Ferromagnetism in the Hubbard Model

– Examples from Models with Degenerate Single-Electron Ground States

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Whether spin-independent Coulomb interaction can be the origin of a realistic ferromagnetism in an itinerant electron system has been an open problem for a long time. Here we study a class of Hubbard models on decorated lattices, which have a special property that the corresponding single-electron Schrödinger equation has N_{d}-fold degenerate ground states. The degeneracy N_{d} is proportional to the total number of sites $|\Lambda|$. We prove that the ground states of the models exhibit ferromagnetism when the electron filling factor is not more than and sufficiently close to $\rho_0 = N_{\mathrm{d}}/(2\,|\Lambda|)$, and paramagnetism when the filling factor is sufficiently small. An important feature of the present work is that it provides examples of three dimensional itinerant electron systems which are proved to exhibit ferromagnetism in a finite range of the electron filling factor. (To appear in Commun. Math. Phys.)

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1 Introduction

1.1 Ferromagnetism in the Hubbard model

In some solids, electronic spins spontaneously align with each other to form strong ferromagnetic ordering. A familiar example is Fe, which maintains long range magnetic order up to the Curie temperature, 1043K. Given the fact that interactions between electrons in a solid are almost spin-independent, the existence of such a strong order may sound as a mystery. As we shall describe below, this has indeed been an interesting open problem in theoretical physics for quite a long time.

In 1928, Heisenberg [8] pointed out that the spin-independent Coulomb interaction between electrons, when combined with the Pauli exclusion principle, can generate effective interaction between electron spins. Heisenberg's picture of ferromagnetism was that the relevant electrons are mostly localized at atomic sites, and their spin degrees of freedom interact with each other via "exchange interaction". It has been realized, however, that his exchange interaction usually has the sign which leads to antiferromagnetic interaction rather than ferromagnetic one. (See [9] for a review.) Nevertheless, Heisenberg's idea still plays a fundamental role in modern theories of ferromagnetism.

A somewhat different approach to ferromagnetism, which was originated by Bloch [2], is to look for a mechanism of ferromagnetism in which the itinerant nature of electrons, as well as the Coulomb interaction and Pauli principle, play fundamental roles. This project, combined with sophisticated band-theoretic techniques, has led to many approximate theories [10]. A common feature of all these theories is that they are based on the Hartree-Fock approximation (*i.e.*, mean field theory) and its perturbative corrections. Although such approximations can lead to reasonable conclusions in some situations, they have serious disadvantage from a theoretical point of view. The basic strategy of the approximations is to treat electrons with up and down spins as different species of particles, and then introduce some self-consistency conditions. By doing this, one severely destroys the original $SU(2)$ invariance of the model and gets Z_2 invariant self-consistent equations. The existence of ferromagnetism then reduces to a problem of spontaneous breakdown of the discrete Z_2 symmetry, which is essentially different from the original problem, a spontaneous breakdown of the continuous $SU(2)$ symmetry. As a consequence, the approximate theories give only two ferromagnetic states with the net magnetization pointing up or down, instead of expected infinitely many states with an arbitrary direction of magnetization. Since a continuous symmetry breaking is a very subtle phenomenon in general, results based on the Hartree-Fock approximation and its improvements are not conclusive enough to answer the fundamental question whether spin-independent Coulomb interaction alone can be the origin of a realistic ferromagnetism in an itinerant electron system. We stress that such a critical point of view has been held by many physicists. See, for example, the review of Herring [10].

Given the subtlety of the problem, it is desirable to have idealized models in which one can develop concrete scenarios for the itinerant electron ferromagnetism. The so called Hubbard model [11, 13] is a simple but nontrivial model suitable for developing such scenarios. There has been a considerable amount of heuristic works (mostly based on the Hartree-Fock approximation and its improvements) devoted to theories of ferromagnetism in the Hubbard model. Since the literature is too large to catalogue here, we only refer to the pioneering work of Kanamori [13] and a review by Herring [10]. The Hartree-Fock approximation applied to the Hubbard model yields the so called Stoner criterion for ferromagnetism [10, 11, 13]. It says that ferromagnetism occurs if $D_{\mathrm{F}}U > 1$, where D_{F} is the single particle-density of states at the fermi level and U is the strength of the Coulomb repulsion. Although this is certainly not true in general, large values of D_{F} and/or U determine the region in parameter space where one may find ferromagnetism.

In 1965, the first rigorous example of ferromagnetism in the Hubbard model was given by Nagaoka [24], and independently by Thouless [31, 17]. It was proved that certain Hubbard models have ground states with saturated magnetization when there is exactly one hole and the Coulomb repulsion is infinite. Recently, it was pointed out that the theorem extends to a general class of models which satisfy a certain connectivity condition [29]. Whether the Nagaoka-Thouless ferromagnetism survives in the models with finite density of holes and/or finite Coulomb repulsion is a very interesting but totally unsolved problem [4, 25, 27, 28, 32].

In 1989, Lieb proved an important theorem on general properties of the ground states of the Hubbard model [18]. As a consequence of the theorem, he showed that a class of Hubbard models on asymmetric bipartite lattices with finite Coulomb interaction have ferromagnetic ground states at half filling. It is sometimes argued that Lieb's examples represent ferrimagnetism (*i.e.*, antiferromagnetism on a bipartite lattice in which the number of the sites in two sublattices are different) rather than ferromagnetism. Although this might be true when the Coulomb repulsion is sufficiently large and the dimension is high enough, we believe mechanisms underlying his examples are much richer in general situations.

A more recent example is due to Mielke, who studied Hubbard models on general line graphs [20, 21]. A special feature of his models is that the single-electron Schrödinger equation corresponding to the Hubbard model has highly degenerate ground states. He proved that these models with nonvanishing Coulomb interaction have ground states with saturated magnetization when the electron number is exactly equal to the dimension of degeneracy of the single-electron ground states. Mielke also extended his results to a finite range of electron filling factor in certain two dimensional models [22]. See [23] for the recent results for a more general class of models.

The latest example is due to Tasaki [30], who proved the existence of ferromagnetism in a class of Hubbard models with nonvanishing Coulomb interaction on decorated lattices. As in the Mielke's models, the class of models have highly degenerate ground states in the corresponding single-electron Schrödinger equation. It was proved that the ground states of the Hubbard model exhibit ferromagnetism in a finite range of electron filling factor. The proof made use of a basis of the single-electron ground states which satisfy certain locality and (reflection) positivity conditions, and a percolation representation for physical quantities. This work covered models in three dimensions as well.

A common feature in the examples of Lieb, Mielke, and Tasaki is that each model has a completely degenerate band in the corresponding single-electron spectrum, and the ferromagnetism (in interacting many electron problem) is proved when the degenerate band is exactly or nearly half-filled. This situation, where D_{F} is infinite, is, in view of the Stoner criterion, in some sense dual to the forementioned theorem of Nagaoka where U is infinite. Possibility of ferromagnetism in systems with a degenerate single-electron band has been discussed for a long time since the pioneering work of Slater, Statz and Koster [26] in 1953. But general consensus on whether ferromagnetism appears or not has been lacking. See Section VIII.2 of [10].

1.2 Purpose of the present paper

The purpose of the present paper is to give further discussions on the ferromagnetism studied in [30]. We do not only present all the detailed analysis announced (but omitted) in [30], but also offer a new proof of the main theorem. Since the new proof is considerably simpler and stronger than the original one, we are able to remove some conditions required in the previous paper. We no longer need the (reflection) positivity condition or the symmetry condition stated in [30], and are able to treat models on an arbitrary decorated lattice.

Our results and their proof demonstrate that there is a mechanism generated by the Coulomb interaction which selects ferromagnetic states as ground states. The mechanism is most clearly seen in the expression of the "spin Hamiltonian" (6.8), where the Hamiltonian for the Coulomb interaction, projected onto a particular subspace, is reduced to that of the ferromagnetic Heisenberg model. This can be regarded as a rigorous example of a "(super) exchange interaction" which is ferromagnetic. The selection mechanism works most effectively when the degenerate single-electron band is nearly half filled (in the sense that the electron number is nearly equal to the dimension of degeneracy in the single-electron ground states), but becomes ineffective when the electron density is too small.

Although the models treated in the present paper are still artificial, we hope that such a selection mechanism generally takes place in a Hubbard model with a large density of states at the bottom of the single-electron energy band. Such a Hubbard model should exhibit ferromagnetism for suitable electron filling factors when the Coulomb interaction is sufficiently large. In other words, we hope the present examples to provide the simplest models in a "universality class" of Hubbard models which exhibit realistic and robust ferromagnetism. The recent numerical and heuristic works of Kusakabe and Aoki [16] for closely related models (which were proposed by the present authors) indeed suggest that the ferromagnetism in the present models is robust and not pathological. It is a challenging problem to extend our results to more general situations.

It is encouraging that ferromagnetism observed in transient metals, like Ni, might have similar properties as our ferromagnetism. The 3d band of Ni has large (single-electron) density of states at the top of the band, and the filling factor of the band is close to one [13]. After the electron-hole transformation, the situation becomes quite similar to that in the models treated in the present paper. When the number of electrons is equal to the degeneracy of the single-electron ground states, our model might also resemble certain ferromagnetic ionic crystals.

A reader might feel that the Hubbard models treated in the present work have "non-standard" hopping matrix elements (including the next nearest neighbor hopping) when compared with the "standard" models with uniform nearest neighbor hoppings. (See eq.(2.3) and Fig. 1.) It should be remarked that, unlike in the lattice field theories, for example, the hopping matrix in the Hubbard model need not be the naive discretization of the Laplacian. It is determined from overlap integrals between electron orbits, and can be quite complicated in general. For example, the typical three-band Hubbard model used to study the normal state of the high-T_{c} superconductors (see *e.g.* [3] and the references therein) contains next-nearest neighbor hoppings and on-site potentials as well and is very similar to our two-dimensional model described in Section 2.1. Another important reason for studying a "nonstandard" model is the remarkable "nonuniversality" of the Hubbard model. These days it is suspected that the simplest Hubbard model with uniform hopping does not exhibit neither ferromagnetism nor superconductivity for reasonable parameter values. This is the case in recent numerical and analytical results for the Hubbard model in infinite dimensions [12]. However the chance is big that a particular version of the Hubbard model with specific hopping matrix (*i.e.*, band structure) and filling factor shows such interesting properties. This is reminiscent of the rich nonuniversal behavior one observes in the actual itinerant electron systems in nature.

The organization of the present paper is as follows. In Section 1.3, we give general definitions of the Hubbard model, and discuss simple construction of ferromagnetic ground states in certain models. In Section 2, we describe our results for a particular Hubbard model, and discuss their physical consequences. The physics of the present paper can be read off from these two sections. Section 3 is devoted to a proof of our main theorem which provides a complete characterization of ground states. In Section 4, we derive percolation representation for various physical quantities, and prove rigorous upper and lower bounds, which have direct physical significance. In Section 5, we calculate correlation functions. In Section 6, we derive a "spin Hamiltonian" and discuss about spin wave excitations.

1.3 Hubbard models with degenerate single-electron ground states

In the present subsection, we will give preliminary discussions on a special class of Hubbard models, in which one can easily construct exact ground states which are ferromagnetic. We shall also give some general definitions.

We take a finite lattice Λ with $|\Lambda|$ sites and consider a Hubbard model on Λ. Throughout the present paper, we denote by $|S|$ the number of elements in a set S. The Hamiltonian is

$$H = H_{\mathrm{hop}} + H_{\mathrm{int}}, \tag{1.1}$$

where

$$H_{\mathrm{hop}} = \sum_{x,y\in\Lambda,\sigma=\uparrow,\downarrow} t_{xy} c^{\dagger}_{x\sigma} c_{y\sigma}, \tag{1.2}$$

and

$$H_{\mathrm{int}} = \sum_{x\in\Lambda} U_x n_{x\uparrow} n_{x\downarrow}. \tag{1.3}$$

As usual $c^{\dagger}_{x\sigma}$ and $c_{x\sigma}$ are the creation and the annihilation operators, respectively, of an electron at site $x\in\Lambda$ with spin $\sigma=\uparrow,\downarrow$. They satisfy the anticommutation relations

$$\{c_{x\sigma}, c^{\dagger}_{y\tau}\} = \delta_{xy}\delta_{\sigma\tau}, \tag{1.4}$$

and

$$\{c_{x\sigma}, c_{y\tau}\} = \{c^{\dagger}_{x\sigma}, c^{\dagger}_{y\tau}\} = 0, \tag{1.5}$$

for any $x, y \in \Lambda$ and $\sigma, \tau =\uparrow, \downarrow$, where $\{A, B\} = AB + BA$. The number operator is defined as

$$n_{x\sigma} = c^\dagger_{x\sigma} c_{x\sigma}. \tag{1.6}$$

The hopping matrix (t_{xy}) is real symmetric, and the on-site Coulomb repulsion U_x is strictly positive. The total electron number operator is

$$\hat{N}_\mathrm{e} = \sum_{x\in\Lambda} (n_{x\uparrow} + n_{x\downarrow}), \tag{1.7}$$

and we denote by N_e its eigenvalue. A standard prescription is to consider the eigenspace of $\hat{N}_\mathrm{e}$ with a given eigenvalue N_e, or to consider certain grand canonical ensemble with the expectation value of $\hat{N}_\mathrm{e}$ fixed. The quantity $N_\mathrm{e}/(2\,|\Lambda|)$ is called the electron filling factor.

We also define the spin operators by

$$S^{(\alpha)}_x = \sum_{\sigma,\tau=\uparrow,\downarrow} c^\dagger_{x\sigma} p^{(\alpha)}_{\sigma\tau} c_{x\tau}/2, \tag{1.8}$$

where $p^{(\alpha)}_{\sigma\tau}$ with $\alpha = 1, 2, 3$ are the Pauli matrices,

$$p^{(1)} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad p^{(2)} = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad p^{(3)} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{1.9}$$

We denote by $S_\mathrm{tot}(S_\mathrm{tot} + 1)$ the eigenvalue of

$$(\mathbf{S}_\mathrm{tot})^2 = \sum_{x,y\in\Lambda} \sum_{\alpha=1,2,3} S^{(\alpha)}_x S^{(\alpha)}_y, \tag{1.10}$$

which is the square of the total spin operator. We say that a state exhibits ferromagnetism if it has S_tot proportional to the system size $|\Lambda|$.

The single-electron Schrödinger equation corresponding to the hopping Hamiltonian (1.2) is

$$\sum_{y\in\Lambda} t_{xy}\varphi_y = \varepsilon\varphi_x, \tag{1.11}$$

where $\varphi_x \in C$, and ε is the single-electron energy. Suppose that our hopping matrix (t_{xy}) has a special property that the (single-electron) ground states of the Schrödinger equation (1.11) are N_d-fold degenerate. We denote the ground state energy by ε_0, and the space of degenerate ground states by $\mathcal{H}_0$. Let $\{\varphi^{(u)}\}_{u\in V}$ be a complete linear independent basis for the space $\mathcal{H}_0$, where V (with $|V| = N_\mathrm{d}$) is the set of indices. The wave function and the creation operator corresponding to a basis state $\varphi^{(u)}$ are denoted as $\{\varphi^{(u)}_x\}_{x\in\Lambda}$ and

$$a^\dagger_{u\sigma} = \sum_{x\in\Lambda} \varphi^{(u)}_x c^\dagger_{x\sigma}, \tag{1.12}$$

respectively.

Consider a ferromagnetic state

$$\Phi_{A\uparrow} = \prod_{u\in A} a^\dagger_{u\uparrow}\Phi_0, \tag{1.13}$$

where A is an arbitrary subset of the index set V, and Φ_0 is the vacuum state, *i.e.*, the state with no electrons. Since the basis $\{\varphi^{(u)}\}_{u\in V}$ is linear independent, the state $\Phi_{A\uparrow}$ is nonvanishing. The electron number of the state $\Phi_{A\uparrow}$ is given by $N_\mathrm{e} = |A|$. By using the commutation relation

$$H_\mathrm{hop} a^\dagger_{u\sigma} = a^\dagger_{u\sigma} H_\mathrm{hop} + \varepsilon_0 a^\dagger_{u\sigma}, \tag{1.14}$$

we find $H_\mathrm{hop}\Phi_{A\uparrow} = N_\mathrm{e}\varepsilon_0\Phi_{A\uparrow}$, where $N_\mathrm{e}\varepsilon_0$ is the lowest possible eigenvalue of H_hop in the subspace with the electron number is fixed to N_e. On the other hand, we already know from the construction that $H_\mathrm{int}\Phi_{A\uparrow} = 0$, where 0 is the minimum possible eigenvalue of H_int. Therefore we have found the following.

Theorem 1.1 *Consider a Hubbard model with the Hamiltonian described by (1.1), (1.2) and (1.3). In the subspace with the electron number fixed to $N_\mathrm{e} \le N_\mathrm{d}$, the ground state energy is $N_\mathrm{e}\varepsilon_0$, and the ferromagnetic state (1.13) with an arbitrary subset $A \subset V$ with $|A| = N_\mathrm{e}$ is a ground state.*

Such a construction of ferromagnetic ground states may be standard, but is not sufficient to draw any meaningful conclusion about the magnetism of the system. A really important (and much more delicate) problem is whether these ferromagnetic states are the only ground states, or what are the other ground states, if any. Note that the single-electron density of states D_F is infinite for $N_\mathrm{e} \le N_\mathrm{d}$. Therefore the Stoner criterion $D_\mathrm{F}U > 1$ predicts the appearance of only the ferromagnetic ground states for any value of $U_x > 0$. But it soon turns out that the situation is not that simple. A trivial counter example is the model with $t_{xy} = 0$ for all x, y, which has the degeneracy $N_\mathrm{d} = |\Lambda|$. Any state with no doubly occupied site is a ground state of this model, so there can be no magnetic ordering. We have paramagnetism, in contrast to the conclusion based on the Stoner criterion.

In the present paper we shall study a class of Hubbard models, in which we can give complete answers to the above questions.

2 Main results and physical consequences

2.1 Definition

In the present section, we discuss our rigorous results and their physical consequences. In order to simplify the discussion, we shall concentrate on the simplest class of models defined on the decorated hypercubic lattice. Many of our results extend to other models with only minor modifications. See the remark at the end of the present subsection.

We shall begin with the definition of the model. Consider a d-dimensional $L \times \cdots \times L$ hypercubic lattice, where L is an even integer, and denote by V the set of sites. We impose periodic boundary conditions. (Note that, in section 1.2, we used the symbol V to denote the index set for the basis states. The reason for using the same symbol for the set of sites will become clear when we construct a basis at the end of Section 2.2.) Let

$$B = \{\{v, w\} \,|\, v, w \in V, |v - w| = 1\}, \tag{2.1}$$

be the set of bonds, where $|v-w|$ denotes the euclidean distance between the sites v and w. For each bond $\{v,w\}$ in B, we denote by $m(v,w)$ the point taken in the middle of the sites v and w. We define

$$M = \{m(v,w)\,|\,\{v,w\}\in B\}, \tag{2.2}$$

and consider the decorated hypercubic lattice $\Lambda = V \cup M$.

We will study the Hubbard model on the lattice Λ. We again write our Hamiltonian as $H = H_{\mathrm{hop}} + H_{\mathrm{int}}$ where

$$H_{\mathrm{hop}} = \sum_{\sigma=\uparrow,\downarrow}\sum_{\{v,w\}\in B} t(c^\dagger_{v\sigma} + c^\dagger_{w\sigma} + \lambda c^\dagger_{m(v,w)\sigma})(c_{v\sigma} + c_{w\sigma} + \lambda c_{m(v,w)\sigma}), \tag{2.3}$$

and

$$H_{\mathrm{int}} = U\sum_{u\in V} n_{u\uparrow}n_{u\downarrow} + U'\sum_{x\in M} n_{x\uparrow}n_{x\downarrow}, \tag{2.4}$$

with $t>0$, $\lambda>0$, $U>0$, and $U'>0$. The case $\lambda<0$ is related to $\lambda>0$ by a unitary transformation. In the case $t<0$, the highest single-particle energy is degenerate. This case can be mapped to $t>0$ by a particle-hole transformation. Note that the above hopping Hamiltonian and interaction Hamiltonian can be written in the form of (1.2) and (1.3) by suitably choosing the hopping matrix (t_{xy}) and the interaction U_x. See Fig. 1.

In general we can take an arbitrary finite lattice V, and construct the corresponding decorated lattice Λ by adding points at the center of each bond in V. The Hamiltonian is defined as in (2.3) and (2.4), but the parameters t, λ, U, and U' can be bond (or site) dependent, provided that they have the required signs. Corollary 2.2 and Theorem 2.3 extend immediately to such general models. If the dimension of V is not less than two, and the coordination number of V is uniformly bounded, one can extend Theorems 2.4 and 2.5 with some extra care.

2.2 Single-electron properties

The special form of the hopping Hamiltonian (2.3) makes the present model fall into the class considered in Section 1.2. To see this, we should study the eigenstates of the single-electron Schrödinger equation (1.11) corresponding to (2.3). A standard way is to use the Fourier transformation to directly solve the eigenvalue problem. One easily finds that the eigenstates can be classified into $(d+1)$-bands, whose dispersion relations are given by

$$\varepsilon_i(k) = \begin{cases} 0 & \text{for } i=1,\\ \lambda^2 t & \text{for } i=2,3,\cdots,d,\\ \lambda^2 t + 2t\sum_{j=1}^{d}(1+\cos k_j) & \text{for } i=d+1, \end{cases} \tag{2.5}$$

where $i=1,2,\cdots,d+1$ is the index for the bands, and $k=(k_1,\cdots,k_d)$ is the wave vector with $-\pi<k_j\le\pi$. Note that the present model has a singular band structure, in which most of the bands are dispersion-less.

Rather than making use of the direct Fourier transformation calculation, however, we here make use of special features of (2.3) to get the following.

Lemma 2.1 *Consider the single-electron Schrödinger equation (1.11) corresponding to the hopping Hamiltonian (2.3). Then the ground states have $\varepsilon = 0$, and are characterized by the condition that*

$$\varphi_v + \varphi_w + \lambda\,\varphi_{m(v,w)} = 0 \tag{2.6}$$

holds for all $\{v, w\} \in B$. The dimension $N_{\rm d}$ of the corresponding eigenspace $\mathcal{H}_0$ is equal to $|V| = L^d$.

Proof: Since the operator $H_{\rm hop}$ is positive semidefinite, the eigenvalues must satisfy $\varepsilon \geq 0$. Let us define a single-electron state as $\Phi = (\sum_{x\in\Lambda}\varphi_x c^\dagger_{x\sigma})\Phi_0$ and note that the Schrödinger equation (1.11) is written as $H_{\rm hop}\Phi = \varepsilon\Phi$. Noting that

$$\begin{aligned}&(c^\dagger_{v\sigma} + c^\dagger_{w\sigma} + \lambda c^\dagger_{m(v,w)\sigma})(c_{v\sigma} + c_{w\sigma} + \lambda c_{m(v,w)\sigma})(\sum_{x\in\Lambda}\varphi_x c^\dagger_{x\sigma})\Phi_0\\ &= (\varphi_v + \varphi_w + \lambda\varphi_{m(v,w)})(c^\dagger_{v\sigma} + c^\dagger_{w\sigma} + \lambda c^\dagger_{m(v,w)\sigma})\Phi_0,\end{aligned} \tag{2.7}$$

we see that the condition (2.6) gives a necessary and sufficient condition for the state Φ to have $\varepsilon = 0$. To get the dimension, one only has to note that the eigenspace is determined by $|\Lambda| - |V|$ independent constraints. ■

¿From Lemma 2.1 and Theorem 1.1, we get the following preliminary result about ferromagnetism.

Corollary 2.2 *In the subspace with the electron number fixed to $N_{\rm e} \leq N_{\rm d}(= L^d)$, the ground state energy of the full Hubbard Hamiltonian H (defined by (2.3) and (2.4)) is* 0*. Among the ground states, there are the ferromagnetic states defined as (1.13).*

Let us construct a basis for the space $\mathcal{H}_0$. We shall label each basis state by a site u in the hypercubic lattice V. For each $u \in V$, we define a single-electron state $\{\varphi^{(u)}_x\}_{x\in\Lambda}$ by

$$\varphi^{(u)}_x = \begin{cases} 1 & x = u \\ -\lambda^{-1} & x = m(u,v)\ \text{for some}\ v \\ 0 & \text{otherwise,}\end{cases} \tag{2.8}$$

which clearly satisfies the condition (2.6). The basis is not orthogonal, but is easily checked to be linear independent. Certain characters of the basis will play central role in the proof of the main theorem in Section 3.

It should be stressed that the locality of our basis (2.8) does not imply that electrons are localized in the present model. One can always take a standard basis states with definite crystal momenta, in which the single-particle states are extended. The actual behavior of electrons should be determined by studying various correlation functions. See discussions in Section 2.3.

2.3 Ferromagnetism for a special electron number

Our first nontrivial result about ferromagnetism deals with the model with a special electron number.

Theorem 2.3 *In the subspace with the electron number fixed to $N_e = N_d (= L^d)$, the ground states of H have $S_{tot} = N_e/2$ and are nondegenerate apart from the $(2S_{tot}+1)$-fold spin degeneracy.*

The theorem will be proved in Section 3.1 as Corollary 3.3. The theorem establishes that the ground states exhibit the maximum possible ferromagnetism. Mielke [20, 21] proved similar result for a general class of Hubbard models on line graphs and on some decorated graphs similar to our model but with additional hopping matrix elements between the sites $m(v,w)$. Recently Mielke [23] extended his results to a general class of Hubbard models with a degenerate single-electron ground states. The result of [23] includes that of both [20, 21] and the above Theorem 2.3. See the remark at the end of Section 3.1 for further discussions. Note that, in the band-theoretic language, the degenerate single-electron ground state band (indexed as $i = 1$ in (2.5)) is exactly half-filled when $N_e = N_d$.

Note that the above theorem applies to the model with $d = 1$ as well. This does not contradict with the general result of Lieb and Mattis [19, 1], which inhibits ferromagnetic order in one dimension, since our model contains non-nearest-neighbor hoppings.

By substituting the definition (2.8) of the basis state into the expression (1.13) of the ferromagnetic ground state, we find that the ground state for $N_e = N_d$ is given by

$$\Phi_{V\uparrow} = \prod_{u\in V} (c^\dagger_{u\uparrow} - \lambda^{-1} \sum_{m;|u-m|=1/2} c^\dagger_{m\uparrow})\Phi_0, \tag{2.9}$$

and its $SU(2)$ rotations.

When the parameter λ is extremely large, the ground state (2.9) has essentially one up electron at each site of the hypercubic lattice V. We will show in Section 5 that the coherence length in the ground state is equal to λ^{-1}. This is extremely short if $\lambda \gg 1$. In this limit, our model resembles that of nearly localized electrons (as in the Heisenberg's work [8]), and the origin of the ferromagnetism may be interpreted as a "super exchange interaction" via the nonmagnetic atom on the site between two magnetic atomic sites. We also expect that the model with $N_e = N_d$ describes a kind of Mott insulator, at least when $\lambda \gg 1$ and $U \gg 1$.

When $\lambda \ll 1$, on the other hand, the coherence length λ^{-1} becomes large, and it is no longer possible to regard the present model as that of localized electrons. It seems that even the simplest model with $N_e = N_d$ contains many interesting physics, which remain to be understood.

2.4 Ferromagnetism in a finite range of electron numbers

Let us investigate whether the ferromagnetism established for the special electron number is stable when the electron number is changed. We stress that any physically realistic model of ferromagnetism should possess such stability. All the theorems presented here will be proved in Section 4.

In Section 3.1, we will find that the ground states of H are highly degenerate for $N_e < N_d$. To get a physically meaningful results, we have to consider the average over the degenerate ground states. Instead of fixing the electron number explicitly, we will employ the grand canonical formalism, and control the expectation value of the electron number by choosing appropriate chemical potential. The reason for using the grand canonical formalism here is mainly technical.

For an arbitrary operator O, we define the grand canonical-like average by

$$\langle O \rangle_\mu = \frac{\mathrm{Tr}[O \exp(\mu \hat{N}_\mathrm{e}) P_0]}{\mathrm{Tr}[\exp(\mu \hat{N}_\mathrm{e}) P_0]}, \tag{2.10}$$

where P_0 is the orthogonal projection operator onto the eigenspace of H with the eigenvalue 0. It is expected that, by choosing a suitable (dimensionless) chemical potential μ in (2.10), we recover zero-temperature properties of the system with a desired electron filling factor. If the electron filling factor had a pathological behavior as a function of μ, the use of the grand canonical formalism could not be justified. The following theorem guarantees that this is not the case.

Theorem 2.4 *For arbitrary values of μ, we have the upper and lower bounds*

$$(1 + \frac{e^{-\mu}}{2})^{-1} \ge \frac{\langle \hat{N}_\mathrm{e} \rangle_\mu}{N_\mathrm{d}} \ge 3^{-d}(1 + \frac{e^{-\mu}}{2})^{-1}. \tag{2.11}$$

In the dimensions $d \ge 2$, there are positive finite constants μ_1, c_1 which depend only on the dimension d, and for any $\mu \ge \mu_1$, we have the lower bound

$$\frac{\langle \hat{N}_\mathrm{e} \rangle_\mu}{N_\mathrm{d}} \ge 1 - c_1 e^{-\mu}. \tag{2.12}$$

The above bounds determine the behavior of the electron filling factor for extreme values of the chemical potential. When μ is negative and its absolute value is large (compared to 1), (2.11) implies

$$\frac{\langle \hat{N}_\mathrm{e} \rangle_\mu}{2|\Lambda|} \approx e^{\mu}. \tag{2.13}$$

When μ is positive and large, (2.11) and (2.12) imply

$$\rho_0 - \frac{\langle \hat{N}_\mathrm{e} \rangle_\mu}{2|\Lambda|} \approx e^{-\mu}, \tag{2.14}$$

where the maximum value of the electron filling factor is defined as $\rho_0 = N_\mathrm{d}/(2\,|\Lambda|) = (2d+2)^{-1}$. The relation $\approx$ means that the both sides behave equally apart from multiplication by a uniformly bounded function of μ.

Now we can state our main theorem.

Theorem 2.5 *In the dimensions $d \ge 2$, there are finite constants c_2, c_3, μ_1, μ_2 (with $c_2, c_3, \mu_1 > 0$ and $\mu_2 < 0$) which depend only on the dimension d and not on the size of the lattice. For any $\mu \ge \mu_1$, we have*

$$S_\mathrm{max}(S_\mathrm{max}+1) \ge \langle (\mathbf{S}_\mathrm{tot})^2 \rangle_\mu \ge S_\mathrm{max}(S_\mathrm{max}+1)(1 - c_2 e^{-\mu}), \tag{2.15}$$

where $S_{\max} = N_{\rm d}/2$. *For any* $\mu \le \mu_2$, *we have*

$$\frac{3}{4}\langle \hat{N}_{\rm e}\rangle_\mu \le \langle (\mathbf{S}_{\rm tot})^2\rangle_\mu \le \frac{3}{4}\langle \hat{N}_{\rm e}\rangle_\mu + c_3|V|e^{2\mu}. \tag{2.16}$$

Note that, when the bounds (2.15) hold, the total spin of the model is proportional to the number of sites $|\Lambda|$. When the bounds (2.16) hold, on the other hand, the total spin is proportional to the square root of $|\Lambda|$. Therefore Theorem 2.5 establishes that the ground states of our Hubbard model exhibit ferromagnetism when the filling factor is not more than and sufficiently close to ρ_0, and paramagnetism when the filling factor is sufficiently small. In the band-theoretic language, ferromagnetism appears when the degenerate ground state band is nearly half-filled.

The requirement that the dimension is not less than two in Theorem 2.5 is essential in controlling ferromagnetic region by using a kind of Peierls argument. (See Section 4.4.) The paramagnetic part (the bounds (2.16)) of Theorem 2.5 easily extends to the case with $d = 1$. We believe that the one-dimensional model exhibits paramagnetism for all the values of $\mu < \infty$.

As we have discussed at the end of Section 1.3, the Stoner criterion from the Hartree-Fock approximation predicts the appearance of only the ferromagnetic ground states for all $\mu < \infty$. Theorem 2.5 clearly shows that this is not the case. For selection of ferromagnetic states to take place, the degenerate single-electron band must be nearly half-filled in the sense that $0 < \rho_0 - \rho \ll 1$. We expect that this feature is universal in the Hubbard models with large single-electron density-of-states. It is interesting that, in perturbative corrections to the Hartree-Fock approximation, one finds somewhat similar conditions in order to ensure sufficiently large "effective" U. See [13] and section X of [10]. See also [15] for a related discussions.

It is an interesting problem whether the ferromagnetism in the present rather artificial model is stable under various perturbations to the Hamiltonian. We believe that the ferromagnetism persists under small perturbations if the on-site Coulomb repulsion is sufficiently large, but we have no rigorous results at the moment. The numerical results of [16] for closely related models (one of which is introduced in [21] and the other is defined at the end of Section 3.1 of the present paper) indicate that the present ferromagnetism is stable under perturbations. It is also important to investigate whether ferromagnetic order in the three dimensional model is present at finite temperatures. Recall that, in one and two dimensions, ferromagnetic order in any Hubbard model is destroyed by thermal fluctuation at finite temperatures [5, 14].

2.5 Other properties

In Subsection 2.3, we argued that the model with the special electron filling factor $\rho = \rho_0$ (which corresponds to $N_{\rm e} = N_{\rm d}$) is likely to be an insulator (at least when $\lambda \gg 1$ and $U \gg 1$). When the filling factor $\rho = \langle \hat{N}_{\rm e}\rangle_\mu/(2\,|\Lambda|)$ is strictly less than ρ_0, on the other hand, band-theoretic intuition suggests that the model describes a metal.

Let $E_{\rm GS}(N_{\rm e})$ be the ground state energy of a Hubbard model with the electron number fixed to $N_{\rm e}$. The charge gap of the model is defined as

$$\Delta_{\rm charge}(N_{\rm e}) = E_{\rm GS}(N_{\rm e}+1) - 2E_{\rm GS}(N_{\rm e}) + E_{\rm GS}(N_{\rm e}-1). \tag{2.17}$$

It is believed that, if a system has nonvanishing charge gap (in the infinite volume limit), it describes an insulator. In our case, we already know from Theorem 2.2 that $E_{\rm GS}(N_{\rm e}) = 0$ for any $N_{\rm e} \le N_{\rm d}$, which means that $\Delta_{\rm charge}(N_{\rm e}) = 0$ for any $N_{\rm e} \le N_{\rm d} - 1$. This might first appear as an indication that the present model describes a ferromagnetic metal when the electron filling factor is strictly smaller than ρ_0. However one must recall that vanishing of the charge gap is a necessary but not a sufficient condition for an electron system to be a conductor. (A trivial example of an insulator with a vanishing charge gap is the model with $H_{\rm hop} = 0$.)

To determine whether the present model is metallic or not, a more elaborate analysis on the transport properties seems necessary. At present we are not able to calculate conductivity (from, e.g., the Kubo formula). We can only calculate certain static correlation functions in the model with $N_{\rm d} - 2d + 1 \le N_{\rm e} \le N_{\rm d}$. See Section 5.

A rotation invariant system with spontaneous ferromagnetic order always has spin wave excitations. In Section 6, we show that the interaction Hamiltonian (2.4), projected onto a certain subspace, becomes

$$P_A H_{\rm int} P_A = 2J(\lambda) \sum_{\langle u,v\rangle} \left(\frac{1}{2} - 2\tilde{\mathbf{S}}_u \cdot \tilde{\mathbf{S}}_v\right) P_A, \tag{2.18}$$

where the summation is over nearest neighbor pairs of sites in V, and $J(\lambda) > 0$. (See Section 6 for definitions.) It is remarkable that (2.18) is nothing but the Hamiltonian of the ferromagnetic Heisenberg model. We expect that the low energy spin excitations of the model are approximately described by the "spin Hamiltonian" (2.18). Then there should be spin wave excitations when the ground states exhibit long range order. When $N_{\rm e} = N_{\rm d}$ (*i.e.*, the degenerate band is exactly half-filled), we prove that there are excited states whose excitation energies are bounded from above by that of the spin wave excitations of the Heisenberg model. See [16] for discussions on low-lying excitations in the closely related Hubbard model with $U = \infty$.

3 Characterization of ground states

3.1 Main theorem

In the present section, we shall state and prove our main theorem. The theorem provides a complete characterization of the ground states when the electron number $N_{\rm e}$ does not exceed the degeneracy $N_{\rm d}$ of the single-electron ground states. This result will be used in Section 4 to prove various bounds for physical quantities. The class of models treated here, which includes the model of Section 2 as a special case, is specified by a set of conditions for a basis $\{\varphi^{(u)}\}_{u\in V}$ of the space $\mathcal{H}_0$ of degenerate single-electron ground states. See B0, B1, and B2 below.

Let Λ be a finite lattice. We consider a Hubbard model on Λ with the Hamiltonian defined by (1.1), (1.2) and (1.3). As in Section 1.2, we denote by $\{\varphi^{(u)}\}_{u\in V}$ a basis for the $N_{\rm d}$-dimensional space $\mathcal{H}_0$ of the single-electron ground states, where V is the index set. Recall that, in Section 2, the symbol V stands both for the (undecorated) hypercubic lattice and for the index set. We stress that this is an accidental coincidence in the model of section 2, and V is not necessarily a set of sites in the present section.

We denote by $a^\dagger_{u\sigma}$ the creation operator defined as in (1.12), which corresponds to a basis state $\varphi^{(u)}$. We have seen in Section 1.2 that the ferromagnetic state (1.13) is an exact ground state of the model. We start from explicit construction of other ground states.

We introduce a notion of connectivity in the index set V by declaring that two indices u and v are directly connected if $\varphi^{(u)}_x\varphi^{(v)}_x \ne 0$ for some site $x\in\Lambda$. Let A be an arbitrary subset of the index set V. The subset A can be uniquely decomposed into a disjoint union of connected components as $A = C_1\cup\cdots\cup C_n$. Note that, in the ground state (1.13), electrons on different connected components may be regarded as not interacting with each other. (Of course this is a basis-dependent observation, which should not be taken literally.) For each $k = 1, 2, \cdots, n$, let us define a subset Λ_k of the lattice Λ by

$$\Lambda_k = \left\{ x\in\Lambda \,\middle|\, \varphi^{(u)}_x \ne 0 \quad \text{for some } u\in C_k \right\}. \tag{3.1}$$

By the definition of connectivity, it immediately follows that $\Lambda_k\cap\Lambda_{k'} = \emptyset$ for $k\ne k'$. We define the spin lowering operator on Λ_k by

$$\hat{S}^-_k = \sum_{x\in\Lambda_k} S^-_x. \tag{3.2}$$

Because of disjointness of the support sets, operators $\hat{S}^-_k$ with different k commute with each other. For $\{m_k\}_{k=1,\cdots,n}$ with $m_k = -|C_k|/2, 1-|C_k|/2, \cdots, |C_k|/2$, we define

$$\Phi_{A,\{m_k\}} = \{\prod_{k=1}^{n} (\hat{S}^-_k)^{(|C_k|/2)-m_k}\}\Phi_{A\uparrow}, \tag{3.3}$$

where $\Phi_{A\uparrow} = \prod_{u\in A} a^\dagger_{u\uparrow}\Phi_0$ is the ferromagnetic ground state defined in (1.13). Note that m_k can be regarded as the total S^z on the sublattice Λ_k.

Lemma 3.1 *In the subspace with the electron number fixed to $N_{\rm e}\le N_{\rm d}$, the state $\Phi_{A,\{m_k\}}$ with arbitrary $A\subset V$ (such that $|A| = N_{\rm e}$) and with arbitrary $\{m_k\}_{k=1,\cdots,n}$ is a ground state of the Hubbard model. The ground state energy is equal to $N_{\rm e}\varepsilon_0$ where ε_0 denotes the single-electron ground state energy.*

Proof: For $u\in C_k$, we have

$$\hat{S}^-_k a^\dagger_{u\uparrow} = a^\dagger_{u\uparrow}\hat{S}^-_k + a^\dagger_{u\downarrow}, \tag{3.4}$$

which means that the states (3.3) are still a linear combinations of the states $(\prod_{u\in A} a^\dagger_{u\sigma(u)})\Phi_0$ with $\sigma(u) = \uparrow,\downarrow$. This proves that $H_{\rm hop}\Phi_{A,\{m_k\}} = N_{\rm e}\varepsilon_0\Phi_{A,\{m_k\}}$. Note that $N_{\rm e}\varepsilon_0$ is the lowest possible eigenvalue of $H_{\rm hop}$. On the other hand the identity $n_{x\uparrow}n_{x\downarrow}S^-_x = 0$ and the fact that $n_{x\uparrow}n_{x\downarrow}\Phi_{A\uparrow} = 0$ immediately imply $n_{x\uparrow}n_{x\downarrow}\Phi_{A,\{m_k\}} = 0$ for any $x\in\Lambda$, and hence $H_{\rm int}\Phi_{A,\{m_k\}} = 0$. Again 0 is the lowest possible eigenvalue of $H_{\rm int}$. ■

The ground states $\Phi_{A,\{m_k\}}$ are not in general eigenstates of the square of the total spin operator $(\mathbf{S}_{\mathrm{tot}})^2$. One can construct eigenstates by taking suitable linear combinations. For example, suppose that A consist of two connected components as $A = C_1 \cup C_2$, and $|C_1| = |C_2| = 2M$. Then the state

$$\sum_{m=-M}^{M} (-1)^m \Phi_{A,\{m,-m\}} \tag{3.5}$$

is a spin-singlet, *i.e.*, an eigenstate of $(\mathbf{S}_{\mathrm{tot}})^2$ with the vanishing eigenvalue. Note that such construction of spin singlet ground states is possible when $|V| - N_{\mathrm{e}}$ is at least of order L^{d-1} (where L is the linear size of the lattice). See [21, 22] for related results.

In order to completely characterize the set of ground states, we require the basis $\{\varphi^{(u)}\}_{u\in V}$ to satisfy the following three conditions.

B0. $\{\varphi^{(u)}\}_{u\in V}$ is a linear independent complete basis of the space $\mathcal{H}_0$. Thus we have $|V| = N_{\mathrm{d}}$. For each $u \in V$, the corresponding wave function $\{\varphi^{(u)}_x\}_{x\in\Lambda}$ is real.

B1. *Quasi locality:* For each $u \in V$, there is a site $x(u) \in \Lambda$ with the properties that $\varphi^{(u)}_{x(u)} \neq 0$ and $\varphi^{(v)}_{x(u)} = 0$ for any $v \neq u$.

B2. *Local connectivity:* For each $x \in \Lambda$, there are at most two indices $u \in V$ such that $\varphi^{(u)}_x \neq 0$.

Then the main theorem of the present section, which will be proved in Section 3.2, is the following.

Theorem 3.2 *Consider a Hubbard model with the Hamiltonian described by (1.1), (1.2) and (1.3). Let ε_0 and $\mathcal{H}_0$ be the ground state energy and the space of the ground states, respectively, of the corresponding single-electron Schrödinger equation (1.11). Suppose that one can find a basis $\{\varphi^{(u)}\}_{u\in V}$ for the space $\mathcal{H}_0$ which satisfies the conditions B0, B1, and B2 stated above. In the subspace with the electron number fixed to $N_{\mathrm{e}} \leq N_{\mathrm{d}}$, the ground state energy is $N_{\mathrm{e}}\varepsilon_0$, and an arbitrary ground state is a linear combination of the states (3.3) with various A (with $|A| = N_{\mathrm{e}}$) and $\{m_k\}$. In the subspace with the electron number fixed to $N_{\mathrm{e}} > N_{\mathrm{d}}$, the ground state energy is strictly larger than $N_{\mathrm{e}}\varepsilon_0$.*

Mielke [22] also gave a somewhat similar complete characterization of the ground states for a class of Hubbard models on two-dimensional line graphs.

Theorem 3.2 alone is not enough to determine magnetic properties of the system. As we have seen by constructing the state (3.5), there are states with small total spins among the degenerate ground states. Whether the system exhibits ferromagnetism depends on how large connected components of a "typical" subset A are. We shall deal with this problem in Section 4. The following special case, which corresponds to the "half-filled degenerate band", can be treated without further analysis.

Corollary 3.3 *Assume the conditions for Theorem 3.2, and that the index set V is connected. In the subspace with the electron number fixed to $N_{\mathrm{e}} = N_{\mathrm{d}}$, the ground states of the Hubbard model have $S_{\mathrm{tot}} = N_{\mathrm{e}}/2$, and are nondegenerate apart form the $(2S_{\mathrm{tot}} + 1)$-fold spin degeneracy.*

Proof: We have $A = V$ because $|A| = |V|$. Since A is connected, (3.3) represents fully ferromagnetic states. ■

Remark: Corollary 3.3, which establishes the existence of ferromagnetism for a special electron number, can be proved in more general settings. In [21], the same statement was proved for the Hubbard models on general line graphs. Let us mention that it is always possible to find a basis that satisfies the conditions B0 and B1. This fact implies that the connectivity of V is necessary and sufficient for the ferromagnetic ground state to be unique in the case $N_{\mathrm{e}} = N_{\mathrm{d}}$. A proof and a basis-independent formulation of this result was given in [23].

We shall briefly describe a class of models similar to the present ones, in which the existence of ferromagnetism can be proved (at least) for special electron numbers. Let the unit cell C consist of n *external* sites $x_1, \ldots, x_n$, and one *internal* site y. (The cell C can be, e.g., a bond, a plaquette, or a cube. Then the external sites are corners, and the internal site is taken at the center of C. When C is a bond, the models reduce to the ones considered in the present paper. One of the models studied in [16] is obtained by letting C a plaquette.) We define the hopping Hamiltonian within the cell as

$$H_{\mathrm{hop}}[C] = t \sum_{\sigma=\uparrow,\downarrow} \left(\sum_{i=1}^{n} c^\dagger_{x_i\sigma} + \lambda c^\dagger_{y\sigma} \right) \left(\sum_{i=1}^{n} c_{x_i\sigma} + \lambda c_{y\sigma} \right), \tag{3.6}$$

where $t, \lambda > 0$. The whole lattice Λ is constructed by assembling together identical copies of the unit cell C. When doing this, an external site may be (or may not be) shared by several distinct unit cells, but an internal site should belong to exactly one unit cell. The total hopping Hamiltonian is

$$H_{\mathrm{hop}} = \sum_j H_{\mathrm{hop}}[C_j], \tag{3.7}$$

where j is the index for the copies of the unit cell. It is easily seen that the single electron ground states have energy $\varepsilon_0 = 0$, and their degeneracy N_{d} is identical to the number of external sites, where an external site which belongs to several different cells is counted only once. When the whole lattice is connected, it can be proved that the Hubbard model (with $U_x > 0$) with the hopping Hamiltonian (3.7) has fully polarized ferromagnetic ground states for $N_{\mathrm{e}} = N_{\mathrm{d}}$. The proof can be done by generalizing the one in the present paper, but it follows immediately from the theorem in [23].

One can also introduce more complicated cell structures and consider various arrangements of cells. The existence of ferromagnetism in the resulting Hubbard model can be proved by the theorem of [23].

3.2 Proof

Following [22], we first introduce some creation and annihilation operators. The Gramm matrix G for the basis $\{\varphi^{(u)}\}_{u\in V}$ is defined as

$$(G)_{uv} = \sum_{x\in\Lambda} \varphi^{(u)}_x \varphi^{(v)}_x. \tag{3.8}$$

Since $\{\varphi^{(u)}\}_{u\in V}$ is linearly independent, the matrix G is regular. We define

$$\kappa_x^{(u)} = \sum_{v\in V} (G^{-1})_{uv}\varphi_x^{(v)}. \tag{3.9}$$

Note that $\{\{\kappa_x^{(u)}\}_{x\in\Lambda}\}_{u\in V}$ also forms a basis of the space $\mathcal{H}_0$. It is easily verified that there are completeness conditions

$$\sum_{x\in\Lambda} \kappa_x^{(u)}\varphi_x^{(v)} = \delta_{uv}, \tag{3.10}$$

and

$$\sum_{u\in V} \kappa_x^{(u)}\varphi_y^{(u)} = \delta_{xy} - \psi_{xy}, \tag{3.11}$$

where

$$\psi_{xy} = \psi_{yx} = \delta_{xy} - \sum_{u,v\in V} \varphi_x^{(u)}(G^{-1})_{uv}\varphi_y^{(v)}. \tag{3.12}$$

Note that ψ_{xy} with a fixed x (or y) defines a state orthogonal to the space $\mathcal{H}_0$ since

$$\sum_{y\in\Lambda} \psi_{xy}\varphi_y^{(u)} = \sum_{y\in\Lambda} \psi_{xy}\kappa_y^{(u)} = 0, \tag{3.13}$$

for any $x \in \Lambda$ and $u \in V$.

Let us define

$$b_{u\sigma} = \sum_{x\in\Lambda} \kappa_x^{(u)} c_{x\sigma} \tag{3.14}$$

and

$$d_{x\sigma} = \sum_{y\in\Lambda} \psi_{xy} c_{y\sigma}. \tag{3.15}$$

¿From (3.10), we find that $b_{u\sigma}$ is the dual of $a^\dagger_{u\sigma}$ in the sense that

$$\left\{b_{u\sigma}, a^\dagger_{v\tau}\right\} = \delta_{uv}\delta_{\sigma\tau}. \tag{3.16}$$

for any $u, v \in V$ and $\sigma, \tau =\uparrow,\downarrow$. The orthogonality (3.13) implies

$$\left\{d_{x\sigma}, a^\dagger_{u\tau}\right\} = \left\{d^\dagger_{x\sigma}, b_{u\tau}\right\} = 0, \tag{3.17}$$

for any $x \in \Lambda$, $u \in V$ and $\sigma, \tau =\uparrow,\downarrow$. Finally from the completeness relation (3.11), we get the expansion formulas

$$\begin{aligned} c^\dagger_{x\sigma} &= \sum_{u\in V} \kappa_x^{(u)} a^\dagger_{u\sigma} + d^\dagger_{x\sigma}, & (3.18)\\ c_{x\sigma} &= \sum_{u\in V} \varphi_x^{(u)} b_{u\sigma} + d_{x\sigma}, & (3.19) \end{aligned}$$

for any $x \in \Lambda$ and $\sigma, \tau =\uparrow,\downarrow$. The formulas (3.18) and (3.19) will turn out to be useful later.

We shall now prove Theorem 3.2. We restrict ourselves to the subspace with the electron number fixed to $N_e \le N_d$. By construction, we already know that the states (3.3) are ground states of the Hubbard model, and the ground state energy is $N_{\mathrm{e}}\varepsilon_0$. We will show that they are the only ground states.

Let Φ be a ground state. Since a ground state satisfies $H_{\mathrm{hop}}\Phi = N_{\mathrm{e}}\varepsilon_0\Phi$, it can be written in the form

$$\Phi = \sum_{A_\uparrow, A_\downarrow} f(A_\uparrow, A_\downarrow) \prod_{u\in A_\uparrow} a^\dagger_{u\uparrow} \prod_{v\in A_\downarrow} a^\dagger_{v\downarrow}\Phi_0, \tag{3.20}$$

where $A_\uparrow$ and $A_\downarrow$ are subsets of V such that $|A_\uparrow|+|A_\downarrow| = N_{\mathrm{e}}$, and $f(A_\uparrow, A_\downarrow)$ is a coefficient.

A ground state must also satisfy $H_{\mathrm{int}}\Phi = 0$, and hence $c_{x\uparrow}c_{x\downarrow}\Phi = 0$ for any $x \in \Lambda$. By substituting the expansion formula (3.19), this necessary condition can be rewritten as

$$\left(\sum_{u\in V} \varphi^{(u)}_x b_{u\uparrow}\right)\left(\sum_{v\in V} \varphi^{(v)}_x b_{v\downarrow}\right)\Phi = 0, \tag{3.21}$$

for any $x \in \Lambda$. We have used $d_{x\sigma}\Phi = 0$, which follows from the anticommutation relation (3.17) and the representation (3.20) of Φ.

We shall first set $x = x(u)$, where $x(u)$ is the site defined in the *quasi locality* condition B1. Then the condition (3.21) becomes

$$(\varphi^{(u)}_{x(u)})^2 b_{u\uparrow}b_{u\downarrow}\Phi = 0. \tag{3.22}$$

By using the anticommutation relations (3.16), we find from (3.22) that the coefficients in (3.20) must satisfy

$$f(A_\uparrow, A_\downarrow) = 0 \tag{3.23}$$

if $A_\uparrow \cap A_\downarrow \neq \emptyset$.

Let $u, v \in V$ be directly connected, and take $x \in \Lambda$ such that $\varphi^{(u)}_x\varphi^{(v)}_x \neq 0$. By using the *local connectivity* B2 and (3.23), we see that the condition (3.21) becomes

$$\varphi^{(u)}_x\varphi^{(v)}_x\left(b_{u\uparrow}b_{v\downarrow} - b_{u\downarrow}b_{v\uparrow}\right)\Phi = 0. \tag{3.24}$$

Again from the anticommutation relations (3.16), we find that

$$f(B_\uparrow \cup \{u\}, B_\downarrow \cup \{v\}) = f(B_\uparrow \cup \{v\}, B_\downarrow \cup \{u\}), \tag{3.25}$$

where $B_\uparrow$ and $B_\downarrow$ are arbitrary subsets of $V\backslash\{u, v\}$ such that $|B_\uparrow|+|B_\downarrow| = N_{\mathrm{e}}-2$. In other words, the coefficients $f(A_\uparrow, A_\downarrow)$ are symmetric under the exchange of spins corresponding to the indices u and v.

Take a subset $A \subset V$ with $|A| = N_{\mathrm{e}}$, and decompose it into connected components as $A = \bigcup_{k=1}^n C_k$. Take $\{m_k\}_{k=1,\cdots,n}$ with $m_k = -|C_k|/2, 1-|C_k|/2, \cdots, |C_k|/2$. By noting that the condition (3.25) is valid for any pair of directly connected indices u, v, we find that the coefficient $f(A_\uparrow, A_\downarrow)$ takes a constant value for those $A_\uparrow$, $A_\downarrow$ such that $A_\uparrow \cap A_\downarrow = \emptyset$, $A_\uparrow \cup A_\downarrow = A$, and $|A_\uparrow \cap C_k| - |A_\downarrow \cap C_k| = 2m_k$ for any $k = 1, \cdots, n$. This proves that any Φ of the form (3.20) satisfying the conditions (3.23) and (3.25) is a linear combination of the states (3.3). The first part of the Theorem 3.2 has been proved.

To prove the second part of Theorem 3.2, fix the electron number $N_{\mathrm{e}} > N_{\mathrm{d}}$, and assume that the ground state energy is still $N_{\mathrm{e}}\varepsilon_0$. Then the condition (3.23), along with the fact that $|A_\uparrow| + |A_\downarrow| > |V|$, immediately leads to $\Phi = 0$.

4 Percolation representation

4.1 Representation

In the present section, we shall prove Theorems 2.4 and 2.5 concerning the behavior of grand canonical average of various quantities. The proofs are based on the complete characterization of the ground states obtained in Section 3 and a percolation analysis.

Throughout the present section, we shall assume for simplicity that the index set V forms a d-dimensional hypercubic lattice (where $d \geq 2$) with periodic boundary conditions, and two sites u and v are directly connected with each other if and only if $|u - v| = 1$. This is precisely the case in the model of Section 2. Generalizations to other models are straightforward.

The strategy to make use of the percolation type analysis in the present context follows that of Mielke's work on the Hubbard models on two dimensional line graphs [22]. Here we shall make the ideas presented in [22] into a rigorous proof, by presenting careful analysis of a non-independent percolation problem. (Unfortunately, the discussion in [22] made use of some properties of the independent percolation. As a consequence, the critical filling factors predicted in [22] are incorrect. We stress, however, that the main body of [22] is completely rigorous, and that the present method can be also applied to the models of [22] to establish rigorously the existence of ferromagnetic order in a finite range of filling factor.)

In the present subsection, we will derive representations for various expectation values in terms of a (non-independent) percolation problem, and give some heuristic discussions about behavior of the system.

We recall from Section 3.1 that the space of (many-electron) ground states of H is spanned by the states

$$\Phi_{A,\{m_k\}} = \{\prod_{k=1}^{n} (\hat{S}_k^-)^{(|C_k|/2)-m_k}\}\Phi_{A\uparrow}, \tag{4.1}$$

where A is an arbitrary sublattice of the hypercubic lattice V. The sets $C_1, \cdots, C_n$ are the connected components of A (in the usual sense), and $m_k = -|C_k|/2, 1-|C_k|/2, \cdots, |C_k|/2$. We first realize the trace in the definition of the grand canonical like average (2.10) by using the complete set of ground states (4.1). For an arbitrary operator O, let us define its matrix element $o(B, \{n_k\}; A, \{m_k\})$ by

$$O\Phi_{A,\{m_k\}} = \Psi + \sum_{B,\{n_k\}} o(B, \{n_k\}; A, \{m_k\})\Phi_{B,\{n_k\}}, \tag{4.2}$$

where Ψ is a state orthogonal to the eigenspace of H with the eigenvalue 0. Since the states (4.1) form a complete basis of the eigenspace, the trace can be realized as

$$\mathrm{Tr}[OP_0] = \sum_{A,\{m_k\}} o(A, \{m_k\}; A, \{m_k\}), \tag{4.3}$$

where the sum is over all the subset $A \in V$ and all the possible $\{m_k\}$.

¿From (4.1) and the definitions (1.6), (1.7) and (1.8), we immediately get

$$\hat{N}_{\mathrm{e}}\Phi_{A,\{m_k\}} = |A|\Phi_{A,\{m_k\}}, \tag{4.4}$$

and

$$(S_{\rm tot}^{(3)})^2\Phi_{A,\{m_k\}} = (\sum_{k=1}^{n} m_k)^2\Phi_{A,\{m_k\}}, \tag{4.5}$$

where $S_{\rm tot}^{(3)} = \sum_{x\in\Lambda} S_x^{(3)}$.

For a fixed subset A, we define the corresponding subtrace by

$$\mathrm{Tr}_A[O] = \sum_{\{m_k\}} o(A,\{m_k\};A,\{m_k\}). \tag{4.6}$$

Straightforward calculations show

$$\begin{aligned}\mathrm{Tr}_A[\exp(\mu\hat{N}_{\rm e})] &= \sum_{m_1=-|C_1|/2}^{|C_1|/2}\cdots\sum_{m_n=-|C_n|/2}^{|C_n|/2}\exp(\mu|A|) \\ &= \prod_{k=1}^{n} e^{\mu|C_k|}(|C_k|+1) = W(A),\end{aligned} \tag{4.7}$$

and

$$\begin{aligned}\mathrm{Tr}_A[(S_{\rm tot}^{(3)})^2\exp(\mu\hat{N}_{\rm e})] &= \sum_{m_1}\cdots\sum_{m_n}(\sum_{k=1}^{n} m_k)^2\exp(\mu|A|) \\ &= W(A)\frac{1}{3}\sum_{k=1}^{n}\frac{|C_k|}{2}\left(\frac{|C_k|}{2}+1\right).\end{aligned} \tag{4.8}$$

¿From the definition (2.10) of the average, and the $SU(2)$ invariance, we get

$$\langle(\mathbf{S}_{\rm tot})^2\rangle_\mu = \frac{1}{Z}\sum_{A\subset V} W(A)\sum_{k=1}^{n}\frac{|C_k|}{2}\left(\frac{|C_k|}{2}+1\right), \tag{4.9}$$

where the "partition function" is given by

$$Z = \sum_{A\subset V} W(A). \tag{4.10}$$

Similarly we have

$$\langle\hat{N}_{\rm e}\rangle_\mu = \frac{1}{Z}\sum_{A\subset V} W(A)\sum_{k=1}^{n}|C_k|. \tag{4.11}$$

Note that the right hand sides of eqs. (4.9) and (4.11) can be regarded as expectation values in a percolation system. The set A may be regarded as a configuration of occupied sites. The probability that a configuration A appears is proportional to the statistical weight $W(A)$ defined in (4.7). Such identification allows us to develop, as in [22], a geometric picture for the ferromagnetic-paramagnetic phase transition observed in the present Hubbard model.

When μ is negative and its absolute value is large (compared to 1), (4.7) suggests that the probability to find a configuration with many occupied sites is relatively small. This means that, among many ground states (4.1), only those with low electron filling factor have main contributions to the grand canonical average. We expect that the percolation system is in its low density phase, where all the connected clusters (which are $C_1, \cdots, C_n$ in our case) have uniformly bounded sizes with large probability. Then the representation (4.9) implies that the square of the total spin is proportional to the system size, which is a characteristic behavior of a paramagnetic phase.

When μ is positive and large, (4.7) suggests that the probability to find a configuration with many occupied sites is large. This indicates that the electron filling factor should be close to its maximum value ρ_0. When the dimension d is not less than the lower critical dimension of the percolation problem, which is two, we expect that the system is in the percolating phase, where one finds an infinitely large connected cluster with probability one. Such a cluster has a dominant contribution in the representation (4.9), and we see that the square of the total spin becomes proportional to the square of the system size. This is the desired ferromagnetic behavior.

Although the present percolation problem is not a simple independent percolation, we can use suitable stochastic geometric techniques to get meaningful bounds for physical quantities. In the following sections, we will make the above heuristic picture into rigorous proofs.

4.2 Universal bounds

We shall prove elementary bounds which are valid for any values of μ.

Since $|C_k| \ge 1$, we see

$$\frac{|C_k|}{2}\left(\frac{|C_k|}{2}+1\right) \ge \frac{3}{4}|C_k|. \tag{4.12}$$

Substituting the bound into (4.9), we immediately get

$$\langle(\mathbf{S}_{\mathrm{tot}})^2\rangle_\mu \ge \frac{3}{4}\langle\hat{N}_{\mathrm{e}}\rangle_\mu, \tag{4.13}$$

for any value of μ. This is the lower bound in (2.16).

We shall prove the upper bound for the electron number in (2.11). Fix a site $u \in V$, and let A be an arbitrary configuration in which u is occupied. By A^* we denote the unique configuration obtained from A by eliminating the site u. Then the weights for two subsets satisfy

$$\frac{W(A^*)}{W(A)} = \frac{\prod_j(|C'_j|+1)}{e^\mu(|C|+1)}, \tag{4.14}$$

where C is the connected cluster in A which contains u, and C'_j are the connected components of $C\backslash\{u\}$. Noting that $|C| = 1 + \sum_j |C'_j|$, the above ratio can be bounded as

$$\frac{W(A^*)}{W(A)} \ge \frac{1+\sum_j |C'_j|}{e^\mu(2+\sum_j|C'_j|)} \ge \frac{1}{2e^\mu}. \tag{4.15}$$

For a general event concerning a configuration A, we define

$$Z_{\mathrm{event}} = \sum_{A\subset V} W(A)\chi[\mathrm{event}], \tag{4.16}$$

where χ is the indicator function, *i.e.*, $\chi[\text{True}] = 1$, $\chi[\text{False}] = 0$. The bound (4.15) implies that

$$\begin{aligned} Z_{u\in A} &= \sum_{A\subset V} W(A)\chi[u\in A] \le 2e^{\mu} \sum_{A\subset V} W(A^*)\chi[u\in A] \\ &= 2e^{\mu} \sum_{A'\subset V} W(A')\chi[u\notin A'] = 2e^{\mu} Z_{u\notin A}, \end{aligned} \tag{4.17}$$

where we have used the fact that, when A runs over all the configurations with $u \in A$, A^* runs over all the configurations with $u \notin A^*$. This immediately implies

$$\langle \chi[u\in A]\rangle_{\mu} = \frac{Z_{u\in A}}{Z_{u\in A} + Z_{u\notin A}} \le \frac{1}{1+e^{-\mu}/2}. \tag{4.18}$$

By summing up the inequality over u, we get

$$\langle \hat{N}_{\mathrm{e}}\rangle_{\mu} \le \frac{|V|}{1+e^{-\mu}/2}, \tag{4.19}$$

which is nothing but the desired upper bound in (2.11).

We shall now prove the lower bound in (2.11). Let b be a $3\times\cdots\times 3$ (hyper-)cubic region in V, and u be the site at the center of b. Take an arbitrary configuration A with $A\cap b = \emptyset$, and let A^* be the unique configuration obtained by adding the site u to A. Then we have $2e^{\mu}W(A) = W(A^*)$. As in the above we see that

$$\langle \chi[A\cap b \ne \emptyset]\rangle_{\mu} = \frac{Z_{A\cap b\ne\emptyset}}{Z_{A\cap b=\emptyset} + Z_{A\cap b\ne\emptyset}} \ge \frac{Z_{A\cap b=u}}{Z_{A\cap b=\emptyset} + Z_{A\cap b=u}} = \frac{1}{1+e^{-\mu}/2}. \tag{4.20}$$

The quantity in the left hand side is the probability that there is at least one occupied site among the 3^d sites in b. By summing up (4.20) over all the nonoverlapping $3\times\cdots\times 3$ (hyper)cubes in V, we get

$$\langle \hat{N}_{\mathrm{e}}\rangle_{\mu} \ge \frac{|V|}{3^d(1+e^{-\mu}/2)}, \tag{4.21}$$

which is the desired lower bound in (2.11).

4.3 Low density bounds

We shall prove the bounds which are valid when the chemical potential μ is negative and its absolute value is large.

Let $\mathcal{C}[A] = \{C_1, \cdots, C_n\}$ be the set of connected clusters in a configuration A. Take a connected set C of sites in V. For any configuration A with $C \in \mathcal{C}[A]$, we denote by A^* the configuration obtained by eliminating C from A. When A runs over all the configurations with $C \in \mathcal{C}[A]$, A^* runs over all the configurations with $\bar{C}\cap A^* = \emptyset$, where $\bar{C}$ is a set obtained by adding neighboring sites to C. We have $W(A) = e^{\mu|C|}(|C|+1)W(A^*)$, and thus

$$\langle \chi[C\in\mathcal{C}[A]]\rangle_{\mu} = \frac{Z_{C\in\mathcal{C}[A]}}{Z_{\bar{C}\cap A\ne\emptyset} + Z_{\bar{C}\cap A=\emptyset}} \le \frac{Z_{C\in\mathcal{C}[A]}}{Z_{\bar{C}\cap A=\emptyset}} = e^{\mu|C|}(|C|+1). \tag{4.22}$$

Note that, when μ is negative and large, the right hand side converges to zero rapidly as the cluster becomes large. ¿From the representations (4.9) and (4.11), we get

$$
\begin{aligned}
\langle(\mathbf{S}_{\mathrm{tot}})^2\rangle_\mu - \frac{3}{4}\langle\hat{N}_{\mathrm{e}}\rangle_\mu &= \sum_{C\subset V}\frac{1}{4}(|C|^2-|C|)\langle\chi[C\in\mathcal{C}[A]]\rangle_\mu \\
&= |V|\sum_{C\ni o}\frac{1}{4}(|C|^2-|C|)\langle\chi[C\in\mathcal{C}[A]]\rangle_\mu,
\end{aligned}
\tag{4.23}
$$

where, in the right hand side, the sum is over all the connected set C which contains a fixed lattice site o. We have made use of the translation invariance to get the final equality. The standard argument shows that the number of such connected C with n sites can bounded from above by a^n where a is a positive constant which depends only on the dimension d. By substituting the bound (4.22) into (4.23), we get

$$
\begin{aligned}
\langle(\mathbf{S}_{\mathrm{tot}})^2\rangle_\mu - \frac{3}{4}\langle\hat{N}_{\mathrm{e}}\rangle_\mu &\le |V|\sum_{n=1}^{\infty}a^n\frac{1}{4}(n^2-n)(n+1)e^{\mu n} \\
&\le c_3\,|V|\,e^{2\mu},
\end{aligned}
\tag{4.24}
$$

where the final bound is valid when $-\mu$ is sufficiently large and the sum converges. Here c_3 is a positive finite constant which depends only on the dimension d. The upper bound in (2.16) has been proved.

4.4 High density bounds

We shall prove the bounds which are valid when μ is positive and large enough. Our proofs are based on a variation of the Peierls argument, which is standard in spin systems [6] and percolation [7]. Let us recall that we have assumed that V is a d-dimensional hypercubic lattice with periodic boundary conditions.

Let $\overline{A} = V\backslash A$, which may be called the set of unoccupied sites, or defects. Again this can be decomposed into connected components as $\overline{A} = D_1\cup\cdots\cup D_m$, and we denote by $\mathcal{D}[A]$ the set $\{D_1,\cdots,D_m\}$. Take a connected set D. The set $V\backslash D$ decouples into several connected components. We call the largest connected component the exterior of D, and other components the interior of D.

Take a connected set D, and let A be an arbitrary configuration with $D\in\mathcal{D}[A]$. We denote by A^* the configuration obtained by adding to A all the sites of D. Let $C_j^D\in\mathcal{C}[A]$ with $j=0,\cdots,p$ be the connected clusters in A which are adjacent to the defect D. We choose the numbering so that C_0^D lies in the exterior of D, and C_j^D with $j=1,\cdots,p$ in the interior. See Fig.2.

Now the ratio of the weights for the configurations A and A^* can be evaluated as

$$
\begin{aligned}
\frac{W(A)}{W(A^*)} &= e^{-\mu|D|}\frac{\prod_{j=0}^{p}(|C_j^D|+1)}{(\sum_{j=0}^{p}|C_j^D|+|D|+1)} \\
&\le e^{-\mu|D|}\prod_{j=1}^{p}(|C_j^D|+1).
\end{aligned}
\tag{4.25}
$$

Since each C_j^D with $j = 1, 2, \cdots, p$ is in the interior of D, it must be surrounded by sites in D. Let d_j be the number of sites in D which are directly surrounding the cluster C_j^D. Then we get the following bound.

$$\begin{aligned}\prod_{j=1}^{p}(|C_j^D|+1) &\leq c' \max_{\{d_1,\cdots,d_p\},d_j\geq 1,\sum_{j=1}^{p}d_j\leq 2|D|}\prod_{j=1}^{p}(d_j)^{d/(d-1)} \\ &\leq c'(\frac{|D|}{p})^{pd/(d-1)} \leq c' \max_q(\frac{|D|}{q})^{qd/(d-1)} \\ &\leq c' \exp[\alpha|D|], \end{aligned} \tag{4.26}$$

where c' is a constant, and $\alpha = d/\{e(d-1)\}$. Thus we get the bound

$$\langle\chi[D \in \mathcal{D}[A]]\rangle_\mu \leq \frac{Z_{D\in\mathcal{D}[A]}}{Z_{D\notin\mathcal{D}[A]}} \leq c' e^{-(\mu-\alpha)|D|}. \tag{4.27}$$

Note that when μ is sufficiently large, the probability to find a larger defect becomes exponentially small.

We will construct a lower bound for the electron number. ¿From the representation (4.11), and the definition of the defects $\{D_1, \cdots, D_m\}$, we get

$$\begin{aligned}|V| - \langle\hat{N}_\mathrm{e}\rangle_\mu &= \frac{1}{Z}\sum_{A\subset V}W(A)\sum_{k=1}^{m}|D_k| = \sum_{D\subset V}\langle\chi[D\in\mathcal{D}[A]]\rangle_\mu|D| \\ &= |V|\sum_{D\ni o}\langle\chi[D\in\mathcal{D}[A]]\rangle_\mu|D|, \end{aligned} \tag{4.28}$$

where the sum in the right hand side is over all the connected sets which contains a fixed lattice site o. We have made use of the translation invariance as in (4.23). ¿From the bound (4.27) and the same entropy estimate as in (4.24), we get

$$|V| - \langle\hat{N}_\mathrm{e}\rangle_\mu \leq |V|\sum_{n=1}^{\infty}a^n n c' e^{-(\mu-\alpha)n} \leq c_1|V|e^{-\mu}, \tag{4.29}$$

where the final inequality holds when μ is large enough and the sum converges, and c_1 is a positive finite constant which depends only on the dimension. Thus we have proved the lower bound (2.12) for the electron number.

We will now prove the lower bound for the total spin in (2.15), which establishes the appearance of ferromagnetism. (Note that the upper bound in (2.15) is trivial.) Let A be a configuration and $\mathcal{D}[A]$ be the set of the corresponding defects. By $\mathrm{ext}(D)$ we denote the exterior of an deffect D. Define

$$C_\mathrm{ext} = \bigcap_{D\in\mathcal{D}[A]}\mathrm{ext}(D), \tag{4.30}$$

which is indeed an element in $\mathcal{C}[A]$. For a connected cluster (defect) D, we denote by $v(D)$ the total number of sites in D and in its interior. Then there is a trivial inequality

$$|C_\mathrm{ext}| \geq |V| - \sum_{D\in\mathcal{D}[A]}v(D). \tag{4.31}$$

¿From (4.31) and the representation (4.9), we now have

$$\begin{aligned}
\langle(\mathbf{S}_{\rm tot})^2\rangle_\mu &\ge \frac{1}{Z}\sum_{A\subset V} W(A)\frac{|C_{\rm ext}|}{2}\left(\frac{|C_{\rm ext}|}{2}+1\right)\\
&\ge \frac{1}{Z}\sum_{A\subset V} W(A)\frac{|V|-\sum v(D)}{2}\left(\frac{|V|-\sum v(D)}{2}+1\right)\\
&\ge \frac{1}{Z}\sum_{A\subset V} W(A)\left\{S_{\rm max}(S_{\rm max}+1)-\left(|V|+\frac{1}{2}\right)\sum_{D\in\mathcal{D}[A]} v(D)\right\}\\
&= S_{\rm max}(S_{\rm max}+1)-\left(|V|+\frac{1}{2}\right)|V|\sum_{D\ni o}\langle\chi[D\in\mathcal{D}[A]]\rangle_\mu v(D), \qquad (4.32)
\end{aligned}$$

where $S_{\rm max}=|V|/2$. The sum in the most right hand side is over all the connected clusters including a fixed lattice site o. We have again made use of the translation invariance as in (4.23) and (4.28). Substituting the bounds $v(D)\le|D|^{d/(d-1)}$ and the entropy estimate (as in (4.24)) into (4.32), we finally get

$$\begin{aligned}
\langle(\mathbf{S}_{\rm tot})^2\rangle_\mu &\ge S_{\rm max}(S_{\rm max}+1)-(|V|+\frac{1}{2})|V|\sum_{n=1}^{\infty}a^n n^{d/(d-1)}e^{-(\mu-\alpha)n}\\
&\ge S_{\rm max}(S_{\rm max}+1)\{1-c_2e^{-\mu}\}, \qquad (4.33)
\end{aligned}$$

for sufficiently large values of μ. Here c_2 is a positive finite constant which depends only on the dimension d. Thus the lower bound in (2.15) is proved.

5 Correlation functions

In the present section, we evaluate electron-electron correlation functions for the model of Section 2 with $N_{\rm d}-2d+1\le N_{\rm e}\le N_{\rm d}$. As we have mentioned in Section 2.3, the result implies that the coherence length in the ground states is λ^{-1}.

Let $\langle\cdots\rangle$ be the usual microcanonical average for some fixed $N_{\rm e}\le N_{\rm d}$. For an arbitrary operator O, it may be expressed as

$$\langle O\rangle=\frac{\sum_{A,\{m_k\};|A|=N_{\rm e}} o(A,\{m_k\};A,\{m_k\})}{\sum_{A,\{m_k\};|A|=N_{\rm e}} 1}. \qquad (5.1)$$

Then one obtains

Lemma 5.1 *If for a given $N_{\rm e}\le N_{\rm d}$ all ground states have the total spin $S_{\rm tot}=N_{\rm e}/2$, then*

$$\sum_\sigma\langle c_{x\sigma}^\dagger c_{y\sigma}\rangle=\frac{N_{\rm e}}{N_{\rm d}}\sum_{u\in V}\kappa_x^{(u)}\varphi_y^{(u)}. \qquad (5.2)$$

Proof: Since the operator $O_{xy}=\sum_\sigma c_{x\sigma}^\dagger c_{y\sigma}$ is $SU(2)$ invariant, it suffices to consider the expectation value in the subspace where all spins are $\uparrow$. We thus get

$$\langle O_{xy}\rangle=\binom{N_{\rm d}}{N_{\rm e}}^{-1}\sum_{A;|A|=N_{\rm e}} o_{xy}(A,\uparrow;A,\uparrow), \qquad (5.3)$$

where $o_{xy}(A,\uparrow;A,\uparrow)$ are the matrix elements of O_{xy} in the subspace with all spins $\uparrow$. Using the expansion formulas (3.18) and (3.19), these matrix elements may be written as

$$\begin{aligned} o_{xy}(A,\uparrow;A,\uparrow) &= \sum_{u,v\in V} \kappa_x^{(u)}\varphi_y^{(v)}\tilde{o}_{uv}(A,\uparrow;A,\uparrow) \\ &= \sum_{u\in V} \kappa_x^{(u)}\varphi_y^{(u)}\tilde{o}_{uu}(A,\uparrow;A,\uparrow), \end{aligned} \tag{5.4}$$

where $\tilde{o}_{uv}(A,\uparrow;A,\uparrow)$ are the matrix elements of $\tilde{O}_{uv}=a_{u\uparrow}^\dagger b_{v\uparrow}$ and we used the relation

$$\tilde{o}_{uv}(A,\uparrow;A,\uparrow)=\delta_{uv}\tilde{o}_{uu}(A,\uparrow;A,\uparrow). \tag{5.5}$$

Now,

$$\begin{aligned} \sum_{A\,;\,|A|=N_\mathrm{e}} \tilde{o}_{uv}(A,\uparrow;A,\uparrow) &= \sum_{A\ni u,|A|=N_\mathrm{e}} 1 \\ &= \binom{N_\mathrm{d}-1}{N_\mathrm{e}-1}, \end{aligned} \tag{5.6}$$

which yields the desired result. ■

Clearly, Lemma 5.1 may be applied in the case $N_\mathrm{e}=N_\mathrm{d}$ if V is connected, and in the case $N_\mathrm{e}=1$, which is trivial. As a consequence we have

Corollary 5.2 *Consider the model of Section 2 in the subspace with the electron number fixed to some value* $N_\mathrm{d}-2d+1\le N_\mathrm{e}\le N_\mathrm{d}$. *Then*

$$\sum_\sigma\langle c_{x\sigma}^\dagger c_{y\sigma}\rangle\simeq\sqrt{\frac{\pi}{2}}(2\pi)^{-d}\lambda^{(d-3)/2}(-1)^{\|x-y\|_1}\,|x-y|^{-(d-1)/2}\exp[-\lambda\,|x-y|] \tag{5.7}$$

for $L\gg 1$ *and* $\lambda\,|x-y|\gg 1$, *where* $\|x\|_1=\sum_{j=1}^d|x_j|$.

Proof: Since any $A\subset V$ with $|V|-2d+1\le|A|$ is connected, we find that any ground state has $S_\mathrm{tot}=N_\mathrm{e}/2$ if $N_\mathrm{d}-2d+1\le N_\mathrm{e}\le N_\mathrm{d}$. This allows us to use Lemma 5.1.

It remains to calculate $\kappa_x^{(y)}$. The Gramm matrix (3.8) for the basis (2.8) is given by

$$(G)_{uv}=\begin{cases}1+2d\lambda^{-2} & \text{if } u=v,\\ \lambda^{-2} & \text{if } |u-v|=1,\\ 0 & \text{otherwise.}\end{cases} \tag{5.8}$$

The inverse can be calculated as

$$(G^{-1})_{uv}=(-1)^{\|u-v\|_1}(2\pi)^{-d}\int_{k\in(-\pi,\pi]^d}d^dk\,\frac{\lambda^2e^{ik\cdot(u-v)}}{\sum_{j=1}^d(2\sin[k_j/2])^2+\lambda^2}. \tag{5.9}$$

The integral $(2\pi)^{-d}\int d^dk$ is a shorthand for the sum $L^{-d}\sum_k$ where $k=(2\pi n_1/L,\ldots,2\pi n_d/L)$ with integers n_j such that $-L/2<n_j\le L/2$. Since the definition (3.9) implies $\kappa_x^{(y)}=(G^{-1})_{yx}$ for $x\in V$, the desired expression for the correlation function (5.7) follows by

combining (5.2), (5.9) and the standard asymptotic evaluation of the integral (sum) in (5.9). ■

Just as one cannot conclude from the vanishing charge gap (2.17) in the case $N_{\rm d}-2d+1 \le N_{\rm e} < N_{\rm d}$ that the system is a metal, one cannot conclude from the exponential decay in (5.7) that the electrons are localized. In the case $N_{\rm e} \le N_{\rm d}$ this exponential decay is due to the ground state degeneracy. λ^{-1} is the phase coherence length and not the localization length.

Before closing the section, let us briefly discuss why we are not able to calculate the correlation function in general situation with $\mu < \infty$. In the grand canonical ensemble, we also have

$$\begin{aligned}\langle c^\dagger_{x\sigma} c_{y\sigma}\rangle_\mu &= \sum_{u,v\in V} \kappa^{(u)}_x \varphi^{(v)}_y \langle a^\dagger_{u\sigma} b_{v\sigma}\rangle_\mu + \sum_{u\in V} \kappa^{(u)}_x \langle a^\dagger_{u\sigma} d_{y\sigma}\rangle_\mu + \sum_{u\in V} \varphi^{(u)}_y \langle d^\dagger_{x\sigma} b_{u\sigma}\rangle_\mu + \langle d^\dagger_{x\sigma} d_{y\sigma}\rangle_\mu \\ &= \sum_{u,v\in V} \kappa^{(u)}_x \varphi^{(v)}_y \langle a^\dagger_{u\sigma} b_{v\sigma}\rangle_\mu . \end{aligned} \tag{5.10}$$

But (5.5) only holds in the subspace with $S_{\rm tot} = N_{\rm e}/2$. The reason is that only in this subspace all the states that can be constructed using the operators $a^\dagger_{u\sigma}$ are ground states of H. Therefore, the dual basis in this subspace is simply given by all the states constructed using the operators $b_{u\sigma}$, and $\tilde{o}_{uv}(A,\uparrow;A,\uparrow)$ has the simple form (5.5). In all the other subspaces with $S_{\rm tot} < N_{\rm e}/2$ the dual basis to the states (3.3) cannot easily be constructed.

The difficulty for the models with $\mu < \infty$ may be expected from a physical point of view. The ground states for $N_{\rm e} = N_{\rm d}$ are essentially the same as that of a noninteracting spinless fermion system. Calculating correlation functions should be of no difficulty. When $\mu < \infty$, on the other hand, the ground states reflect strong correlation effect, and have quite nontrivial structure. Though the expression for the ground state (3.3) appears rather simple in the nonorthogonal basis, it will become highly complicated when expressed in the standard orthogonal basis.

6 Spin Hamiltonian and spin wave excitations

In the present section, we rigorously derive a "spin Hamiltonian" of our Hubbard model. More precisely we show that the interaction Hamiltonian $H_{\rm int}$, when projected onto a certain subspace which includes ground states, exactly reduces to the Hamiltonian of the ferromagnetic Heisenberg model. In the model with exactly half-filled degenerate band, we prove that there is a set of low energy excited states whose excitation energies are bounded from above by that of the spin wave excitations of the Heisenberg model. This result suggests that our Hubbard model has a "normal" spin excitation structure. Based on a trial state calculation, Kusakabe and Aoki recently [16] argued that the closely related Hubbard model with $U = \infty$ has low-lying excitations which are expected for a "normal" itinerant electron system with ferromagnetic order.

We first discuss the general class of models as in Section 3. For a subset $A \subset V$, we define a (non-orthogonal) projection operator P_A by the following procedure. Given an arbitrary state Φ, we can uniquely decompose it as

$$\Phi = \Psi + \sum_{A_\uparrow, A_\downarrow} f(A_\uparrow, A_\downarrow) \prod_{u \in A_\uparrow} a^\dagger_{u\uparrow} \prod_{v \in A_\downarrow} a^\dagger_{v\downarrow} \Phi_0, \tag{6.1}$$

where Ψ is orthogonal to the space with $H_{\rm hop}\Phi = N_{\rm e}\varepsilon_0\Phi$. We define

$$P_A\Phi = \sum_{A_\uparrow, A_\downarrow;\, A_\uparrow \cup A_\downarrow = A,\, A_\uparrow \cap A_\downarrow = \emptyset} f(A_\uparrow, A_\downarrow) \prod_{u \in A_\uparrow} a^\dagger_{u\uparrow} \prod_{v \in A_\downarrow} a^\dagger_{v\downarrow} \Phi_0. \tag{6.2}$$

By using the expansion formulas (3.18) and (3.19), we get

$$n_{x\uparrow}n_{x\downarrow} = (\sum_q \kappa^{(q)}_x a^\dagger_{q\uparrow} + d^\dagger_{x\uparrow})(\sum_r \varphi^{(r)}_x b_{r\uparrow} + d_{x\uparrow})(\sum_s \kappa^{(s)}_x a^\dagger_{s\downarrow} + d^\dagger_{x\downarrow})(\sum_t \varphi^{(t)}_x b_{t\downarrow} + d_{x\downarrow}). \tag{6.3}$$

Let a site $x \in \Lambda$ be such that there is an index $u \in V$ with $x(u) = x$, where $x(u)$ is defined in the *quasi locality* condition B1 in Section 3.1. Then from (6.3) we get

$$P_A n_{x\uparrow}n_{x\downarrow} P_A = P_A \sum_{q,s \in V} \kappa^{(q)}_x \varphi^{(u)}_x \kappa^{(s)}_x \varphi^{(u)}_x a^\dagger_{q\uparrow} b_{u\uparrow} a^\dagger_{s\downarrow} b_{u\downarrow} P_A = 0. \tag{6.4}$$

Next take a site $x \in \Lambda$ such that there are indices $u, v \in V$ with $\varphi^{(u)}_x \varphi^{(v)}_x \neq 0$. ¿From the *local connectivity* condition B2 and (6.3), we have

$$\begin{aligned} P_A n_{x\uparrow}n_{x\downarrow} P_A &= P_A \sum_{q,r,s,t \in V} \kappa^{(q)}_x \varphi^{(r)}_x \kappa^{(s)}_x \varphi^{(t)}_x a^\dagger_{q\uparrow} b_{r\uparrow} a^\dagger_{s\downarrow} b_{t\downarrow} P_A \\ &= \kappa^{(u)}_x \kappa^{(v)}_x \varphi^{(u)}_x \varphi^{(v)}_x (a^\dagger_{u\uparrow} b_{u\uparrow} a^\dagger_{v\downarrow} b_{v\downarrow} + a^\dagger_{u\uparrow} b_{v\uparrow} a^\dagger_{v\downarrow} b_{u\downarrow} \\ &\quad + a^\dagger_{v\uparrow} b_{u\uparrow} a^\dagger_{u\downarrow} b_{v\downarrow} + a^\dagger_{v\uparrow} b_{v\uparrow} a^\dagger_{u\downarrow} b_{u\downarrow}) P_A. \end{aligned} \tag{6.5}$$

Let us introduce spin operators for the state $\varphi^{(u)}$ by

$$\tilde{S}^{(\alpha)}_u = \sum_{\sigma,\tau = \uparrow,\downarrow} a^\dagger_{u\sigma} p^{(\alpha)}_{\sigma\tau} b_{u\tau}/2, \tag{6.6}$$

where $p^{(\alpha)}_{\sigma\tau}$ with $\alpha = 1, 2, 3$ are the Pauli matrices (1.9). The operators $\tilde{S}^{(\alpha)}_u$ are not self-adjoint, but have exactly the same algebraic structure (*i.e.*, commutation relations) as the standard spin operators. Using these operators, (6.5) can be rewritten as

$$P_A n_{x\uparrow}n_{x\downarrow} P_A = \kappa^{(u)}_x \kappa^{(v)}_x \varphi^{(u)}_x \varphi^{(v)}_x \left(\frac{1}{2} - 2\tilde{\mathbf{S}}_u \cdot \tilde{\mathbf{S}}_v\right) P_A. \tag{6.7}$$

By substituting (6.7) into the definition (1.3) of the interaction Hamiltonian, we get the desired "spin Hamiltonian"

$$P_A H_{\rm int} P_A = \sum_{u,v \in V} J_{uv} \left(\frac{1}{2} - 2\tilde{\mathbf{S}}_u \cdot \tilde{\mathbf{S}}_v\right) P_A, \tag{6.8}$$

where the "exchange interaction" is given by

$$J_{uv} = \sum_x U_x \kappa^{(u)}_x \kappa^{(v)}_x \varphi^{(u)}_x \varphi^{(v)}_x. \tag{6.9}$$

If the "exchange interaction" J_{uv} is nonnegative, the "spin Hamiltonian" (6.8) is nothing but the Hamiltonian of the ferromagnetic Heisenberg model. We expect that the "spin Hamiltonian" (6.8) approximately describes low energy excited states which involve only spin degrees of freedom.

In [30] it was shown that a class of models with certain global symmetry has $J_{uv} > 0$ for directly connected u, v. The proof of ferromagnetism in [30] was based on this observation. Note, however, that the proof in Section 3.2 no longer requires symmetry conditions.

We can explicitly evaluate J_{uv} for the model of Section 2. By combining the definition (2.8) of the basis state $\varphi_x(u)$, the definition (3.9) of $\kappa_x^{(u)}$, and the formula (5.9) for $(G^{-1})_{uv}$, we get

$$J_{uv} = \begin{cases} J(\lambda) > 0 & \text{if } |u-v| = 1, \\ 0 & \text{otherwise,} \end{cases} \tag{6.10}$$

where

$$\begin{aligned} J(\lambda) &= U' \left((2\pi)^{-d} \int_{k \in (-\pi,\pi]^d} d^d k \frac{1-\cos(k_1)}{\sum_{j=1}^d (2\sin(k_j/2))^2 + \lambda^2} \right)^2 \\ &\simeq \begin{cases} U' C_d & \text{as } \lambda \downarrow 0, \\ U' \lambda^{-4} & \text{for } \lambda \gg 1. \end{cases} \end{aligned} \tag{6.11}$$

The constant C_d depends only on the dimension d.

The form of the "spin Hamiltonian" (6.8) suggests that the model has spin wave excitations when there is a ferromagnetic order in the ground states. For the model with $N_{\mathrm{e}} = N_{\mathrm{d}}$, we can prove the existence of low energy excited states as follows.

Theorem 6.1 *Consider the model of Section 2 in the subspace with the electron number fixed to $N_{\mathrm{e}} = N_{\mathrm{d}}$. To each wave vector $k = (2\pi n_1/L, \ldots, 2\pi n_d/L) \neq (0, \ldots, 0)$ with integers $-L/2 < n_j \leq L/2$, there corresponds an excited state whose excitation energy is bounded from above by a function $E_L(k)$. In the infinite volume limit $L \to \infty$, $E_L(k)$ converges to an analytic function $E(k)$ which satisfies*

$$E(k) = J(\lambda)|k|^2 + O(|k|^4). \tag{6.12}$$

Recall that the dispersion relation of the spin wave excitations for the Heisenberg Hamiltonian (6.8) is

$$E_{\mathrm{SW}}(k) = 2J(\lambda) \sum_{j=1}^{d} (1 - \cos k^{(j)}), \tag{6.13}$$

which has the same asymptotic behavior as (6.12).

Proof: Let us define the "one magnon state" by

$$\Psi_k = \sum_{u \in V} e^{ik\cdot u} \tilde{S}_u^- \Phi_{V\uparrow}, \tag{6.14}$$

where $\tilde{S}_u^- = \tilde{S}_u^{(1)} - i\tilde{S}_u^{(2)} = a_{u\downarrow}^\dagger b_{u\uparrow}$, and $\Phi_{V\uparrow} = \prod_{v\in V} a_{v\uparrow}^\dagger \Phi_0$. Note that Ψ_k with different k are orthogonal to each other, and Ψ_k with $k \neq (0, \ldots, 0)$ is orthogonal to the ground states. If we denote the energy expectation value as

$$E_L(k) = \frac{(\Psi_k, H\,\Psi_k)}{(\Psi_k, \Psi_k)}, \tag{6.15}$$

the first part of the theorem follows from the standard variational argument.

It now remains to evaluate $E_L(k)$. As for the denominator of (6.15), we have

$$\begin{aligned}(\Psi_k, \Psi_k) &= \sum_{u,v} e^{ik\cdot(v-u)}(a^\dagger_{u\downarrow}b_{u\uparrow}\Phi_{V\uparrow}, a^\dagger_{v\downarrow}b_{v\uparrow}\Phi_{V\uparrow}) \\ &= \sum_{u,v} e^{ik\cdot(v-u)}(G)_{uv}(G^{-1})_{uv}(\Phi_{V\uparrow}, \Phi_{V\uparrow}) \\ &= L^d \sum_u e^{-ik\cdot u}(G)_{uo}(G^{-1})_{uo}(\Phi_{V\uparrow}, \Phi_{V\uparrow}), \end{aligned} \tag{6.16}$$

where o denotes an arbitrary fixed site in V. The second line of (6.16) follows from the anticommutation relations $\{a_{u\sigma}, a^\dagger_{v\tau}\} = (G)_{uv}\delta_{\sigma\tau}$, $\{b_{u\sigma}, b^\dagger_{v\tau}\} = (G^{-1})_{uv}\delta_{\sigma\tau}$, and the relations $b^\dagger_{u\uparrow}\Phi_{V\uparrow} = a_{u\downarrow}\Phi_{V\uparrow} = 0$. The third line follows from the translation invariance.

The numerator of (6.15) can be evaluated in a similar manner, although the calculation is more complicated. By using the representation (6.3), we have

$$\begin{aligned}(\Psi_k, n_{x\uparrow}n_{x\downarrow}\Psi_k) &= \sum_{u,v} e^{ik\cdot(v-u)} \sum_{q,r,s,t} \kappa^{(q)}_x\varphi^{(r)}_x\kappa^{(s)}_x\varphi^{(t)}_x(a^\dagger_{u\downarrow}b_{u\uparrow}\Phi_{V\uparrow}, a^\dagger_{q\uparrow}b_{r\uparrow}a^\dagger_{s\downarrow}b_{t\downarrow}a^\dagger_{v\downarrow}b_{v\uparrow}\Phi_{V\uparrow}) \\ &= \sum_{u,v} e^{ik\cdot(v-u)} \sum_{q,r,s,t} \kappa^{(q)}_x\varphi^{(r)}_x\kappa^{(s)}_x\varphi^{(t)}_x\delta_{vt}(G)_{us}\{\delta_{qr}(G^{-1})_{uv} - \delta_{qv}(G^{-1})_{ur}\} \\ &\quad \times(\Phi_{V\uparrow}, \Phi_{V\uparrow}) \\ &= \sum_{u,v,r,s} e^{-ik\cdot u}(e^{ik\cdot v} - e^{ik\cdot r})\kappa^{(r)}_x\varphi^{(r)}_x\kappa^{(s)}_x\varphi^{(v)}_x(G)_{us}(G^{-1})_{uv}(\Phi_{V\uparrow}, \Phi_{V\uparrow}) \\ &= L^d \sum_{u,r,s} e^{-ik\cdot u}(1 - e^{ik\cdot r})\kappa^{(r)}_x\varphi^{(r)}_x\kappa^{(s)}_x\varphi^{(o)}_x(G)_{us}(G^{-1})_{uo}(\Phi_{V\uparrow}, \Phi_{V\uparrow}). \end{aligned} \tag{6.17}$$

Summing up (6.17) over x, dividing the result by (6.16), and noting that $H_{\rm hop}\Psi_k = 0$, we finally get

$$E_L(k) = \frac{\sum_{x\in\Lambda}\sum_{u,r,s\in V} e^{-ik\cdot u}(1 - e^{ik\cdot r})U_x\kappa^{(r)}_x\varphi^{(r)}_x\kappa^{(s)}_x\varphi^{(o)}_x(G)_{us}(G^{-1})_{uo}}{\sum_{u\in V} e^{-ik\cdot u}(G)_{uo}(G^{-1})_{uo}}, \tag{6.18}$$

which converges to an analytic function of k as $L \to \infty$. By expanding (6.18) in k, we find

$$\begin{aligned} E(k) &= \frac{\frac{1}{2}\sum_x\sum_{u,r,s}(k\cdot r)^2U_x\kappa^{(r)}_x\varphi^{(r)}_x\kappa^{(s)}_x\varphi^{(o)}_x(G)_{us}(G^{-1})_{uo}}{\sum_u(G)_{uo}(G^{-1})_{uo}} + O(|k|^4) \\ &= J(\lambda)|k|^2 + O(|k|^4), \end{aligned} \tag{6.19}$$

which is the desired estimate. ■

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Figure Captions

Fig.1 The decorated square lattice. The hopping matrix elements are given by $t_{xy} = t$ for a black line, $t_{xy} = \lambda t$ for a gray line, $t_{xx} = 4t$ for a site x of the square lattice, and $t_{xx} = \lambda^2 t$ for a site x at the middle of a bond, where $t, \lambda > 0$. The on-site Coulomb repulsion is nonvanishing for any site. It is proved that the ground states exhibit ferromagnetism when the electron filling factor ρ is not more than and sufficiently close to $\rho_0 = 1/6$, and paramagnetism when ρ is sufficiently small.

Fig.2 The defect $D \in \mathcal{D}[A]$ and nearby clusters. The white regions represent the occupied sites.