Ferromagnetism in the Hubbard Models with Degenerate Single-Electron Ground States

Hal Tasaki

Department of Physics, Gakushuin University, Mejiro, Toshima-ku, Tokyo 171, Japan

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We study a class of Hubbard models in which the corresponding single-electron ground states have bulk degeneracy. We prove that the ground states of the models exhibit ferromagnetism when the electron filling factor is not more than and sufficiently close to $\rho_0=|V|/2|\Lambda|$ (where $|V|$ is the dimension of degeneracy and $|\Lambda|$ is the number of sites), and exhibit paramagnetism when the filling factor is sufficiently small. This is the first time that a three-dimensional itinerant-electron system is proved to exhibit ferromagnetism in a finite range of the electron filling factor.

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The derivation of ferromagnetism from a reasonably fundamental model of itinerant electrons, such as the Hubbard model [1], is a challenging problem in theoretical and mathematical physics. Rigorous examples of ferromagnetic ground states in certain Hubbard models have been obtained by Nagaoka [2], Lieb [3], and Mielke [4]. Each of these results covers a general class of models satisfying certain conditions, but works only for a special value of the electron number. Recently Mielke has extended his results to a finite range of the filling factor in two-dimensional models [5].

In the present Letter, we study a class of Hubbard models in which the corresponding single-electron ground states have bulk degeneracy (as in the Mielke's models [4,5]). We prove that the (many-electron) ground states exhibit ferromagnetism when the electron filling factor is not more than and sufficiently close to $\rho_0=|V|/2|\Lambda|$ (where $|V|$ is the dimension of degeneracy and $|\Lambda|$ is the number of sites in the lattice), and exhibit paramagnetism when the filling factor is sufficiently small. As far as we know, this is the first time that a three-dimensional itinerant-electron system is proved to exhibit ferromagnetism in a finite range of the electron filling factor.

Our results indicate that there is a mechanism generated by electron interactions which selects ferromagnetic states as ground states. The mechanism is most clearly seen in Eq. (14) where the Hamiltonian for the Coulomb interaction, represented in a certain nonorthogonal basis, is reduced to that of the ferromagnetic Heisenberg model. This can be regarded as a rigorous example of exchange interactions which are ferromagnetic. The selection mechanism works most effectively when the degenerate single-electron states are nearly "saturated," but becomes ineffective when the electron density is too small. Although the models treated in the present paper are still artificial, we expect 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, provided that a certain saturation condition is satisfied and the Coulomb interaction is sufficiently large. We hope that the present examples shed light on mechanisms of the actual ferromagnetism observed in, e.g., transient metals [6].

Here we describe our results for the simplest class of models. Generalizations and some technical details of the proofs will appear elsewhere [7].

Consider the d-dimensional hypercubic lattice with periodic boundary conditions [8]. We denote by V the (ordered) set of sites (denoted as u, v, w, ...) and by B the set of bonds (i.e., unoriented pairs of neighboring sites) in the lattice. 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. M is the set of $m(v,w)$ for all the bonds in B.

We consider the Hubbard model [9] on the decorated lattice $\Lambda=V\cup M$ with the Hamiltonian $H=H_{\rm hop}+H_{\rm int}$ where

$$H_{\rm hop}=\sum_{\sigma=\uparrow,\downarrow}\sum_{\{v,w\}\in B} t(c_{v\sigma}^{\dagger}+c_{w\sigma}^{\dagger}+\lambda c_{m(v,w)\sigma}^{\dagger})(c_{v\sigma}+c_{w\sigma}+\lambda c_{m(v,w)\sigma}),\quad H_{\rm int}=U\sum_{u\in V} n_{u\uparrow}n_{u\downarrow}+U'\sum_{x\in M} n_{x\uparrow}n_{x\downarrow}, \tag{1}$$

with $t>0$, $\lambda>0$, $U>0$, and $U'>0$ (see Fig. 1). As usual $c_{x\sigma}^{\dagger}$, $c_{x\sigma}$, and $n_{x\sigma}=c_{x\sigma}^{\dagger}c_{x\sigma}$ are the creation, the annihilation, and the number operators, respectively, of an electron at site x (in Λ) with spin σ. The total electron number operator is $N_e=\sum_{x\in\Lambda}(n_{x\uparrow}+n_{x\downarrow})$, and the electron filling factor is $\rho=N_e/2|\Lambda|$. (In general $|X|$ denotes the number of sites in a lattice X.) We define the spin operators by $S_x^{+}=c_{x\uparrow}^{\dagger}c_{x\downarrow}$, $S_x^{-}=(S_x^{+})^{\dagger}$, $S_x^{3}=(n_{x\uparrow}-n_{x\downarrow})/2$. The square of the total spin operator is given by $(\mathbf{S}_{\rm tot})^2=\sum_{x,y\in\Lambda}\{(S_x^{+}S_y^{-}+S_x^{-}S_y^{+})/2+S_x^{3}S_y^{3}\}$.

The single-electron eigenstate $\{\varphi_x\}_{x\in\Lambda}$ corresponding to $H_{\rm hop}$ is determined by the Schrödinger equation

$$H_{\rm hop}\sum_x \varphi_x c_{x\sigma}^{\dagger}\Phi_0=\varepsilon\sum_x \varphi_x c_{x\sigma}^{\dagger}\Phi_0, \tag{2}$$

where Φ_0 is the vacuum state. In the present model, the minimum eigenvalue of (2) is $\varepsilon=0$, and the corresponding eigenfunctions (single-electron ground states) are characterized by the property that $\varphi_v+\varphi_w+\lambda\varphi_{m(v,w)}=0$ for all $\{v,w\}\in B$. We shall construct a complete (but not orthonormal) basis of the eigenspace with $\varepsilon=0$, which

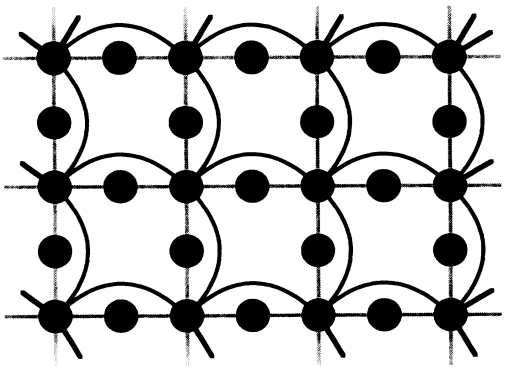

FIG. 1. The decorated square lattice. The hopping matrix elements are given by $t_{xy}=t$ for a black line, $t_{xy}=\lambda t$ for a gray line, $t_{xx}=4t$ for a site x of the square lattice, and $t_{xx}=\lambda^2 t$ for a site x at the middle of a bond, where $t,\lambda>0$. The on-site Coulomb repulsion 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 $\rho_0=\frac{1}{6}$, and exhibit paramagnetism when ρ is sufficiently small.

turns out to be $|V|$ dimensional. For each $u\in V$, we define a single-electron state $\{\varphi_x^{(u)}\}_{x\in\Lambda}$ by $\varphi_x^{(u)}=1$ if $x=u$, $\varphi_x^{(u)}=-1/\lambda$ if $x=m(u,v)$ for some v, and $\varphi_x^{(u)}=0$ for other x. We define the corresponding creation operator by $a_{u\sigma}^\dagger=\sum_x\varphi_x^{(u)}c_{x\sigma}^\dagger$. Note that the locality of our basis states does not imply that the electrons are localized, since one can always take extended basis states with definite crystal momenta. In [7] we show that the coherence length of the model can become much larger than the lattice spacing.

Let A be an arbitrary subset (sublattice) of V which is not necessarily connected. The state (with $|A|$ electrons)

$$\Phi_{A\uparrow}=\prod_{u\in A}a_{u\uparrow}^\dagger\Phi_0 \tag{3}$$

clearly satisfies $H_{\rm hop}\Phi_{A\uparrow}=0$, where 0 is the minimum possible eigenvalue of $H_{\rm hop}$. The Pauli principle implies that state (3) has no site with two electrons, and thus satisfies $H_{\rm int}\Phi_{A\uparrow}=0$, where 0 is again the minimum possible eigenvalue of $H_{\rm int}$. We see that the ferromagnetic state $\Phi_{A\uparrow}$ is an exact ground state of the full Hubbard Hamiltonian H. Such construction of a ferromagnetic ground state may be standard, but it does not lead to any strong conclusions about the magnetism of the system since there may be (and are) many other ground states.

From the above construction (3), we have found that the ground-state energy of H is 0 for the electron numbers $N_e\le|V|$. We shall investigate the properties of the ground states of H when this condition is satisfied. Employing the standard grand canonical formalism, we define

$$\langle O\rangle_\mu={\rm Tr}_0[O\exp(\mu N_e)]/{\rm Tr}_0[\exp(\mu N_e)]\,, \tag{4}$$

where O is an arbitrary operator, and the trace is taken over all the (many-electron) states with $H\Phi=0$ (as is indicated by the subscript 0). By choosing a suitable (dimensionless) chemical potential μ in (4), we recover zero-temperature properties of the system with a desired electron filling factor [10]. In the limit $\mu\to\infty$, the filling factor takes the maximum value $\rho_0=|V|/2|\Lambda|$. Our main results are the following.

Theorem 1.—In the dimensions $d\ge2$, there are finite constants c,c',μ_1,μ_2 (with $\mu_1>0>\mu_2$) which depend only on d and not on the size of the lattice. For any $\mu\ge\mu_1$, we have

$$S_{\max}(S_{\max}+1)\ge\langle(\mathbf{S}_{\rm tot})^2\rangle_\mu\ge S_{\max}(S_{\max}+1)(1-ce^{-\mu})\,, \tag{5}$$

where $S_{\max}=|V|/2$. For any $\mu\le\mu_2$, we have

$$\tfrac{3}{4}\langle N_e\rangle_\mu\le\langle(\mathbf{S}_{\rm tot})^2\rangle_\mu\le\tfrac{3}{4}\langle N_e\rangle_\mu+c'|V|e^{2\mu}\,. \tag{6}$$

The theorem 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. We expect that, in three (and higher) dimensions, the ferromagnetism persists at finite temperatures [11]. When $\mu<\infty$ the ground-state energy does not change under small variation of the filling factor, i.e., the charge gap is vanishing. Although one might expect that the present models are ferromagnetic metals, we note that the vanishing charge gap is necessary but not sufficient for an electron system to be a conductor. See [7] for further discussions on this point.

Recall that the standard mean-field (or the Hartree-Fock) approximation [1] predicts the existence of only the ferromagnetic ground states whenever D_F (the single-electron density of states at the Fermi level) is large. We have large (actually infinite) D_F for $\rho\le\rho_0$, but Theorem 1 tells us that it is not enough to guarantee the appearance of ferromagnetism. For selection of ferromagnetic states to take place, the degenerate single-electron band must be nearly "saturated" in the sense that $\rho\lesssim\rho_0$. We expect that this feature is universal in the Hubbard models with large single-electron density of states [12].

The proof of Theorem 1 is based on complete characterization of the ground states for $N_e\le|V|$. Let us begin by constructing ground states other than (3). A sublattice A (of V) can be uniquely decomposed into a disjoint union of connected components as $A=C_1\cup\cdots\cup C_n$ where all the sites in each A_k are connected via (paths of) bonds in B. Note that, in the ground state (3), electrons on different connected components may be regarded as not interacting with each other. (Of course this is a basis-dependent observation, and should not be taken literally.) For each k $(=1,\ldots,n)$, let Λ_k be a subset of Λ obtained by adding to A_k the sites in M which are nearest neighbors of sites in A_k. It is not hard to show that the state

$$\prod_{k=1}^{n}\left(\sum_{x\in\Lambda_k} S_x^-\right)^{m_k}\Phi_{A\uparrow}\,, \tag{7}$$

with $m_k=0,1,\ldots,|C_k|$ is also a ground state of H. Although state (7) is not an eigenstate of $(\mathbf{S}_{\rm tot})^2$, one can construct eigenstates by taking suitable linear combinations. One finds [7] that there even appear spin-singlet ground states when $|V|-N_e$ is at least of order L^{d-1} (where L is the linear size of the lattice). See Ref. [4] for related results.

The following theorem provides the desired complete characterization of the ground states. Mielke [5] also gave a similar complete characterization of the ground states in Hubbard models on two-dimensional line graphs.

Theorem 2.—Any state Φ with $H\Phi=0$ is a linear combination of the states (7) with various A and $\{m_k\}$.

As a special case of Theorem 2, one finds that the ground states have maximum possible spin and are nondegenerate (apart from the trivial spin degeneracy) when $N_e=|V|$, i.e., the degenerate single-electron ground states are perfectly "saturated." This fact can be proved for a general class of models including the present one [7]. Mielke [4] proved the same fact for a general class of Hubbard models on line graphs.

The proof of Theorem 1 is based on Theorem 2. We shall leave the complete proof to [7], and briefly discuss the basic idea. By using (7) we can express the expectation value of the square of the total spin as

$$\langle(\mathbf{S}_{\rm tot})^2\rangle_\mu=\frac{1}{Z}\sum_{A\subset V}W(A)\sum_{k=1}^{n}\frac{|C_k|}{2}\left(\frac{|C_k|}{2}+1\right), \tag{8}$$

where $W(A)=\prod_{k=1}^{n}e^{\mu|C_k|}(|C_k|+1)$, $Z=\sum_{A\subset V}W(A)$, and the sum is over all the subsets A of V. Representation (8) can be regarded as describing a kind of (interacting) percolation problem on the lattice V, in which the subset A corresponds to the configuration of "occupied" sites. The probability that a configuration A appears is proportional to $W(A)$. By employing suitable stochastic geometric techniques [7], we can control the percolation problem in certain regions of the parameter μ. For sufficiently large μ, it is shown that the occupied sites form a large percolating cluster. Then the representation (8) implies that this cluster carries a bulk magnetic moment. For sufficiently small μ, the occupied sites do not percolate any more, and (8) implies a paramagnetic behavior.

Proof of Theorem 2.—Note that any state Φ with $H_{\rm hop}\Phi=0$ is a linear combination of the basis states

$$\prod_{u\in A}a_{u\uparrow}^\dagger\prod_{u\in A'}a_{u\downarrow}^\dagger\Phi_0\,, \tag{9}$$

where A,A' are arbitrary subsets of V. When Φ further satisfies $H_{\rm int}\Phi=0$, a basis state (9) which has nonvanishing contribution to Φ cannot have a common element in A and A'. To see this assume that v appears in both A and A'. Then we see that the basis state (9) with A,A' contains a nonvanishing component

$$c_{v\uparrow}^\dagger c_{v\downarrow}^\dagger\left(\prod_{u\in A,\,u\neq v}a_{u\uparrow}^\dagger\right)\left(\prod_{u\in A',\,u\neq v}a_{u\downarrow}^\dagger\right)\Phi_0\,.$$

To get $H_{\rm int}\Phi=0$, the state Φ cannot contain such a term with a doubly occupied site. Since it is impossible to cancel this term with the basis states (9) with other A,A', the conclusion follows.

Thus we see that any Φ with $H\Phi=0$ is decomposed as $\Phi=\sum_{A\subset V}\Phi_A$ where each Φ_A (with A being a subset of V) is a linear combination of the basis states

$$\Phi_{A,\sigma}=\prod_{u\in A}a_{u\sigma(u)}^\dagger\Phi_0\,, \tag{10}$$

where a "spin configuration" $\sigma=\{\sigma(u)\}_{u\in A}$ is a collection of spin indices $\sigma(u)=\uparrow,\downarrow$. We further claim that each Φ_A satisfies $H\Phi_A=0$, i.e., is itself a ground state. To see this assume that, for some Φ_A and $x\in M$, we have $n_{x\uparrow}n_{x\downarrow}\Phi_A\neq0$. Let $\{v,w\}$ be the unique bond in B such that $x=m(v,w)$. Then Φ_A must have a nonvanishing component $c_{x\uparrow}^\dagger c_{x\downarrow}^\dagger\prod_{u\in A,\,u\neq v,w}c_{u\sigma(u)}^\dagger\Phi_0$. For the linear combination Φ to become a ground state, such a component must be canceled by other $\Phi_{A'}$ with $A'\neq A$, but this is impossible.

Therefore, to prove Theorem 2, it suffices to show that any ground state Φ_A which is a linear combination of the basis states (10) with a fixed A can be decomposed into a linear combination of the ground states (7). Let us define the projection operator onto the space spanned by (10). Given an arbitrary (many-electron) state Ψ, we first perform a standard orthogonal projection onto the space with $H_{\rm hop}=0$. We expand the resulting state in the basis (9), and then throw away all the basis states not in (10). We write the resulting state as $P_A\Psi$.

Let $x\in M$, and take the bond $\{v,w\}$ as the above. By applying the operator $n_{x\uparrow}n_{x\downarrow}$ onto the basis state (10), we get

$$n_{x\uparrow}n_{x\downarrow}\Phi_{A,\sigma}=\mathrm{sgn}(v,w)\lambda^{-2}c_{x\sigma(v)}^\dagger c_{x\sigma(w)}^\dagger\prod_{u\in A,\,u\neq v,w}a_{u\sigma(u)}^\dagger\Phi_0 \tag{11}$$

where $\mathrm{sgn}(v,w)$ is the fermionic sign we get by bringing v,w in front. Because of the linear independency of the single-electron states $a_{u\sigma}^\dagger$, we have a unique expansion

$$c_{x\sigma}^\dagger=\sum_{u\in V}\kappa_u^{(x)}a_{u\sigma}^\dagger+b_\sigma^{(x)\dagger}\,, \tag{12}$$

where $b_\sigma^{(x)\dagger}$ is the creation operator for a single-electron state orthogonal to the space with $H_{\rm hop}=0$. Consider the one-to-one map $V\to V$ generated by the reflection with respect to the hyperplane including x and orthogonal to the bond $\{v,w\}$. Since the expansion (12) must be invariant under the map, we see that the coefficients in (12) satisfy $\kappa_v^{(x)}=\kappa_w^{(x)}$, and hence the (reflection) positivity [13] $K=\lambda^{-2}\kappa_v^{(x)}\kappa_w^{(x)}>0$.

By substituting the expansion (12) into (11) and applying the projection P_A, we find

$$P_A n_{x\uparrow} n_{x\downarrow} \Phi_{A,\sigma} = \mathrm{sgn}(v,w) K (a^\dagger_{v\sigma(v)} a^\dagger_{w\sigma(w)} + a^\dagger_{w\sigma(v)} a^\dagger_{v\sigma(w)}) \prod_{u \in A,\, u \neq v,w} a^\dagger_{u\sigma(u)} \Phi_0 = K(\Phi_{A,\sigma} - \Phi_{A,E_{vw}\sigma}) , \quad (13)$$

where $E_{vw}\sigma$ is a spin configuration obtained from σ by exchanging $\sigma(v)$ and $\sigma(w)$. By summing up (13), we get

$$P_A H_{\mathrm{int}} \Phi_{A,\sigma} = U' K \sum_{v,w \in A,\, \{v,w\} \in B} (\Phi_{A,\sigma} - \Phi_{A,E_{vw}\sigma}) , \quad (14)$$

which is nothing but the action of the ferromagnetic Heisenberg Hamiltonian for a spin system defined on the lattice A.

Suppose that a state $\Phi_A = \sum_\sigma f_\sigma \Phi_{A,\sigma}$ satisfies $H_{\mathrm{int}}\Phi = 0$. Since we must have $P_A H_{\mathrm{int}} \Phi = 0$, (14) implies that the coefficients f_σ satisfy $\sum_{v,w \in A,\, \{v,w\} \in B} U' K (f_\sigma - f_{E_{vw}\sigma}) = 0$ for all σ. This implies that

$$2 \sum_\sigma \left\{ f_\sigma \sum_{v,w \in A,\, \{v,w\} \in B} (f_\sigma - f_{E_{vw}\sigma}) \right\} = \sum_\sigma \sum_{v,w \in A,\, \{v,w\} \in B} (f_\sigma - f_{E_{vw}\sigma})^2 = 0 .$$

It follows that f_σ takes a constant value for those σ which can be mapped onto each other by successive application of the exchange operator E_{vw}. It is not hard to see that any state with such coefficients f_σ is a linear combination of the ground states (7).

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[3] E. H. Lieb, Phys. Rev. Lett. **62**, 1201 (1989).

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[5] A. Mielke, "Exact ground states for the Hubbard model on the Kagomé lattice" (to be published). Although the main body of Mielke's paper is perfectly rigorous, it seems that his conclusions based on the percolation analogy require minor modifications. By employing the grand canonical formalism like ours, for example, it can be proved that his model exhibits ferromagnetism in a range of the chemical potential.

[6] The $3d$ band of Ni is believed to have a large single-electron density of states at the top of the band, and the filling factor is close to 1. After the hole-particle transformation, the situation becomes quite similar to that considered here.

[7] H. Tasaki (to be published).

[8] By the present method, one can treat any connected lattice with the property that, for each bond $\{v,w\}$ in B, one can take a one-to-one map $V \to V$ which preserves the lattice structure and switches v and w.

[9] Somewhat similar models are discussed in U. Brandt and A. Giesekus, Phys. Rev. Lett. **68**, 2648 (1992).

[10] Theorem 1 would be less meaningful if the filling factor $\rho = \langle N_e \rangle_\mu / 2|\Lambda|$ had pathological dependence on μ. In [7] I will show this is not the case by proving that $\rho_0 - \rho \approx e^{-\mu}$ for $\mu \gg 1$ and $\rho \approx e^{\mu}$ for $\mu \ll -1$.

[11] It is known that in one and two dimensions, ferromagnetism is always destroyed by thermal fluctuation at finite temperatures. See D. K. Ghosh, Phys. Rev. Lett. **27**, 1584 (1971); T. Koma and H. Tasaki, Phys. Rev. Lett. **68**, 3248 (1992).

[12] In both of the examples by Lieb [3] and Mielke [4,5], the single-electron ground states are degenerate and these states are perfectly or nearly "saturated." For related discussions, see K. Kusakabe and H. Aoki, J. Phys. Soc. Jpn. **61**, 1165 (1992).

[13] By using the equation $\kappa_u^{(x)} + \lambda^{-2} \sum_{u' \text{ s.t. } \{u,u'\} \in B} (\kappa_u^{(x)} + \kappa_{u'}^{(x)}) = \delta_{u,v} + \delta_{u,w}$, one can prove the positivity for some models without reflection symmetry [7].

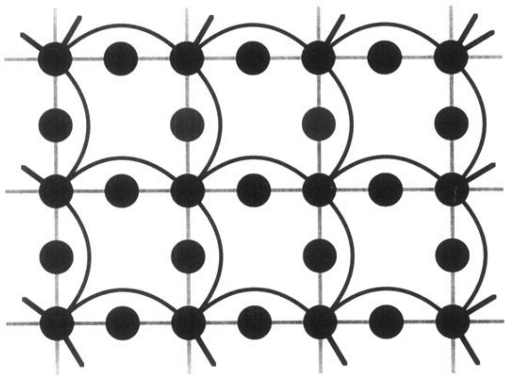

FIG. 1. The decorated square lattice. The hopping matrix elements are given by $t_{xy}=t$ for a black line, $t_{xy}=\lambda t$ for a gray line, $t_{xx}=4t$ for a site x of the square lattice, and $t_{xx}=\lambda^2 t$ for a site x at the middle of a bond, where $t,\lambda>0$. The on-site Coulomb repulsion 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 $\rho_0=\frac{1}{6}$, and exhibit paramagnetism when ρ is sufficiently small.