \tag{6·13}$$

where $t > 0$ is a constant. Then the main result of Ref. 14) is the following.

Theorem 6.2 (Mielke's flat-band ferromagnetism) *Suppose that the graph G is twofold connected.***) *Consider the above Hubbard model with $N_{\rm e} = M(G)$. Then for any $U > 0$, the ground states of the model have total spin $S_{\rm tot} = S_{\max} (= N_{\rm e}/2)$, and are nondegenerate apart from the trivial $(2S_{\max} + 1)$-fold degeneracy.*

This theorem applies to the Hubbard model defined on various line graphs, a typical one being the kagomé lattice of Fig. 11.

*) G is bipartite if it can be decomposed into two disjoint sublattices as $G = A \cup B$ with the property that any edge in E joins a vertex in A with a vertex in B.

**) A graph is twofold connected if and only if one cannot make it disconnected by the removal of a single vertex.

6.6. *Beyond flat-band ferromagnetism*

Let us once again take a look at the mechanism by which ferromagnetism is generated in a flat-band model. Reflecting the bulk degeneracy in the single-electron ground states, the ground states of the non-interacting model with $H = H_{\rm hop}$ are highly degenerate. There are ground states for any possible values of total spin $S_{\rm tot}$, including the smallest $S_{\rm tot} = 0$ or $1/2$ and the maximum $S_{\rm tot} = S_{\rm max} (= N_{\rm e}/2)$. When we introduce the Hubbard interaction $H_{\rm int}$, the energy of the ferromagnetic ground states (of $H_{\rm hop}$) do not change since ferromagnetic states *do not feel* on-site repulsion. These observations are indeed trivial. A truly nontrivial point (which is proved by imposing some conditions on models) is that all the other ground states of $H_{\rm hop}$ receive extra energy from $H_{\rm int}$, and the ferromagnetic ground states become the only ground states of $H = H_{\rm hop} + H_{\rm int}$.

In this sense, the flat-band ferromagnetism certainly takes into account nontrivial interplay of $H_{\rm hop}$ and $H_{\rm int}$. However, there is no true "competition" between $H_{\rm hop}$ and $H_{\rm int}$. The ferromagnetic ground states are already present in the $U = 0$ model among highly degenerate ground states. The only role of the interaction is to lift the degeneracy, and "select" the ferromagnetic ground states as the only ground states. This is why flat-band ferromagnetism takes place for any $U > 0$.

As we have seen in Theorem 3.2, we never realize saturated ferromagnetism for values of U which are too small in a system without bulk degeneracy in the single-electron ground states. Of course, the bulk degeneracy in a flat-band model is far from being robust, and it is easily destroyed by adding to the hopping matrix T an arbitrarily small generic perturbation. Then, an essential question is whether ferromagnetism found in a flat-band model remains stable after adding a small perturbation to T which makes the lowest band "nearly flat." If the ferromagnetism were unstable against perturbations, we would have to conclude that flat-band ferromagnetism is a mere mathematical game.

It was conjectured[7),8)] that the flat-band ferromagnetism is stable against small perturbations to the hopping Hamiltonian. Among the main arguments used in that discussion was that an approximate low-energy effective Hamiltonian of the flat-band model has the precise form of the ferromagnetic Heisenberg spin system. Kusakabe and Aoki[48),49)] made the first systematic study about 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 evidence that ferromagnetism remains stable if we add sufficiently small perturbations to the hopping matrix, thus making the lowest flat band "nearly flat".

As for rigorous results, stability of ferromagnetism under a single-spin flip is proved in Refs. 16) and 17) for the model obtained by adding an *arbitrary* small translation invariant perturbation to the hopping matrix of the translation invariant flat-band Hubbard model of §6.1. Although this only establishes the local stability of flat-band ferromagnetism, it is a remarkable nonperturbative result which applies to a robust class of models. Given the global stability of ferromagnetism in the original flat-band model, the local stability of ferromagnetism in a nearly-flat-band

model provides very strong evidence that the nearly-flat-band model indeed exhibits globally stable ferromagnetism.

Finally, the problem of stability of ferromagnetism was completely solved in Refs. 18) and 19) for a special class of models. Let us explain the results briefly.

Take the same lattice Λ as in §6.2, i.e., the d-dimensional decorated hypercubic lattice. We define special perturbations to the hopping amplitudes as follows. For each $z \in \mathcal{E}$, we let

$$s_{x,y}^{(z)} = -s\mu_x^{(z)}\mu_y^{(z)}, \tag{6·14}$$

where

$$\mu_x^{(z)} = \begin{cases} \lambda & \text{if } x = z; \\ 1 & \text{if } x \text{ is an internal site adjacent to } z; \\ 0 & \text{otherwise.} \end{cases} \tag{6·15}$$

Here $s > 0$ is a new constant, and $\lambda > 0$ is the same as in §6.1.

Then the hopping matrix $\mathsf{T} = (t_{x,y})_{x,y\in\Lambda}$ of the perturbed models is defined by*)

$$t_{x,y} = \sum_{j=1}^{M} t_{x,y}^{(j)} + \sum_{z\in\mathcal{E}} s_{x,y}^{(z)} + (\lambda^2 s - 2dt)\delta_{x,y}, \tag{6·16}$$

where $t_{x,y}^{(j)}$ is the same as in (6·2). This $t_{x,y}$ can be written more explicitly as

$$t_{x,y} = \begin{cases} \lambda(t+s) & \text{if } |x-y| = 1/2; \\ t & \text{if } x, y \in \mathcal{E} \text{ and } |x-y| = 1; \\ -s & \text{if } x, y \in \mathcal{I} \text{ and } |x-y| = 1 \text{ or } 1/\sqrt{2}; \\ (\lambda^2 - 2d)t + (\lambda^2 - 2)s & \text{if } x = y \in \mathcal{I}; \\ 0 & \text{otherwise.} \end{cases} \tag{6·17}$$

As can be seen also from Fig. 12, this model contains nearest-neighbor hoppings and some next-nearest-neighbor hoppings (but not more than that). The amplitudes for the different hoppings and the on-site potential must satisfy special relations because there are only three controllable parameters, $t > 0$, $s > 0$ and $\lambda > 0$.

The single-electron energy bands of the model can be easily obtained. There are $(d+1)$ bands with dispersion relations

$$\varepsilon_j(k) = \begin{cases} -2d(t+s) - 2s\sum_{\mu=1}^{d} \cos k_\mu & \text{if } j = 1; \\ \lambda^2(t+s) - 2dt & \text{if } j = 2, \cdots, d; \\ \lambda^2(t+s) + 2t\sum_{\mu=1}^{d} \cos k_\mu & \text{if } j = d+1. \end{cases} \tag{6·18}$$

If $d > 1$, the middle bands with $j = 2, \cdots, d$ have constant values (i.e., are flat and degenerate), reflecting the geometry of the decorated hypercubic lattice.**) For us it is crucial that the most important lowest band has a healthy non-constant dispersion.

*) The term with the Kronecker delta is included only to make the expression (6·17) simpler and is not essential.

**) It is possible to design short range perturbations to T which make these bands non-flat and non-degenerate, while allowing Theorem 6.3 to hold.

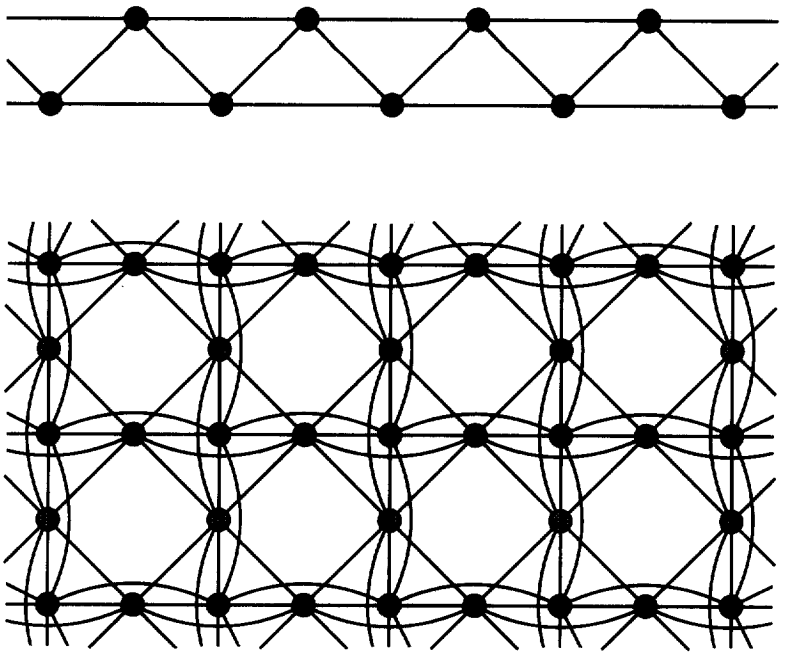

Fig. 12. The d-dimensional decorated hypercubic lattice with the nearest-neighbor and the next-nearest-neighbor hoppings for $d = 1$ and 2. These models is obtained by adding special perturbations to the models (a) and (b) in Fig. 9, respectively. In a range of parameters, we can prove that the corresponding Hubbard model with sufficiently large but finite U exhibits ferromagnetism even when the lowest band is not flat.

We consider the Hubbard model on Λ with the above $t_{x,y}$ and electron number $N_e = |\mathcal{E}| = L^d$. If $s = 0$, the model exhibits the flat-band ferromagnetism of Theorem 6.1 for any $U > 0$. When $s > 0$ and the lowest band is no longer flat, the model exhibits Pauli paramagnetism for $U = 0$. Moreover, from the elementary variational estimate of Theorem 3.2, we find that the model does not exhibit ferromagnetism when $U < 4ds$. We can say that there is a true "competition" between H_{hop} and H_{int} in this model. If the model exhibits ferromagnetism, it must be in a non-perturbative region with sufficiently large U. The following theorem establishes such a non-perturbative statement in the case that the lowest band is sufficiently flat.

Theorem 6.3 (Ferromagnetism in non-singular Hubbard models) *Consider the above Hubbard model with electron number $N_e = |\mathcal{E}| = L^d$, and let*[*)] *$\lambda > 0$. If s/t is sufficiently small, and U/t is sufficiently large, the ground states have total spin $S_{\text{tot}} = S_{\max}(= N_e/2)$, and are non-degenerate apart from the trivial $(2S_{\max} + 1)$-fold degeneracy.*

*) In Ref. 18), we presented a complete proof for $d = 1$ which, however, assumed $\lambda > \lambda_c > 0$. The improved proof in Ref. 19) applies to general d and only requires $\lambda > 0$.

For given $d \geq 1$ and $\lambda > 0$, the range of s/t and U/t in which the theorem holds can be determined by finite calculations which can be (in principle) executed by a computer. This means that one can construct a computer-aided proof if one desires. We have only performed very elementary calculations for $d = 1$ with a personal computer. When we set $\lambda = \sqrt{2}$ (in which case $t_{x,x} = 0$ for all x), the theorem is valid, for example,*) if $s/t \leq 0.4$ and $U/t \geq 40$.

Although the model is rather artificial, this is the first rigorous example of saturated ferromagnetism in a non-singular Hubbard model in which we must deal with the competition between H_{int} and H_{hop}. If we further have $s/t \ll 1$, $U/t \gg 1$ and $\lambda \gg 1$, it has also been proved that low-lying excitation above the ground state has a normal dispersion relation of spin-wave excitations.[18),17)] Starting from a Hubbard model of itinerant electrons, the existence of a "healthy" ferromagnetism has been established rigorously.

Recently, Penc, Shiba, Mila and Tsukagoshi[50)] made a systematic study of related one-dimensional Hubbard models and found various pieces of evidence suggesting that the ferromagnetism in these models is indeed robust.

§7. Possible experimental realizations of (nearly-)flat-band ferromagnetism

7.1. *Ferromagnetism in* $La_4Ba_2Cu_2O_{10}$

In 1990 (when the only example of saturated ferromagnetism in the Hubbard model was that of Nagaoka), Mizuno, Masuda, Hirabayashi, Tanaka, Hasegawa and Mizutani[51),52)] reported that the tetragonal cuprate $La_4Ba_2Cu_2O_{10}$ (also called La_2BaCuO_5), which we shall abbreviate as La422, exhibits ferromagnetism.**) A series of experiments[51)-53)] has revealed that La422 is an ideal insulating ferromagnet with Curie temperature 5.2 K, where most of the magnetic moment comes from the spin 1/2 moments of the Cu^{2+} ions.

The origin of the ferromagnetic coupling between Cu-ions within the ab-plane of La422 is expected to be described by the GKA rules,[52),54)] which involve exchange interactions between excited orbital states and ground orbital states. Ferromagnetic coupling along the c-axis seems to require more careful treatment. Along the c-axis, La422 forms a characteristic chain structure consisting of Cu, O and La. This is shown in Fig. 13. Interestingly enough, we see La and O forming a triangular structure similar to those in the (nearly-)flat-band models of §6. We stress that there are experimental results which strongly indicate that the existence of La is essential for the occurrence of ferromagnetism. One such result is the observation that the cuprate Nd_2BaCuO_5, which has the same crystal structure as La422, exhibits antiferromagnetic ordering.[55),56)] It is pointed out that the essential difference is

*) For sufficiently large U, the theorem is valid for $t = 1.6s$, in which case the lower band occupies more than 1/4 of the whole range of the single-electron energy spectrum (including the gap). In this case the lower band may not even be "nearly-flat".

**) Ferromagnetism was discovered while investigating the superconductor $LaBa_2Cu_3O_{7-y}$.

that Nd has a magnetic moment, while La does not. This point is supported by the result[57] that ferromagnetism remains stable upon partial replacement of La in La422 by Eu, which has no magnetic moment. Another such result is from NMR measurement in La422 that there is a large hyperfine field at La sites.[58] This suggests that the magnetic moments are not sharply localized at Cu-sites, but partially exist on La-sites as well (exactly as in the (nearly-)flat-band models).

On the other hand, a band calculation based on the Local Density Approximation (LDA)[59] revealed that two bands of La422 near the fermi level are almost flat.*)

These observations about the lattice structure and the band structure may be regarded as clues that the ferromagnetism in La422 is related to the ferromagnetism in the Hubbard model with (nearly-)flat-band. As far as the present author knows, this possible relation was first realized by Hirabayashi.[60]

In fact it is not hard to construct a flat-band Hubbard model on the lattice of Fig. 13 where hopping amplitudes are nonvanishing only on the bonds in the figure. We can prove that the model exhibits ferromagnetism when the number of electrons is identical to the number of Cu-sites in the lattice.

This theoretical result, however, seems to be almost irrelevant to the ferromagnetism in La422. Analysis of the orbital structures of La422[54] suggests that a simplified **) but reasonable tight-binding description of the system is given by the lattice structure of Fig. 13 with one non-degenerate orbit per each site, and with the electron number equal to the number of Cu-sites plus the twice the number of O-sites. (In other words, originally Cu orbits are singly occupied, O orbits are doubly occupied, and La orbits are empty.) Then the resulting ferromagnetism is expected to be a "partial ferromagnetism" in which only spins from Cu-sites align ferromagnetically. Unfortunately, we still do not know how to treat such partial ferromagnetism theoretically.

Nevertheless we believe that there is a deep relation between the ferromagnetism

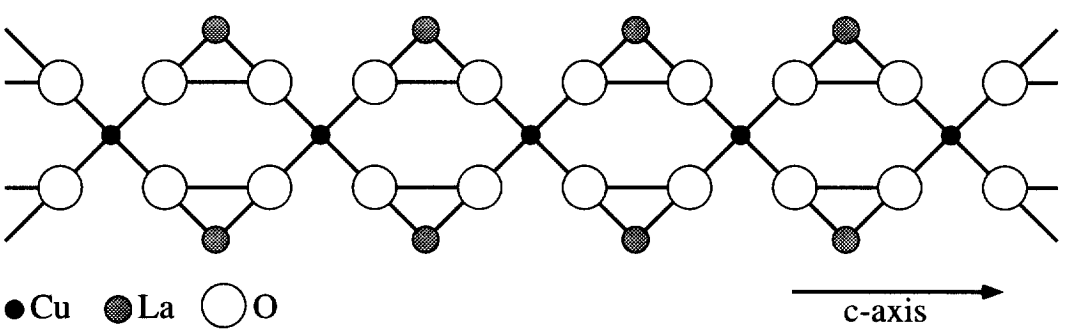

Fig. 13. A chain of Cu, O and La formed along the c-axis of La422. One finds a triangular structure formed by La and O, which reminds us of the (nearly-)flat-band models of §6.

*) In LDA calculations, the Coulomb interaction between electrons is supposed to be taken into account in a certain self-consistent manner. Therefore the flatness of two bands in the LDA calculation does not directly indicate that the corresponding tight-binding model has a flat band.

**) This model is a slight simplification of the tight-binding model discussed in Ref. 54).

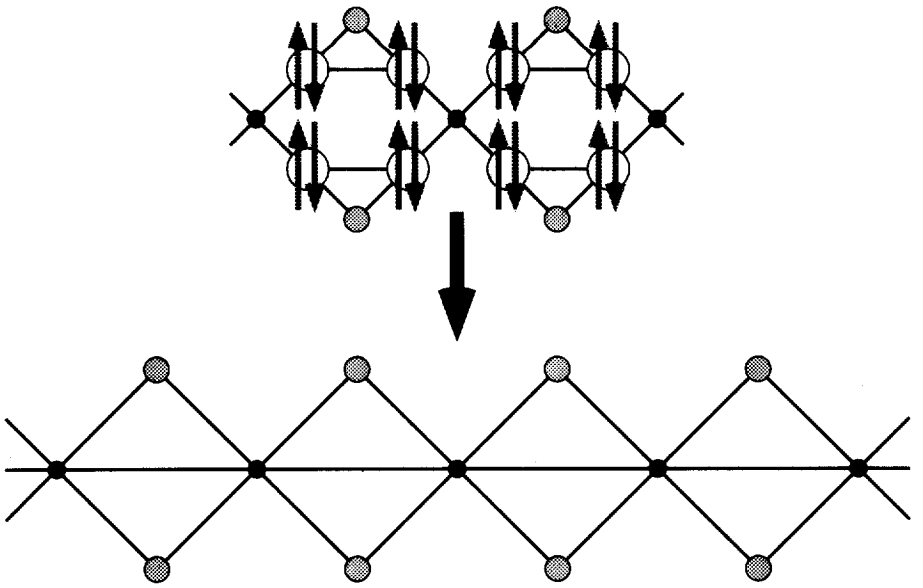

Fig. 14. In the second order perturbation in $1/\epsilon_O$, the model of Fig. 13 reduces to a Hubbard model on the Cu-La chain in the figure with the electron number equal to the number of the Cu-sites. The new model falls into the class of (nearly-)flat-band ferromagnetism for suitable hopping amplitudes. This observation provides a crude link between the ferromagnetism in La422 and the (nearly-)flat-band ferromagnetism.

in La422 and that in Hubbard models with (nearly-)flat-bands. It is a challenging problem to further investigate this relation both from the above described tight-binding model*) and from a continuum model.

If one wishes to see a more direct connection between the ferromagnetism in La422 and the (nearly-)flat-band ferromagnetism, one may try reducing the above Hubbard model to a simpler one by relying on some approximate argument. For example, one can consider the limit in which the on-site potential ϵ_O for O-sites (which is $t_{x,x}$, with x being an O-site) is negative, and its absolute value is much larger than other $|t_{x,y}|$. In this limit, all the O-sites are doubly occupied, and electrons (including those on Cu- and La-sites) cannot move on the lattice. If we consider a perturbation expansion in $1/\epsilon_O$ up to second order, there arise effective hoppings between Cu-sites and La-sites, and between nearby Cu-sites. The model then reduces to an effective model with Cu-sites and La-sites, as in Fig. 14, with the electron number equal to the number of the Cu-sites. For suitable values of hopping amplitudes, the model falls into the class of (nearly-)flat-band ferromagnetism of §6. This observation provides a crude link between the ferromagnetism in La422 and the (nearly-)flat-band ferromagnetism.

*) Apart from numerical experiments (which are always possible), systematic perturbative calculations of "effective Hamiltonian" along the line of Refs. 50) and 54) are also possible and may be enlightening.

7.2. *Possible ferromagnetism in quantum wires*

Recent developments in nanotechnology are making it possible to design various atomic scale structures which should show nontrivial quantum behavior. In Ref. 61), Watanabe, Ichimura, Onogi, Ono, Hashizume, and Wada made a theoretical study of the electronic properties of Ga adsorbates around dangling-bond wires on an H-terminated Si surface, and pointed out the possibility of ferromagnetism. The effective tight-binding model (which is not quite faithful to the actual lattice structure) used in Ref. 61) has the lattice and hopping structure shown in Fig. 15 and has electron number*) $N_e = N_s/3$.

It is possible to construct Hubbard models with exactly the same hopping structure so that the models have flat lowest bands.[62] Let the lattice be $\Lambda = \{1, 2, \ldots, N_s\}$, where N_s is a multiple of three, and impose periodic boundary conditions. The Hamiltonian is then

$$\begin{aligned} H = & t \sum_{j=1}^{N_s/3} \sum_{\sigma=\uparrow,\downarrow} (\lambda c_{3j-1,\sigma} + c_{3j-2,\sigma} + c_{3j,\sigma})^\dagger (\lambda c_{3j-1,\sigma} + c_{3j-2,\sigma} + c_{3j,\sigma}) \\ & + s \sum_{j=1}^{N_s/3} \sum_{\sigma=\uparrow,\downarrow} (c_{3j,\sigma} + c_{3j+1,\sigma})^\dagger (c_{3j,\sigma} + c_{3j+1,\sigma}) \\ & + U \sum_{j=1}^{N_s/3} (n_{3j-2,\uparrow} n_{3j-2,\downarrow} + n_{3j,\uparrow} n_{3j,\downarrow}) + U' \sum_{j=1}^{N_s/3} n_{3j-1,\uparrow} n_{3j-1,\downarrow}, \end{aligned} \tag{7·1}$$

with $t, s, U, U' > 0$ and $\lambda \neq 0$. This model has a flat lowest band with energy 0. For electron number $N_e = N_s/3$, one can prove that the model exhibits ferromagnetism.[62] Since the discussion about the robustness of the flat-band ferromagnetism applies to the present models as well, the present ferromagnetism is also expected to be stable against perturbations.

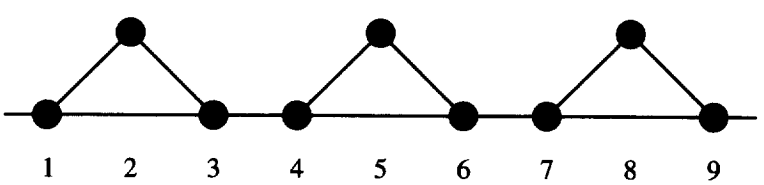

Fig. 15. The effective tight-binding model for the "quantum wire." It is possible to design Hubbard model with the same structure which shows flat-band ferromagnetism.[62]

*) To be precise, 5/6-filling with $N_e = 5N_s/3$ was considered in Ref. 61). This electron number is changed into $N_e = N_s/3$ by using the hole-particle transformation. (See Appendix B.) One should note that the hole-particle transformation does not only change the signs of the hopping amplitudes, but it also introduces a difference in on-site potentials when $U \neq U'$ in the Hamiltonian (7·1).

§8. Towards metallic ferromagnetism

8.1. *Conjectures and some evidence*

Metallic ferromagnetism is a fascinating phenomenon in which electrons exhibiting ferromagnetism contribute to electric conductivity as well. Whether such simple models as the single-orbital Hubbard model can describe metallic ferromagnetism is an unsolved and intriguing problem.

Nagaoka's ferromagnetism is certainly motivated by metallic ferromagnetism, and we believe it reveals some important aspects of a possible mechanism of metallic ferromagnetism. But for the models where the theorem is proved, the only dynamical freedom comes form the motion of the single "hole." We cannot expect the single hole to contribute to appreciable electric current in a bulk system.

In the flat-band models of §6.1 and the related nearly-flat band models of §6.6, 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.

In the flat-band models of §6.2 defined in dimensions greater than one, the existence of ferromagnetism is proved[7),8)] for (not too small) electron numbers less than $|\mathcal{E}|$. There is a similar rigorous result for Mielke's model in two dimensions.[15)] We expect the models to describe a kind of metallic ferromagnetism, but the situation is not clear because of pathological degeneracy in the (many-body) ground states. In any case, the flat-band models, which are quite useful in describing the origin of exchange interaction in certain systems, are too singular to discuss electric conductivity.

Promising candidates of simple models exhibiting metallic ferromagnetism are the nearly-flat-band models (obtained by adding perturbations to the flat-band models) at filling factor $\nu = N_e/(2N_s)$ different from $\nu_0 = |\mathcal{E}|/(2N_s)$. For the case $\nu < \nu_0$, the approximate projection method (similar to those described in Refs. 8) and 17), but based on a local Wannier basis) indicates that the low energy effective theory of these models is represented by the ferromagnetic t-J models in any dimension.[19)] (The definition of the ferromagnetic t-J model can be found in §8.2.) This observation leads us to the conjecture that these models exhibit metallic ferromagnetism at least when $\nu < \nu_0$ is not too small and the model is sufficiently close to a flat-band model.

Penc, Shiba, Mila and Tsukagoshi[50)] made a detailed study of related problems in one dimension, and found both theoretical and numerical evidences that the model exhibits metallic ferromagnetism for arbitrary filling factor within the range $0 < \nu < \nu_0 = 1/4$. That the ferromagnetism is stable for an arbitrarily small density reflects the special character of one-dimensional systems as noted in §3.3. Sakamoto and Kubo[63)] also found strong numerical evidence that related one-dimensional models exhibit metallic ferromagnetism for $0 < \nu < \nu_0$.

Watanabe and Miyashita[64),65)] treated the one-dimensional flat-band Hubbard model of §6.2 for a filling factor ν in the range $1/2 > \nu > \nu_0 = 1/4$. Since the

lower band is totally filled for such electron densities, the flatness of the lower band is regarded as irrelevant. Note that the case with $N_e = N_s - 1$ is nothing but Nagaoka's ferromagnetism; we have come back to Nagaoka's ferromagnetism following a different path! Watanabe and Miyashita found numerical evidence that the model exhibits metallic ferromagnetism for all densities they considered.

A different (but in some sense related) candidate for a model with metallic ferromagnetism is the so-called t-t' model. It is defined on the one-dimensional lattice $\Lambda = \{1, \dots, N_s\}$, and its hopping amplitudes are defined by $t_{x,x+1} = t_{x+1,x} = -t$, $t_{x,x+2} = t_{x+2,x} = t'$ for all $x \in \Lambda$ and $t_{x,y} = 0$ otherwise. From a first order perturbation theory, it was suggested[66),67)] that the model with $U = \infty$ exhibits ferromagnetism if $t' > 0$. By considering a continuum limit theory, Müller-Hartmann[68)] argued that the model exhibits metallic ferromagnetism when $4t' > |t| > 0$, $U = \infty$, and the electron density is sufficiently low. There is numerical evidence that the t-t' model exhibits ferromagnetism.[26),69)]

Kohno[70)] discussed the possibility of metallic ferromagnetism in the Hubbard model on a ladder. Both perturbation theory and numerical calculations suggest that metallic ferromagnetism appears for electron numbers satisfying $N_s/2 < N_e < N_s$. It is interesting that, in this model, itinerant electrons in upper bands play essential roles in generating ferromagnetism.

Unfortunately, none of the above conjectures have yet been confirmed rigorously.*)

8.2. *Ferromagnetic t-J model*

In the present and following sections, we discuss some rigorous results concerning (metallic) ferromagnetism in one-dimensional models with $U \to \infty$ related to the Hubbard model. Thanks to the special nature of one-dimensional models, all the results can be obtained by straightforward applications of the Perron-Frobenius theorem. As far as we know, such an application of the Perron-Frobenius theorem to metallic ferromagnetism in one dimension was developed in the pioneering work of Kubo,[72)] where he studied the double exchange model. Although the results we shall discuss appear to be somewhat similar to the conjectures in the previous section, we still have no idea if they shed light on the truly fascinating problem of metallic ferromagnetism in the Hubbard model.

We first discuss the ferromagnetic t-J model. This is not an interesting model (in one dimension), but helps us in illustrating the basic structure of the proof that we use for other models. Unlike the Hubbard model, this model contains spin-

*) In a fermion system on a finite lattice, a formal perturbation series alway converges because the operators are finite dimensional. Then one might think that the first order perturbation theories of Refs. 66), 67) and 70) imply weak rigorous results that a finite model exhibits ferromagnetism for sufficiently small t'/t (or $t_\parallel/t_\perp$). However, this is not the case since there are no estimates of the energy difference between the ground state and the first excited state, and there remains a possibility that the higher order perturbations change the nature of the ground state for any small values of the expansion parameter. The situation is different from that of Nagaoka's ferromagnetism, where the result for $U = \infty$ automatically implies the same result for sufficiently large U (in a finite system). For an example of rigorous (and general) perturbation theory for quantum many-body systems, see Ref. 71).

spin interactions which explicitly favor ferromagnetism. The problem is whether ferromagnetism is realized in the presence of hopping. As we shall see (and is well-known), the problem is trivial in one dimension.

Consider the one-dimensional lattice $\Lambda = \{1, \ldots, N_s\}$. The Hamiltonian of the ferromagnetic t-J model is

$$H = -t\sum_{x=1}^{N_s}\sum_{\sigma=\uparrow,\downarrow}(c_{x,\sigma}^{\dagger}c_{x+1,\sigma} + \text{h.c.}) - J\sum_{x=1}^{N_s}\left(\hat{\mathbf{S}}_x \cdot \hat{\mathbf{S}}_{x+1} - \frac{n_x n_{x+1}}{4}\right) + U\sum_{x=1}^{N_s} n_{x,\uparrow}n_{x,\downarrow}, \tag{8·1}$$

with $t > 0$, $J > 0$. Here h.c. represents the hermitian conjugate. We let $U \to \infty$ to inhibit double occupancies. We use periodic boundary conditions and identify the site N_s+1 with 1. The spin operator at site x is defined as $\hat{\mathbf{S}}_x = \sum_{\sigma,\tau} c_{x,\sigma}^{\dagger}(p^{(\alpha)})_{\sigma,\tau}\, c_{x,\sigma}$. (See (3·1).)

Theorem 8.1 (Ferromagnetism in the one-dimensional ferromagnetic t-J model) *Assume that the electron number N_e satisfies $N_e \leq N_s$ and is odd.*) Then the ground states of the present t-J model have total spin $S_{tot} = S_{max}(= N_e/2)$, and are non-degenerate apart from the trivial $(2S_{max}+1)$-fold degeneracy.*

Proof: The proof is based on an elementary observation which one may call a rigorous "spin-charge separation" argument. (See Ref. 50) and references therein.) To take into account the $U \to \infty$ limit (with the help of Lemma 4.2), we use as our basis the collection of the states (2·10) with $x_1 < x_2 < \cdots < x_{N_e}$ and $\sigma_j = \uparrow, \downarrow$ such that $S_{tot}^{(3)} = \sum_{j=1}^{N_e}\sigma_j = 1/2$. The theory of angular momenta ensures that any eigenstate of H has its copy in the sector with the lowest $|S_{tot}^{(3)}|$. This sector is spanned by this basis. We first claim that all the matrix elements of H in the present basis are nonpositive. As for the hopping term, this is trivial since there is no exchange in electron ordering and one does not have to worry about fermion signs.**) As for the exchange term, this is easily verified by using the identity $\hat{\mathbf{S}}_x \cdot \hat{\mathbf{S}}_{x+1} = (\hat{S}_x^{+}\hat{S}_{x+1}^{-} + \hat{S}_x^{-}\hat{S}_{x+1}^{+})/2 + \hat{S}_x^{(3)}\hat{S}_{x+1}^{(3)}$. It is also verified that all the basis states are connected via nonvanishing matrix elements of H. Note that the existence of the exchange term is essential for this property. Therefore we can readily apply the Perron-Frobenius theorem (Theorem 4.3) to conclude that the ground state Φ_{GS} is unique (in this sector), and it is a linear combination of all the basis states with positive coefficients.

This fact indeed implies that for Φ_{GS}, $S_{tot} = S_{max}$. To see this, we first note that uniqueness of the ground state implies that Φ_{GS} is an eigenstate of $(\hat{\mathbf{S}}_{tot})^2$. We then take a reference state $\Phi = \left(\hat{S}_{tot}^{-}\right)^{(N_e-1)/2}\left(\prod_{x=1}^{N_e} c_{x,\uparrow}^{\dagger}\right)\Phi_{vac}$, which obviously has $S_{tot}^{(3)} = 1/2$ and $S_{tot} = S_{max}$. Clearly Φ is written as a linear combination of basis

*) We can allow any $N_e \leq N_s$ if we use open boundary conditions. Peculiar dependence of the nature of the ground states on the parity of the electron number and boundary conditions is related to the appearance of spiral states. (See Refs. 72), 73), 50) and 65).)

**) Hops between sites 1 and N_e are exceptional, but these do not produce any signs if N_e is odd. When N_e is even, such hops generate a "wrong" sign for the Perron-Frobenius theorem. This "frustration" can be regarded as the origin of the spiral states.[72),73),50),65)]

states (2·10) with nonnegative coefficients. Thus we see $\langle \Phi, \Phi_{\rm GS} \rangle \neq 0$, which implies that $S_{\rm tot} = S_{\rm max}$ also holds for $\Phi_{\rm GS}$. ■

Once knowing that the ground states have $S_{\rm tot} = S_{\rm max}$, we can look at the ground state with $S^{(3)}_{\rm tot} = S_{\rm max}$. Then it is apparent that the term $(\hat{\mathbf{S}}_x \cdot \hat{\mathbf{S}}_{x+1} - n_x n_{x+1}/4)$ always vanishes, and hence the ground state is identical to that of $H_{\rm hop}$. Then we have the exact expression for the ground state

$$\Phi_{\rm GS} = \left(\prod_{k \text{ s.t. } |k| \le k_{\rm F}} C^\dagger_\uparrow(\eta^{(k)}) \right) \Phi_{\rm vac}, \tag{8·2}$$

where $\eta^{(k)}$ is the plane wave state (2·5), and $k_{\rm F} = \pi(N_{\rm e} - 1)/(2L)$ is the fermi momentum. The ground state allows gapless (charge) excitations, and hence describes a metallic system.

Unfortunately, the above theorem and proof do not shed *any* light on the corresponding problems in higher dimensions, which are much more important and interesting. The proof for the one-dimensional case relies heavily on the fact that essentially no nontrivial spin exchanges take place when $U = \infty$ and $J = 0$. The system suddenly becomes ferromagnetic when we turn on arbitrarily small $J > 0$.

In the corresponding problem in higher dimensional lattices (or even on slightly more complicated one-dimensional lattices, like a ladder), there are highly nontrivial exchange processes even for $J = 0$. There is no guarantee that one gets ferromagnetism when introducing an explicit ferromagnetic interaction, $J > 0$. We of course believe that the ferromagnetic t-J models in higher dimensions also exhibit ferromagnetism for sufficiently large J/t and $\rho = N_{\rm e}/N_{\rm s}$, but we have no idea how one can prove such a statement. Although "proving ferromagnetism in the ferromagnetic t-J models" might sound like a tautology at first glance, it is indeed a very difficult and deep problem, whose solution should shed light on various aspects of strongly interacting itinerant electron systems.

8.3. *Hubbard model with correlated hopping*

In this section, we discuss an artificial model which (like the Hubbard model, and unlike the t-J model) have no interactions explicitly favoring ferromagnetism, but in which we can still prove the appearance of (probably metallic) ferromagnetism in a wide range of parameters and electron density.

Take the one-dimensional lattice $\Lambda = \{1, \dots, N_{\rm s}\}$ with even $N_{\rm s}$, and impose periodic boundary conditions by identifying $N_{\rm s} + x$ with x. We consider the Hamiltonian

$$\begin{aligned} H = & -t \sum_{x=1}^{N_{\rm s}} \sum_{\sigma=\uparrow,\downarrow} (c^\dagger_{x,\sigma} c_{x+1,\sigma} + \text{h.c.}) + t' \sum_{j=1}^{N_{\rm s}/2} \sum_{\sigma=\uparrow,\downarrow} (c^\dagger_{2j,\sigma} c_{2j+2,\sigma} n_{2j+1} + \text{h.c.}) \\ & + U \sum_{x=1}^{N_{\rm s}} n_{x,\uparrow} n_{x,\downarrow}, \end{aligned} \tag{8·3}$$

where we set $t > 0$, $t' > 0$. We will take the $U \to \infty$ limit.

This resembles the Hubbard model with next-nearest-neighbor hopping, but the hopping term with t' has an extra number operator $n_{2j+1} = n_{2j+1,\uparrow} + n_{2j+1,\downarrow}$. Thus a hop between $2j$ and $2j+2$ is possible only when $2j+1$ is occupied by an electron. Note, however, that such density-dependent hopping terms themselves are completely spin-independent, and do not prefer ferromagnetism. Nevertheless we have the following.

Theorem 8.2 (Ferromagnetism in the model with correlated hopping) *Consider the model (8·3) in the limit $U \to \infty$ with any odd electron number N_e. Then the ground states have total spin $S_{tot} = S_{max} (= N_e/2)$, and are non-degenerate apart from the trivial $(2S_{max}+1)$-fold degeneracy.*

Proof: Exactly as in the proof of Theorem 8.1, we take account of the $U \to \infty$ limit by using the basis states (2·10) with $x_1 < x_2 < \cdots < x_{N_e}$ and $\sigma_j = \uparrow, \downarrow$ such that $S_{tot}^{(3)} = \sum_{j=1}^{N_e} \sigma_j = 1/2$. It is again trivial to check that the nearest-neighbor hopping terms in (8·3) have nonpositive matrix elements. By definition, an electron hops between even sites x and $x+2$ only when $x+1$ is occupied. Then, such a hop is always associated with a change of ordering in electrons. (See Fig. 16.) This yields a minus sign, resulting again in nonpositive matrix elements.

It remains to prove that all the basis states (with $S_{tot}^{(3)} = 1/2$) are connected with each other by nonvanishing matrix elements. However, this is already proved in the one hole case in §4.3, and extensions to the multiple holes are trivial. Thus we can apply the Perron-Frobenius theorem exactly as in the proof of Theorem 8.1. ■

We believe that the ferromagnetic ground states of the present model have a metallic character. But this is not as obvious as in the case of the t-J model. The model remains strongly interacting in the sector with $S_{tot}^{(3)} = S_{max}$, and it is not easy to investigate the properties of the ground states.

It is clear that the above theorem extends to much more general models with additional density-density interactions and on-site potential provided that there are nearest-neighbor and next-nearest-neighbor (possibly site-dependent) hoppings with the correct signs. An interesting extension is obtained by replacing the second sum in (8·3) over even sites with a sum over all the sites as

$$H_1 = -t \sum_{x=1}^{N_s} \sum_{\sigma=\uparrow,\downarrow} (c_{x,\sigma}^\dagger c_{x+1,\sigma} + \text{h.c.}) + t' \sum_{x=1}^{N_s} \sum_{\sigma=\uparrow,\downarrow} (c_{x,\sigma}^\dagger c_{x+2,\sigma} n_{x+1} + \text{h.c.}) + U \sum_{x=1}^{N_s} n_{x,\uparrow} n_{x,\downarrow}. \tag{8·4}$$

This defines a translation invariant model which resembles the t-t' model. Of course the same proof as above shows that the model exhibits ferromagnetism for $U = \infty$.

To see the relation between the model (8·4) and the t-t' model, consider the Hamiltonian

$$H_2 = H_1 + t'' \sum_{x=1}^{N_s} \sum_{\sigma=\uparrow,\downarrow} \{c_{x,\sigma}^\dagger c_{x+2,\sigma} (1 - n_{x+1}) + \text{h.c.}\}. \tag{8·5}$$

When $t'' = t'$, this becomes the Hamiltonian of the t-t' model, while it defines a controllable model (8·4) when $t'' = 0$. One finds that the t''-term in (8·5) (along

with other terms) generates an antiferromagnetic interaction. Therefore in order to control the possible ferromagnetism in the t-t' model, one has to deal with the competition between the t'-term and the t''-term in (8·5), which seems to be a nontrivial task.*)

8.4. *Limiting U-V model*

We consider another toy model (which perhaps is slightly less artificial than the one in the previous section) obtained by adding a strong nearest-neighbor repulsion to the Hubbard model. Again we can prove the existence of (metallic) ferromagnetism easily.

Take the one-dimensional lattice $\Lambda = \{1, \dots, N_s\}$ with even N_s, and impose periodic boundary conditions. We consider a model with electron number N_e in the range $N_s > N_e > N_s/2$, and with the Hamiltonian

$$H = -t \sum_{x=1}^{N_s} \sum_{\sigma=\uparrow,\downarrow} (c_{x,\sigma}^\dagger c_{x+1,\sigma} + \text{h.c.}) + t' \sum_{j=1}^{N_s/2} \sum_{\sigma=\uparrow,\downarrow} (c_{2j,\sigma}^\dagger c_{2j+2,\sigma} + \text{h.c.})$$
$$+U \sum_{x=1}^{N_s} n_{x,\uparrow} n_{x,\downarrow} + V \left\{ \left(\sum_{x=1}^{N_s} n_x n_{x+1} \right) - (2N_e - N_s) \right\}, \tag{8·6}$$

where we require $t > 0$ and $t' > 0$. We will consider the $U, V \to \infty$ limits. The new nearest neighbor repulsion term is normalized so that the minimum energy for this term is zero. Note that the hopping amplitudes in the above model can be gauge transformed**) to satisfy the condition for Nagaoka's theorem.

As in the Hubbard model, none of the terms in (8·6) explicitly favor ferromagnetism. Nevertheless we can prove that they together generate ferromagnetism.

Theorem 8.3 (Ferromagnetism in the limiting U-V model)
Consider the model (8·6) in the limits $U \to \infty$ and $V \to \infty$ with odd N_e such that $N_s > N_e > N_s/2$. Then the ground states have total spin $S_{\text{tot}} = S_{\max} (= N_e/2)$, and are non-degenerate apart from the trivial $(2S_{\max} + 1)$-fold degeneracy.

Proof: We take into account the $V \to \infty$ limit exactly as in Lemma 4.2. Now our basis states are (2·10) with $x_1 < x_2 < \cdots < x_{N_e}$ and $\sigma_j = \uparrow, \downarrow$, where $x_1, \dots, x_{N_e}$ must further satisfy the condition that the nearest-neighbor repulsion term in (8·6) is minimized. When $N_e > N_s/2$, this condition implies that there can be no neighboring holes in the relevant basis states. This guarantees that an electron hops between even sites x and $x+2$ only when $x+1$ is occupied. (See Fig. 16.) The remainder of the proof is the same as that of Theorem 8.2. ■

Again, this result can be extended to various more complicated models.

Note that the nature of the model is quite different for electron numbers $N_e \leq N_s/2$ (in which case we drop $-(2N_e - N_s)$ from the Hamiltonian (8·6)). In the limits $U \to \infty$ and $V \to \infty$, configurations with neighboring electrons are inhibited,

*) One does not face this competition in first order perturbation theory.[66),67)]

**) Take Λ' in Appendix A as the set of even sites.

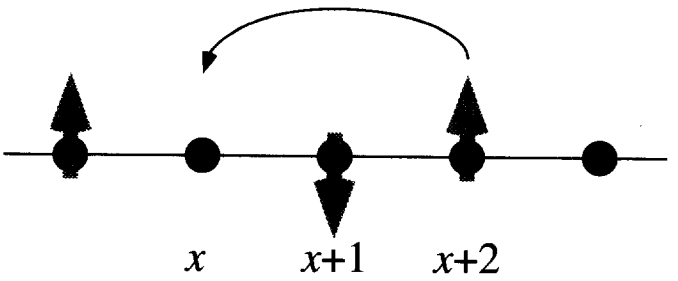

Fig. 16. The essential electron exchange process in the correlated hopping model and the limiting U-V model. In the limiting U-V model with $N_e > N_s/2$, sites $x-1$ and $x+1$ must be occupied when x is empty. Then the ordering of electrons always changes when an electron hops from $x+2$ to x. In the model with correlated hopping, the same fact is guaranteed by the definition.

and hence exchange processes never take place. In this case the model should exhibit paramagnetism. This is consistent with a numerical work[74] where a shift in the ferromagnetic region as a result of finite V is reported for $N_e \leq N_s/2$. We expect that a finite value of V enlarges the region of ferromagnetism for $N_s/2 < N_e < N_s$.

Appendix A
—— *Gauge Transformation* ——

The signs of the hopping amplitude $t_{x,y}$ can be partially changed by means of gauge transformations. Let Λ' be an arbitrary subset of Λ. We define the new operators $\tilde{c}_{x,\sigma}$ by $\tilde{c}_{x,\sigma} = -c_{x,\sigma}$ if $x \in \Lambda'$ and $\tilde{c}_{x,\sigma} = c_{x,\sigma}$ if $x \notin \Lambda'$. Since $\tilde{c}_{x,\sigma}$ also satisfy the canonical anticommutation relations (2·6) and (2·7), we can use these operators to describe the system. Then the hopping Hamiltonian (2·26) is written as

$$H_{\text{hop}} = \sum_{\substack{x,y\in\Lambda \\ \sigma=\uparrow,\downarrow}} t'_{x,y}\tilde{c}^{\dagger}_{x,\sigma}\tilde{c}_{y,\sigma}, \tag{A·1}$$

with $t'_{x,y} = t_{x,y}$ if both x and y are in Λ' or if neither x nor y is in Λ', and $t'_{x,y} = -t_{x,y}$ if exactly one of x and y is in Λ'.

The model is said to be bipartite when there is a subset Λ' with the property that $t_{x,y} = 0$ if both x and y are in Λ' or if neither x nor y is in Λ'. In a bipartite system, we can use the above gauge transformation to change the signs of all the hopping amplitudes. A typical example is the model on the simple cubic lattice with only nearest-neighbor hoppings.

Appendix B
—— *Hole-Particle Transformation* ——

Let us discuss a simple and standard transformation which maps a Hubbard model onto a different Hubbard model with (usually) different electron number.

We define the new operators $\tilde{c}_{x,\sigma}$ by $\tilde{c}_{x,\sigma} = c^{\dagger}_{x,\sigma}$. This simply means that we

switch the creation and the annihilation operators. Since the $\tilde{c}_{x,\sigma}$ also satisfy the canonical anticommutation relations (2·6) and (2·7), we can use these operators to describe the system. From (2·6), the new number operator $\tilde{n}_{x,\sigma} = \tilde{c}^{\dagger}_{x,\sigma}\tilde{c}_{x,\sigma}$ is related to the original number operator by $\tilde{n}_{x,\sigma} = 1 - n_{x,\sigma}$. Therefore the new total electron number $\tilde{N}_{\rm e}$ (which is an eigenvalue of $\sum_{x\in\Lambda,\sigma=\uparrow,\downarrow}\tilde{n}_{x,\sigma}$) is related to the original electron number by $\tilde{N}_{\rm e} = 2N_{\rm s} - N_{\rm e}$.

The hopping Hamiltonian (2·26) is written as

$$H_{\rm hop} = \sum_{\substack{x,y\in\Lambda\\ \sigma=\uparrow,\downarrow}} (-t_{x,y})\tilde{c}^{\dagger}_{x,\sigma}\tilde{c}_{y,\sigma} + 2\sum_{x\in\Lambda} t_{x,x}, \tag{B·1}$$

and the interaction Hamiltonian (2·31) as

$$\begin{aligned} H_{\rm int} &= U\sum_{x\in\Lambda}(1-\tilde{n}_{x,\uparrow})(1-\tilde{n}_{x,\downarrow}) \\ &= U\sum_{x\in\Lambda}\tilde{n}_{x,\uparrow}\tilde{n}_{x,\downarrow} - U\sum_{\substack{x\in\Lambda\\ \sigma=\uparrow,\downarrow}}\tilde{n}_{x,\sigma} + N_{\rm s}U. \end{aligned} \tag{B·2}$$

Note that (B·2) has exactly the same form as the original interaction Hamiltonian (2·31), apart from the constant term and the term proportional to the total electron number, which simply shift the total energy.

Appendix C
—— *Positive Semidefinite Operators* ——

We summarize the definition and elementary properties of positive semidefinite operators (or matrices) which we used in the main body of the paper. They should be well-known to readers with a mathematical background.

Let $\mathcal{H}$ be a finite dimensional Hilbert space with inner product $\langle\cdot,\cdot\rangle$. In the paper, $\mathcal{H}$ may be $\mathcal{H}_{N_{\rm e}}$ or $\mathfrak{h}$.

Definition C.1 (Positive semidefiniteness) *For an operator (or matrix) on $\mathcal{H}$, we write $A \geq 0$ and say A is positive semidefinite if A is self-adjoint (or hermitian) and we have $\langle\Phi, A\Phi\rangle \geq 0$ for any $\Phi \in \mathcal{H}$. For two self-adjoint operators A and B, we write $A \geq B$ if $A - B \geq 0$.*

The following statement is easily proved by diagonalizing A.

Lemma C.2 (Positive semidefiniteness and eigenvalues) *A self-adjoint operator (or a hermitian matrix) A is positive semidefinite if and only if all the eigenvalues of A are nonnegative.*

The following lemma provides a standard way of constructing a positive semidefinite operator.

Lemma C.3 *Let B be an arbitrary operator (or matrix) on $\mathcal{H}$. Then $A = B^{\dagger}B$ is positive semidefinite.*

Proof: Observe that for any Φ, we have $\langle \Phi, B^\dagger B \Phi \rangle = \langle B\Phi, B\Phi \rangle \geq 0$. ■

Conversely, any $A \geq 0$ can be expressed as $A = B^2$ with some $B \geq 0$. This is most easily verified by diagonalizing A.

The following lemma is used repeatedly in the main body of the paper.

Lemma C.4 (The sum of positive semidefinite operators) *If $A \geq 0$ and $B \geq 0$, we have $A + B \geq 0$.*

Proof: Assume that $A + B$ has an eigenstate Φ with a negative eigenvalue. Then we get $0 > \langle \Phi, (A+B)\Phi \rangle = \langle \Phi, A\Phi \rangle + \langle \Phi, B\Phi \rangle \geq 0$, which is a contradiction. ■

The following is trivial if we expand Φ into eigenstates of A.

Lemma C.5 *Let $A \geq 0$. Then $\langle \Phi, A\Phi \rangle = 0$ is equivalent to $A\Phi = 0$.*

The following lemma is also useful.

Lemma C.6 *Let $A_i \geq 0$ for $i = 1, \ldots, n$. Then $\sum_{i=1}^n A_i \Phi = 0$ implies $A_i \Phi = 0$ for each $i = 1, \ldots, n$.*

Proof: Since $\sum_{i=1}^n A_i \Phi = 0$, we have $0 = \langle \Phi, \sum_{i=1}^n A_i \Phi \rangle = \sum_{i=1}^n \langle \Phi, A_i \Phi \rangle$. By noting that $\langle \Phi, A_i \Phi \rangle \geq 0$, this means $\langle \Phi, A_i \Phi \rangle = 0$ for each $i = 1, \ldots, n$. We then use Lemma C.5. ■

We finally state the following lemma, which sometimes provides us with a powerful information.

Lemma C.7 *Assume that $A \geq 0$ is expressed as $A = B^\dagger B$ where B is not necessarily self-adjoint. Then $A\Phi = 0$ implies $B\Phi = 0$.*

Proof: Since $B^\dagger B \Phi = 0$, we have $0 = \langle \Phi, B^\dagger B \Phi \rangle = \langle B\Phi, B\Phi \rangle$ which means $B\Phi = 0$. ■

Appendix D
—— *Explicit Construction of the Hilbert Space and Fermion Operators* ——

In §2.2, we first introduced the algebra of fermion operators, and then defined the Hilbert space by operating (a representation of) the algebra onto a single state Φ_{vac}. There is no problem in making the discussion mathematically rigorous since both the algebra and the Hilbert space are finite dimensional. However, readers familiar with fields like functional analysis might feel more comfortable if the Hilbert space is first defined explicitly and then the operators are defined. Here we explicitly define the Hilbert space and the fermion operators following the standard approach.*)

Let $\tilde{\Lambda} = \Lambda \times \{\uparrow, \downarrow\}$ be the configuration space for a single electron. We denote its elements as**) $u, u_1, u_2, \cdots \in \tilde{\Lambda}$. The Hilbert space for a single electron is $\ell^2(\tilde{\Lambda}; \mathbb{C})$.

*) For more details, see, for example, §5.2 of Ref. 75).

**) Of course $u = (x, \sigma)$ with $x \in \Lambda$ and $\sigma = \uparrow, \downarrow$.

For $n = 0, 1, \ldots, 2N_{\rm s}$, we define the n-electron Hilbert space $\mathcal{H}_n$ by $\mathcal{H}_0 = \mathbb{C}$, and

$$\mathcal{H}_n = P_- \underbrace{\ell^2(\tilde{\Lambda};\mathbb{C}) \otimes \cdots \otimes \ell^2(\tilde{\Lambda};\mathbb{C})}_{n}, \tag{D·1}$$

where P_- is the projection operator onto functions which are antisymmetric under exchanges of any two variables. More precisely, it is defined as

$$P_-\psi(u_1, \ldots, u_n) = \frac{1}{n!} \sum_{p:(1,\ldots,n)\to(p(1),\ldots,p(n))} (-1)^p \psi(u_{p(1)}, \ldots, u_{p(n)}), \tag{D·2}$$

where p is summed over all permutations of $(1, \ldots, n)$, and $(-1)^p$ denotes the parity of p.

We now define the fermion operators. For $\psi \in \mathcal{H}_0$, we let $c_u\psi = 0$. For $\psi \in \mathcal{H}_n$ with $n \geq 1$, we let

$$(c_u\psi)(u_1, \ldots, u_{n-1}) = \sqrt{n}\, \psi(u, u_1, \ldots, u_{n-1}), \tag{D·3}$$

where $c_u\psi \in \mathcal{H}_{n-1}$. On $\psi \in \mathcal{H}_n$ with $n < 2N_{\rm s}$, the adjoint operator $c_u^\dagger$ acts as

$$(c_u^\dagger\psi)(u_1, \ldots, u_{n+1}) = \frac{1}{\sqrt{n+1}} \sum_{j=1}^{n+1} (-1)^{j+1} \delta_{u,u_j} \psi(u_1, \ldots, u_{j-1}, u_{j+1}, \ldots, u_{n+1}), \tag{D·4}$$

where $c_u^\dagger\psi \in \mathcal{H}_{n+1}$. For $\psi \in \mathcal{H}_{2N_{\rm s}}$, we let $c_u^\dagger\psi = 0$.

It is natural to regard the operators $c_u : \mathcal{H}_n \to \mathcal{H}_{n-1}$ and $c_u^\dagger : \mathcal{H}_n \to \mathcal{H}_{n+1}$ as acting on the Fock space

$$\mathcal{F} = \bigoplus_{n=0}^{2N_{\rm s}} \mathcal{H}_n. \tag{D·5}$$

Finally, we take a basis state (say 1) of the Hilbert space $\mathcal{H}_0 = \mathbb{C}$, and identify it with $\Phi_{\rm vac}$. Then it is not difficult to check that states of the form (2·10) form a basis of the Hilbert space $\mathcal{H}_{N_{\rm e}}$.

As examples, let us calculate $f = (c_v^\dagger\Phi_{\rm vac}) \in \mathcal{H}_1$ and $g = (c_w^\dagger f) = (c_w^\dagger c_v^\dagger \Phi_{\rm vac}) \in \mathcal{H}_2$, where we understand that $\Phi_{\rm vac} = 1$. From (D·4), we have $f(u_1) = (c_v^\dagger 1)(u_1) = \delta_{v,u_1}$. Similarly we get

$$\begin{aligned} g(u_1, u_2) &= (c_w^\dagger f)(u_1, u_2) \\ &= \frac{1}{\sqrt{2}} \{\delta_{w,u_1} f(u_2) - \delta_{w,u_2} f(u_1)\} \\ &= \frac{1}{\sqrt{2}} (\delta_{w,u_1}\delta_{v,u_2} - \delta_{w,u_2}\delta_{v,u_1}). \end{aligned} \tag{D·6}$$

Note that g is antisymmetric under the exchange of the names of the two particles. This is a special case of more general states

$$(c_{v_1}^\dagger \cdots c_{v_n}^\dagger \Phi_{\rm vac})(u_1, \ldots, u_n) = \frac{1}{\sqrt{n!}} \begin{vmatrix} \delta_{v_1,u_1} & \delta_{v_2,u_1} & \cdots & \delta_{v_n,u_1} \\ \delta_{v_1,u_2} & \delta_{v_2,u_2} & \cdots & \delta_{v_n,u_2} \\ \vdots & \vdots & \ddots & \vdots \\ \delta_{v_1,u_n} & \delta_{v_2,u_n} & \cdots & \delta_{v_n,u_n} \end{vmatrix}, \tag{D·7}$$

which are known as the Slater determinant states.

Appendix E
—— *Band Structures in Single-Electron Energy Spectra* ——

Here we explain (for readers without background in condensed matter physics) the notion of band structure in a single-electron problem. The readers will find the notion quite elementary,*) especially in a tight-binding model.

We realize the lattice Λ as a subset of the d-dimensional $L \times \cdots \times L$ torus

$$T_L = \left\{ (x_1, \ldots, x_d) \,\middle|\, 0 \le x_j < L \right\} = \mathbb{R}^d/\sim, \tag{E·1}$$

where the identification $\sim$ is defined by $x \sim y \Longleftrightarrow x - y \in L\mathbb{Z}^d$. Here L is a positive integer. Let the unit cell $\mathcal{U} \subset [0,1)^d$ be a set of finite points (sites). The number of sites $|\mathcal{U}|$ in the unit cell will determine the number of bands. Assume that the lattice Λ can be written as

$$\Lambda = \left\{ x + z \,\middle|\, x \in \mathcal{U}, z \in \{0, 1, \ldots, L-1\}^d \right\}. \tag{E·2}$$

We then assume that the hopping matrix $\mathsf{T} = (t_{x,y})_{x,y\in\Lambda}$ has translational invariance**)

$$t_{x,y} = t_{x+z,y+z} \tag{E·3}$$

for any $x, y \in \Lambda$ and $z \in \mathbb{Z}^d$. We note that perfect translational invariance is never possible in real physical systems which always have boundaries.***) We often take artificial periodic boundary conditions because we want to concentrate on universal behavior taking place in the bulk of the system.

We are interested in the eigenvalue problem $\varepsilon\boldsymbol{\varphi} = \mathsf{T}\boldsymbol{\varphi}$ or

$$\varepsilon\varphi_x = \sum_{y\in\Lambda} t_{x,y}\,\varphi_y \tag{E·4}$$

for a single electron. The translational invariance (E·3) suggests that we look for eigenstates in the form

$$\varphi_x = e^{ik\cdot x} v_{u(x)}, \tag{E·5}$$

where $k \in \mathcal{K}$ is a wave vector, $u(x)$ is the unique element in $\mathcal{U}$ such that $x - u(x) \in \mathbb{Z}^d$, and $\mathbf{v} = (v_u)_{u\in\mathcal{U}}$ is a $|\mathcal{U}|$-dimensional vector. The set of wave vectors $\mathcal{K}$ consists of $k = ((2\pi/L)n_1, \ldots, (2\pi/L)n_d)$ with $n_j = 0, \pm 1, \ldots, \pm\{(L/2) - 1\}, L/2$ (where we assume L to be even). By substituting (E·5) into (E·4), we get

$$\varepsilon\, v_u = \sum_{u'\in\mathcal{U}} \tau^{(k)}_{u,u'}\, v_{u'}, \tag{E·6}$$

*) In the band theory of electrons in solids, one usually talks about band structures in an "effective single-electron problem" (defined through complicated self-consistency arguments) in interacting many-electron problems. To explain this theory is beyond the scope of the present article (and the ability of the author).

**) We of course identify $x + z$ and $y + z$ as elements in T_L by using the identification $\sim$ if necessary.

***) The presence of boundaries does not change the band structure drastically, but introduces extra eigenstates which mainly live on the boundaries. Analysis of single-particle eigenstates may not be easy.

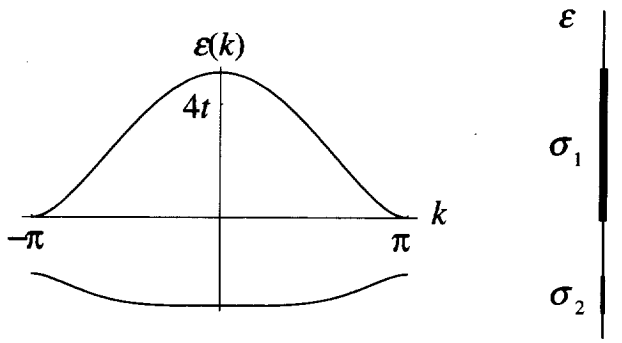

Fig. 17. The dispersion relations and the corresponding band structure of the simple one-dimensional model with next-nearest-neighbor hoppings with $t = t'/2 > 0$ and $V = 0$. The spectrum consists of the two bands separated by a finite band gap.

with

$$\tau^{(k)}_{u,u'} = \sum_{y\in\Lambda \text{ s.t. } u(y)=u'} t_{u,y}\, e^{ik\cdot(y-u)}. \tag{E·7}$$

For each $k \in \mathcal{K}$, (E·6) has $|\mathcal{U}|$ eigenvalues that we denote as $\varepsilon_j(k)$ with $j = 1, \ldots, |\mathcal{U}|$. We can choose $\varepsilon_j(k)$ so that $\varepsilon_j(k)$ is an analytic function of $k \in (-\pi, \pi]^d$ for each j. Consequently, the spectrum of the hopping matrix T is decomposed as

$$\sigma(\mathsf{T}) = \bigcup_{j=1}^{|\mathcal{U}|} \sigma_j(\mathsf{T}), \tag{E·8}$$

with $\sigma_j(\mathsf{T}) = \{\varepsilon_j(k) \,|\, k \in \mathcal{K}\}$. Each $\sigma_j(\mathsf{T})$ is called an *energy band*. The function $\varepsilon_j(k)$ is called the *dispersion relation* of the j-th band.

Let us discuss a simple example with two bands. Let $d = 1$, and take $\mathcal{U} = \{0, 1/2\}$. The resulting lattice is $\Lambda = \{0, 1/2, 1, 3/2, \ldots, L - (1/2)\}$. We define the hopping matrix $\mathsf{T} = (t_{x,y})_{x,y\in\Lambda}$ by $t_{x,y} = t'$ if $|x - y| = 1/2$, $t_{x,y} = t$ if $x, y \in \mathbb{Z}$ and $|x - y| = 1$, $t_{x,x} = V$ if $x + 1/2 \in \mathbb{Z}$, and $t_{x,y} = 0$ otherwise. Then the eigenvalue equation (E·6) becomes

$$\varepsilon \begin{pmatrix} v_0 \\ v_{1/2} \end{pmatrix} = \begin{pmatrix} 2t\cos k & 2t'\cos(k/2) \\ 2t'\cos(k/2) & V \end{pmatrix} \begin{pmatrix} v_0 \\ v_{1/2} \end{pmatrix}. \tag{E·9}$$

The two eigenvalues of (E·9) define two dispersion relations

$$\varepsilon_{1,2}(k) = \frac{1}{2}\left\{V + 2t\cos k \mp \sqrt{(V - 2t\cos k)^2 + (4t'\cos(k/2))^2}\right\}. \tag{E·10}$$

(See Fig. 17.)

Consider special cases where the parameters t' and V can be written as $t' = \lambda t$ and $V = (\lambda^2 - 2)t$ with the parameter $\lambda > 0$. Then (E·10) becomes $\varepsilon_1(k) = -2t$ and $\varepsilon_2(k) = \lambda^2 t + 2t\cos k$. The model becomes the flat-band model*) discussed in §6.3.

*) We recover the dispersion relation at the end of §6.3 if we shift the energy by $2t$.

Appendix F
—— *Proof of Theorem 3.3* ——

We describe estimates required for the proof of Theorem 3.3. Although the calculations are straightforward, they illustrate some standard techniques we encounter in many-fermion problems and may serve as a good exercise for beginners.

First note that the sate Ψ defined in (3·6) satisfies $n_{x,\downarrow}n_{y,\downarrow}\Psi = 0$ for any $x \neq y$ since there is only one $\downarrow$ electron. Then the definition (3·9) of the variational state $\tilde{\Psi}$ simplifies as

$$\tilde{\Psi} = P_0\Psi = (1-\hat{\nu})\Psi, \tag{F·1}$$

with $\hat{\nu} = \sum_{x\in\Lambda} n_{x,\uparrow}n_{x,\downarrow}$. To evaluate the energy expectation value of (3·11), we observe that

$$\left\langle \tilde{\Psi}, \tilde{\Psi} \right\rangle = \langle P_0\Psi, P_0\Psi\rangle = \langle \Psi, P_0\Psi\rangle = 1 - \langle \Psi, \hat{\nu}\Psi\rangle\,, \tag{F·2}$$

and

$$\begin{aligned}\left\langle \tilde{\Psi}, H_{\rm hop}\tilde{\Psi} \right\rangle &= \langle \Psi, (1-\hat{\nu})H_{\rm hop}(1-\hat{\nu})\Psi\rangle \\ &= \langle \Psi, H_{\rm hop}\Psi\rangle - \langle \Psi, \hat{\nu}H_{\rm hop}\Psi\rangle - \langle \Psi, H_{\rm hop}\hat{\nu}\Psi\rangle + \langle \Psi, \hat{\nu}H_{\rm hop}\hat{\nu}\Psi\rangle \\ &= E_\Psi(1 - 2\langle \Psi, \hat{\nu}\Psi\rangle) + \langle \Psi, \hat{\nu}H_{\rm hop}\hat{\nu}\Psi\rangle\,, \end{aligned} \tag{F·3}$$

where we used $H_{\rm hop}\Psi = E_\Psi\Psi$ and $\langle \Psi, \Psi\rangle = 1$. Thus we need to estimate the quantities $\langle \Psi, \hat{\nu}\Psi\rangle$ and $\langle \Psi, \hat{\nu}H_{\rm hop}\hat{\nu}\Psi\rangle$.

The best way to evaluate these quantities is to go into a Fourier representation and express everything in terms of the $a_{j,\sigma}$ operators of (2·27). By using the completeness relation $\sum_{j=1}^{N_s}(\psi_{x'}^{(j)})^*\psi_x^{(j)} = \delta_{x,x'}$, we find the inverse of (2·27) is

$$c_{x,\sigma} = \sum_{j=1}^{N_s} \psi_x^{(j)} a_{j,\sigma}. \tag{F·4}$$

This leads us to the representations

$$\hat{\nu} = \sum_{p,q,r,s=1}^{N_s} V_{p,q,r,s} a_{p,\uparrow}^\dagger a_{q,\uparrow} a_{r,\downarrow}^\dagger a_{s,\downarrow}, \tag{F·5}$$

with

$$V_{p,q,r,s} = \sum_{x\in\Lambda} (\psi_x^{(p)})^* \psi_x^{(q)} (\psi_x^{(r)})^* \psi_x^{(s)}, \tag{F·6}$$

and

$$H_{\rm hop} = \sum_{j=1}^{N_s} \sum_{\sigma=\uparrow,\downarrow} \varepsilon_j\, a_{j,\sigma}^\dagger a_{j,\sigma}. \tag{F·7}$$

All we have to do now is to substitute (F·5) and (F·7) into the desired quantities, and use the anticommutation relations $\{a_{j,\sigma}, a_{k,\tau}\} = 0$, $\{a_{j,\sigma}^\dagger, a_{k,\tau}\} = \delta_{j,k}\delta_{\sigma,\tau}$, the definition (3·6) of Ψ, and the fact that $a_{j,\sigma}\Phi_{\rm vac} = 0$. Then we obtain

$$\langle \Psi, \hat{\nu}\Psi\rangle = \sum_{p=1}^{N_e-1} V_{p,p,1,1}$$

$$= \sum_{x\in\Lambda} \left(|\psi_x^{(1)}|^2 \sum_{p=1}^{N_e-1} |\psi_x^{(p)}|^2 \right), \tag{F·8}$$

$$\left\langle \Psi, \hat{\nu} H_{\rm hop}^{\uparrow} \hat{\nu}\Psi \right\rangle = \left(\sum_{j=1}^{N_e-1} \varepsilon_j \right) \langle \Psi, \hat{\nu}\Psi \rangle - \sum_{x\in\Lambda} \left(|\psi_x^{(1)}|^2 \sum_{p=1}^{N_e-1} \varepsilon_p |\psi_x^{(p)}|^2 \right) + \sum_{x\in\Lambda} \left(t_{x,x} |\psi_x^{(1)}|^2 \sum_{p=1}^{N_e-1} |\psi_x^{(p)}|^2 \right), \tag{F·9}$$

and

$$\begin{aligned} \left\langle \Psi, \hat{\nu} H_{\rm hop}^{\downarrow} \hat{\nu}\Psi \right\rangle &= \sum_{x,y\in\Lambda} \left\{ t_{x,y} \left(\sum_{p=1}^{N_e-1} |\psi_x^{(p)}|^2 \right) \left(\sum_{q=1}^{N_e-1} |\psi_y^{(q)}|^2 \right) (\psi_x^{(1)})^* \psi_y^{(1)} \right\} \\ &\quad + \sum_{x,y\in\Lambda} \left\{ t_{x,y} \left(\sum_{p=1}^{N_e-1} (\psi_x^{(p)})^* \psi_y^{(p)} \right) \left(\sum_{q=N_e}^{N_s} \psi_x^{(q)} (\psi_y^{(q)})^* \right) (\psi_x^{(1)})^* \psi_y^{(1)} \right\} \\ &= \sum_{x\in\Lambda} \left\{ t_{x,x} \left(\sum_{p=1}^{N_e-1} |\psi_x^{(p)}|^2 \right) |\psi_x^{(1)}|^2 \right\} + R, \end{aligned} \tag{F·10}$$

with

$$\begin{aligned} R = &\sum_{\substack{x,y\in\Lambda \\ \text{s.t. } x\neq y}} \left\{ t_{x,y} \left(\sum_{p=1}^{N_e-1} |\psi_x^{(p)}|^2 \right) \left(\sum_{q=1}^{N_e-1} |\psi_y^{(q)}|^2 \right) (\psi_x^{(1)})^* \psi_y^{(1)} \right\} \\ &- \sum_{\substack{x,y\in\Lambda \\ \text{s.t. } x\neq y}} \left\{ t_{x,y} \left(\sum_{p=1}^{N_e-1} (\psi_x^{(p)})^* \psi_y^{(p)} \right) \left(\sum_{q=1}^{N_e-1} \psi_x^{(q)} (\psi_y^{(q)})^* \right) (\psi_x^{(1)})^* \psi_y^{(1)} \right\}, \end{aligned} \tag{F·11}$$

where we have used the fact that $\sum_{p=1}^{N_s} \varepsilon_p (\psi_x^{(p)})^* \psi_y^{(p)} = t_{x,y}$ and $\sum_{p=1}^{N_s} (\psi_x^{(p)})^* \psi_y^{(p)} = \delta_{x,y}$. We also made the obvious decomposition $H_{\rm hop} = H_{\rm hop}^{\uparrow} + H_{\rm hop}^{\downarrow}$.

By collecting all the estimates, we get

$$\begin{aligned} \Delta E &= \frac{\left\langle \tilde{\Psi}, H_{\rm hop} \tilde{\Psi} \right\rangle}{\left\langle \tilde{\Psi}, \tilde{\Psi} \right\rangle} - E_{\rm ferro} \\ &= \varepsilon_1 - \varepsilon_{N_e} + \frac{2(\bar{t} - \varepsilon_1) \langle \Psi, \hat{\nu}\Psi \rangle}{1 - \langle \Psi, \hat{\nu}\Psi \rangle} + \frac{R}{1 - \langle \Psi, \hat{\nu}\Psi \rangle}, \end{aligned} \tag{F·12}$$

with

$$\bar{t} = \frac{\sum_{x\in\Lambda} \left(t_{x,x} |\psi_x^{(1)}|^2 \sum_{p=1}^{N_e-1} |\psi_x^{(p)}|^2 \right)}{\sum_{x\in\Lambda} \left(|\psi_x^{(1)}|^2 \sum_{p=1}^{N_e-1} |\psi_x^{(p)}|^2 \right)} \le \max_{x\in\Lambda} t_{x,x}. \tag{F·13}$$

To proceed further, we assume that there is a constant $\alpha > 0$ independent of x, N_s and $p = 1, \ldots, N_s$, and we have*)

$$|\psi_x^{(p)}| \leq \frac{\alpha}{\sqrt{N_s}}. \tag{F·14}$$

Note that if the model possesses translational invariance as in Appendix E, then the bound is true with $\alpha = \sqrt{|U|}$. We also assume that $\max_{x\in\Lambda} t_{x,x}$, $\max_{x\in\Lambda} \sum_{y\in\Lambda} |t_{x,y}|$, and ε_1 converge to finite quantities as $N_s \to \infty$, which is again trivially valid in translation invariant models. With the requirement (F·14), we obtain $|R| \leq \text{const}\, \rho^2$, which means that R gives only negligible contributions for small ρ. Since we also find $\langle \Psi, \hat{\nu}\Psi \rangle \propto \rho$, the bound (F·12) implies the desired estimate (3·11).

It is a pleasure to thank Izumi Hirabayashi and Koichi Kusakabe for valuable discussions related to the material in §7.1, and Shun-Qing Shen for valuable discussions about the t-t' model. I also thank Fumihiko Nakano and Yuuki Watanabe for various useful comments on the manuscript.

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