

Ferromagnetism in the Hubbard model with orbital degeneracy in infinite dimensions

Tsutomu Momoi and Kenn Kubo

Institute of Physics, University of Tsukuba, Tsukuba, Ibaraki 305-8571, Japan

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We study the ferromagnetism due to orbital degeneracy in the Hubbard model in infinite dimensions. The model contains the intraorbital repulsion U , the interorbital repulsion U' , the exchange J (Hund coupling) and the pair hopping J' , where all of them originate from the on-site Coulomb interaction. The ground state of the effective one-site problem was obtained by exact diagonalizations of finite clusters. At the $\frac{1}{4}$ filling, we found two insulating phases; one is a ferromagnetic phase with alternating orbital order and the other is antiferromagnetic with uniform orbital order. If electrons are doped into the $\frac{1}{4}$ filling, the ferromagnetic phase still survives and becomes metallic, while the antiferromagnetic phase disappears. This result indicates that a double-exchange mechanism is relevant to stabilize metallic ferromagnetism in infinite dimensions.

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Many investigations have been done on the Hubbard model to clarify whether the Coulomb interaction can realize ferromagnetism in itinerant electron systems. They revealed that the simple single-band Hubbard model on the hypercubic lattice does not easily show ferromagnetism and that some additional properties are necessary to stabilize ferromagnetism. There are several proposals for such properties. One is the special lattice structure (or band structure) which favors ferromagnetism. For example, ferromagnetism on the fcc lattice¹ and of the flat (or nearly flat) band model^{2,3} are discussed in this context. Another is the existence of the orbital degeneracy.⁴⁻⁶ It was argued that the on-site Hund coupling between electrons in degenerate orbitals creates indirect ferromagnetic coupling between conduction electrons.⁶

Numerical study of strongly correlated electron systems is quite difficult in higher dimensions than one. In the infinite-dimensional ($d=\infty$) limit, however, it is manageable with the aid of recently developed technique.⁷ In this limit we can treat quantum fluctuations completely, by taking local interactions into account exactly, and we can neglect spatial fluctuations. Monte Carlo simulations of the $d=\infty$ single-band Hubbard model revealed that any ferromagnetic phase does not appear on the hypercubic lattice⁸ and, on the other hand, metallic ferromagnetism occurs on the fcc-type lattice.⁹ These two results clearly show the lattice-structure dependence for the appearance of the ferromagnetism. The purpose of this paper is to clarify whether the itinerant ferromagnetism appears due to orbital degeneracy in infinite dimensions.

We study the Hubbard model with doubly degenerate orbitals at each site on the hypercubic lattice. The Hamiltonian is given by

$$\begin{aligned}
 H = \sum_{m=1,2} \left\{ -\frac{t}{2\sqrt{d}} \sum_{\substack{(i,j) \in \text{NN} \\ \sigma=\uparrow,\downarrow}} (c_{im\sigma}^\dagger c_{jm\sigma} + \text{H.c.}) \right. \\
 \left. - \mu \sum_{i,\sigma} n_{im\sigma} + U \sum_i n_{im\uparrow} n_{im\downarrow} \right\} \\
 + U' \sum_{i,\sigma,\sigma'} n_{i1\sigma} n_{i2\sigma'} - J \sum_{i,\sigma,\sigma'} c_{i1\sigma}^\dagger c_{i1\sigma'} c_{i2\sigma'}^\dagger c_{i2\sigma} \\
 - J' \sum_i (c_{i1\uparrow}^\dagger c_{i1\downarrow}^\dagger c_{i2\uparrow} c_{i2\downarrow} + \text{H.c.}), \quad (1)
 \end{aligned}$$

where $c_{im\sigma}$ ($c_{im\sigma}^\dagger$) denotes the annihilation (creation) operator of the electron at site i with orbital m ($=1$ or 2) and spin σ . The number operator is denoted by $n_{im\sigma}$. All the interaction terms in Eq. (1) originate from the Coulomb interaction between electrons at the same site. We treat every interaction exactly. Generally interaction parameters satisfy the relation $U \geq U' \geq J \approx J'$. A symmetry argument leads to the relation $U = U' + 2J$.¹⁰ Hopping terms are scaled with the dimensionality d so that the one-electron density of states (DOS) behaves as $D(\varepsilon) = \exp(-\varepsilon^2/t^2)/t\sqrt{\pi}$ in the limit $d \rightarrow \infty$.

The double-exchange mechanism due to strong Hund coupling J was proposed to produce itinerant ferromagnetism for $n > 1$, where n denotes electron density per site.⁴⁻⁶ At the $\frac{1}{4}$ filling ($n=1$) the ground state is expected to be insulating in the strong-coupling limit. In this case the effective interaction due to virtual hoppings of electrons favor a ferromagnetic ground state with alternating orbital order.¹¹⁻¹⁴ In one dimension, the ferromagnetism was found numerically near $n=1$,¹⁵⁻¹⁹ and shown rigorously for general n in the strong-coupling limit.^{20,17} For higher dimensions, it is not yet clear whether ferromagnetic order appears. Inagaki and Kubo obtained ferromagnetic phases on the simple cubic lattice for $J'=0$ using the Hartree-Fock approximation.²¹ However, it is not quite clear how the predicted metallic ferromagnetism in three dimensions is stable, since the local quantum fluctuations and the pair-hopping (J') term, both of which suppress the magnetic order, are neglected in their study. Effects of orbital degeneracy were also studied with a $d=\infty$ two-band model in the anisotropic (Ising) limit of Hund coupling and $J'=0$.²²⁻²⁴

In this paper we study the model (1) in infinite dimensions near the quarter filling. We present the one-site effective action of the model (1) and study the ground-state properties using the exact diagonalization method. We found a metallic ferromagnetic phase for electron doped cases, e.g., $n=1.2$, which indicates that the double-exchange mechanism can stabilize ferromagnetism in infinite dimensions. At the $\frac{1}{4}$ filling, the ground state shows a metal-insulator transition at a finite parameter U . A phase diagram with both ferromagnetic and antiferromagnetic phases is obtained for $n=1$. The phase diagram is consistent with a mean-field theory based on the perturbational treatment from the strong-coupling limit.

To derive the one-site effective action of the present model, we employ the cavity method.⁷ Taking the trace for all degrees of freedom except for those on site 0, we obtain the effective action

$$\exp[-S_{\text{eff}}(c_{0m\sigma}^\dagger, c_{0m\sigma})] \equiv \frac{Z_{\text{eff}}}{Z} \int \prod_{i \neq 0} \prod_{m,\sigma} Dc_{im\sigma}^\dagger Dc_{im\sigma} e^{-S}, \quad (2)$$

where the partition function of the model is written as a functional integral over Grassman variables. Generally, S_{eff} is an infinite series of multiples of Grassman variables at various times. In the $d = \infty$ limit, the action becomes quite simple as

$$S_{\text{eff}} = -\beta \sum_{m=1,2} \sum_{\sigma=\uparrow,\downarrow} \sum_{\omega_n} c_{0m\sigma}^\dagger(i\omega_n) \mathcal{G}_{0m\sigma}^{-1}(i\omega_n) c_{0m\sigma}(i\omega_n) + \int_0^\beta d\tau H_{\text{int}}(c_{0m\sigma}^\dagger(\tau), c_{0m\sigma}(\tau)), \quad (3)$$

where H_{int} denotes the local interaction on the site 0, and $\mathcal{G}_{0m\sigma}$ satisfies the relation

$$\mathcal{G}_{0m\sigma}(i\omega_n) = [G_{m\sigma}(i\omega_n)^{-1} + \Sigma_{m\sigma}(i\omega_n)]^{-1}. \quad (4)$$

To derive Eqs. (3) and (4), we have used the facts that the self-energy is independent of momentum and that $\langle c_i^\dagger c_j \rangle \sim (1/\sqrt{d})^{|i-j|}$, which applies for large d .

Here we briefly explain the method for calculating the ground state. This one-site effective action can be approximated by the following two-channel impurity model:

$$H = \sum_{m=1,2} \sum_{\sigma=\uparrow,\downarrow} \left\{ \sum_{p=2,n_s} \varepsilon_{pm\sigma} a_{pm\sigma}^\dagger a_{pm\sigma} - \mu c_{m\sigma}^\dagger c_{m\sigma} + \sum_{p=2,n_s} V_{pm\sigma} (a_{pm\sigma}^\dagger c_{m\sigma} + \text{H.c.}) \right\} + U \sum_m n_{m\uparrow} n_{m\downarrow} + U' \sum_{\sigma,\sigma'} n_{1\sigma} n_{2\sigma'} - J \sum_{\sigma,\sigma'} c_{1\sigma}^\dagger c_{1\sigma'} c_{2\sigma'}^\dagger c_{2\sigma} - J' (c_{1\uparrow}^\dagger c_{1\downarrow}^\dagger c_{2\uparrow} c_{2\downarrow} + \text{H.c.}), \quad (5)$$

where $a_{pm\sigma}$ ($c_{m\sigma}$) denotes the annihilation operator of the conduction (impurity) electron with channel m and spin σ . The effective action of the impurity site has the same form as Eq. (3) with

$$\mathcal{G}_{m\sigma}^{\text{imp}}(i\omega_n) = \left[i\omega_n + \mu - \sum_{p=2,n_s} \frac{V_{pm\sigma}^2}{i\omega_n - \varepsilon_{pm\sigma}} \right]^{-1} \quad (6)$$

instead of $\mathcal{G}_{0m\sigma}(i\omega_n)$. Conduction electrons have $n_s - 1$ orbitals. The effective action (3) can be well approximated with the impurity model (5), if we increase n_s and select the most suitable parameters ($\varepsilon_{pm\sigma}, V_{pm\sigma}$) so that $\mathcal{G}_{m\sigma}^{\text{imp}}$ satisfies the self-consistency condition (4). We numerically diagonalize the impurity model (5) with the Lanczos method and obtain the ground state under the self-consistency condition (4). It has been shown that this method works well and the ground state can be accurately described even with small number $n_s = 5$ or 6 .⁷ In spatially uniform ground states the

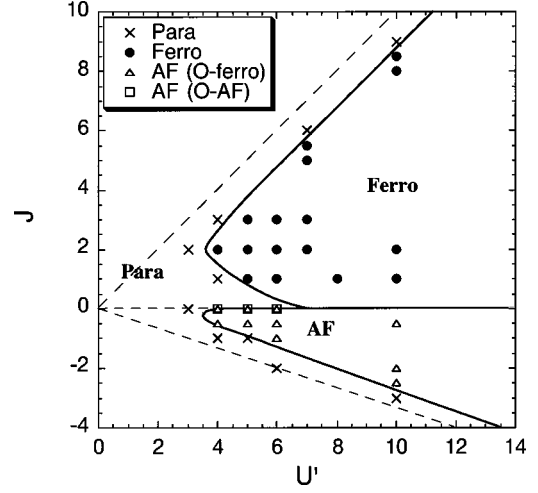


FIG. 1. Magnetic phase diagram at the $\frac{1}{4}$ filling ($n=1$). Parameters are fixed as $U=U'+2J$ and $J=J'$.

Green function is related to the self-energy with $G_{m\sigma}(\mathbf{k}, i\omega_n)^{-1} = (G_0)^{-1} - \Sigma - \varepsilon_{\mathbf{k}}$, where $G_0 = 1/(i\omega_n + \mu)$ and $\varepsilon_{\mathbf{k}} = d^{-1/2} \sum_{\mu=1}^d \cos k_{\mu}$. We also consider states with two-sublattice structures. The Green function from l sublattice to l' sublattice, $G_{m\sigma}^{ll'}(\mathbf{k}, i\omega_n)$, has the form

$$\begin{pmatrix} (G_0)^{-1} - \Sigma^A & -\varepsilon_{\mathbf{k}} \\ -\varepsilon_{\mathbf{k}} & (G_0)^{-1} - \Sigma^B \end{pmatrix}^{-1}. \quad (7)$$

We have two effective actions for two sublattices. The self-consistency condition is unchanged as $\mathcal{G}_{0m\sigma}^l(i\omega_n) = [G_{m\sigma}^{ll}(i\omega_n)^{-1} + \Sigma_m^l(i\omega_n)]^{-1}$, where $\mathcal{G}_{0m\sigma}^l(i\omega_n)$ denotes the dynamical mean field applied to the sublattice l .

We study the ground states at the fillings $n=1, 1.2$, and 0.8 , controlling the chemical potential. Parameters are set as $U=U'+2J$ and $J=J'$. Both spatially uniform states and those with the two-sublattice structure are considered. Numerical calculations were done for $n_s=5$ or $n_s=6$. We mostly studied the system with $n_s=5$ and confirmed phase boundaries using the system with $n_s=6$. We found that n_s dependence of the ground state is small and the phase diagrams are the same between the cases $n_s=5$ and 6 .

For the $\frac{1}{4}$ filling, we found three ground-state phases, i.e., paramagnetic, ferromagnetic, and antiferromagnetic ones. We obtained the phase diagram shown in Fig. 1. Though J will be positive in real systems, we consider both positive and negative J to clarify the effects of Hund coupling. Near the phase boundary, two (or three) solutions coexist and their energies cross over. We selected the ground state comparing the energies and determined the phase diagram.

For a wide parameter region, we found a ferromagnetic phase. This state has an orbital super-lattice structure. The pseudospin $\tau_i^z = \sum_{\sigma} (n_{i1\sigma} - n_{i2\sigma})/2$, which represents the orbital degree of freedom, is antiferromagnetically ordered. In this phase the compressibility, $dn/d\mu$, is always vanishing and hence the ground state is insulating (see Fig. 2). Thus magnetic transition and metal-insulator transition occur at the same coupling parameter. The magnetization is hardly reduced from the full polarization. For example, the magnetization per site ($=N_e$) is $\langle M \rangle / N_e = 0.5000$ for $U=18$, $U'=10$, and $J=4$, where N_e denotes the number of electrons.

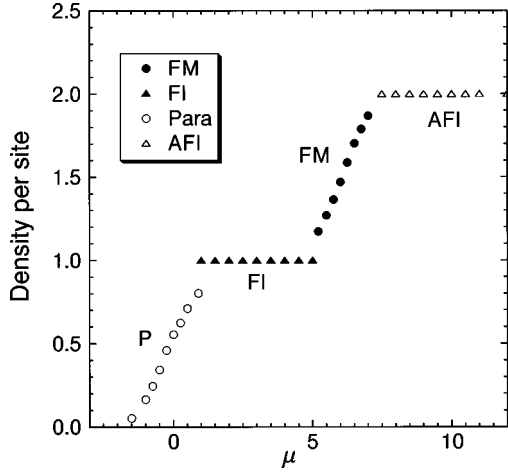


FIG. 2. Chemical potential dependence of the electron density at the parameters $U=18$, $U'=10$, and $J=J'=4$. Magnetic order of each state is written by FM, P, FI, and AFI. FM and P denote ferromagnetic and paramagnetic metal, respectively. FI means ferromagnetic insulator with alternating orbital order and AFI denotes antiferromagnetic insulator with no orbital order.

Rigorously speaking the spins cannot be fully polarized in the $d \rightarrow \infty$ limit because of the Gaussian DOS.²⁵ Since the reduction is too small, it is invisible within accuracy of the present calculation.

Another insulating phase appears for negative J . In this phase the ground state has antiferromagnetic long-range order and also uniform orbital order. The sublattice magnetization per site is very close to $\frac{1}{2}$.

The phase boundaries of the above two phases are well understood in terms of the effective Hamiltonian in the strong-coupling limit. We start from the ground states in the atomic limit ($t=0$) and treat the hopping term as a perturbation.¹² Then the second-order perturbation leads to the following effective Hamiltonian for spin operators S_i and pseudospin operators τ_i :¹²

$$\begin{aligned}
 H_{\text{eff}} = & -\frac{t^2}{2d} \sum_{\langle i,j \rangle} \left[\frac{4U}{U^2 - J'^2} \left(\frac{1}{4} + \tau_i^z \tau_j^z \right) \left(\frac{1}{4} - \mathbf{S}_i \cdot \mathbf{S}_j \right) \right. \\
 & - \frac{2J'}{U^2 - J'^2} \left(\tau_i^- \tau_j^- + \tau_i^+ \tau_j^+ \right) \left(\frac{1}{4} - \mathbf{S}_i \cdot \mathbf{S}_j \right) \\
 & + \frac{2U'}{U'^2 - J^2} \left\{ \frac{1}{4} - \tau_i^z \tau_j^z - 2(\tau_i \cdot \tau_j - \tau_i^z \tau_j^z) \left(\frac{1}{4} + \mathbf{S}_i \cdot \mathbf{S}_j \right) \right\} \\
 & \left. + \frac{2J}{U'^2 - J^2} \left\{ \tau_i^z \tau_j^z - \tau_i \cdot \tau_j + 2 \left(\frac{1}{4} - \tau_i^z \tau_j^z \right) \left(\frac{1}{4} + \mathbf{S}_i \cdot \mathbf{S}_j \right) \right\} \right]. \quad (8)
 \end{aligned}$$

Clearly, spin interactions have $SO(3)$ symmetry and, under the conditions $U=U'+2J$ and $J=J'$, pseudospin interactions also have $SO(2)$ rotational symmetry about the y axis. The derivation of Eq. (8) is valid for $-U'/3 < J < U'$, where intermediate states have higher energy than the unperturbed ground states. The perfect ferromagnetic state with perfect antiferromagnetic pseudospin order has the energy $-t^2/(2U'-2J)$ per site, while that of the Néel state with perfect ferromagnetic pseudospin order is $-t^2U/(2U^2$

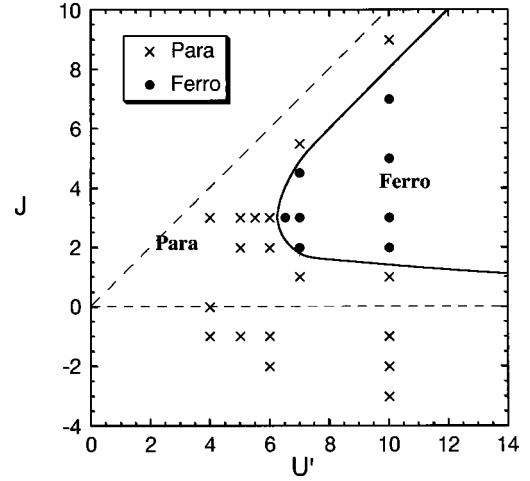


FIG. 3. Magnetic phase diagram at the filling $n=1.2$. Parameters are fixed as $U=U'+2J$ and $J=J'$.

$-2J^2$). Thus the ferromagnetic state has a lower energy for $0 < J < U'$ and the antiferromagnetic state is lower for $-U'/3 < J < 0$. We see in Fig. 1 that the phase boundaries are close to the three lines $J = -U'/3$, $J=0$, and $J=U'$. The present result reflects the fact that the mean-field theory is exact in infinite-dimensional localized spin models.

In order to examine the effects of electron doping to the ordered states at the $\frac{1}{4}$ filling, we studied the case with $n=1.2$. At this filling we obtained two metallic phases, both of which are spatially uniform, i.e., the ferromagnetic phase and the paramagnetic one (see Fig. 3). We could not find any antiferromagnetic phase at this filling. The transition from the paramagnetic phase to the ferromagnetic one is of first order. Both ferromagnetic and paramagnetic states exist as solutions of the self-consistency equations in a region close to the phase boundary and their energies cross over at the phase boundary.

The ferromagnetic state is metallic, since it has finite compressibility (Fig. 2), and it has no orbital ordering. The reduction of magnetization is larger than the insulating ferromagnet at the $\frac{1}{4}$ filling. For example, $\langle M \rangle / N_e = 0.341$ for $U=18$, $U'=10$, and $J=4$ at $n=1.2$. The area of the ferromagnetic phase is reduced in the phase diagram compared to that of the insulating ferromagnetic phase at the $\frac{1}{4}$ filling. On the other hand, the antiferromagnetic phase completely disappears at this filling. This result is consistent with the well-known fact that the itinerancy of electrons (or holes) is hardly compatible with the antiferromagnetic long-range order.

As a hole-doped case, we study the ground state for $n=0.8$. At this filling we found only metallic ground states which are translationally invariant. We could not find any magnetically ordered phase for $J \leq U' \leq 20$. Disappearance of antiferromagnetism is understood as the result of the itinerancy of the holes. Self-consistent solutions that show ferromagnetism also appear for large U' , e.g., $U'=10$, but have slightly higher energy than that of the paramagnetic states. Since the probability of double occupancy is low for $n < 1$, the double-exchange mechanism due to Hund coupling is less effective than in the case with $n > 1$ and hence ferromagnetism may disappear. The ferromagnetic ground state however appears even for $n < 1$ in one dimension.^{17,19} This

discrepancy may be understood with the argument that higher dimensionality destroys the perfect ferromagnetism,^{25,26} though we need more study to conclude the absence of the metallic ferromagnetism at less than $\frac{1}{4}$ filling for strong coupling.

In this study, we found the metallic ferromagnetism, in which spins are partially polarized, for positive J only at more than $\frac{1}{4}$ filling ($n = 1.2$). This result should be compared with the single-band Hubbard model, which does not show ferromagnetism.⁸ This indicates that the double-exchange mechanism due to the Hund-coupling favors ferromagnetism and realizes metallic ferromagnetism for strong but finite coupling in infinite dimensions. The ferromagnetism appears in a parameter region where $0 < J < U'$. We did not search for ground states with larger sublattice structures in the

present study. Hence possibility of incommensurate states still remains. Further extension of the study in infinite dimensions and also a reliable phase diagram of the metallic ferromagnetism in one dimension, which is still not available, will be useful to gain insight into the role of the orbital degeneracy in the metallic ferromagnetism in two and/or three dimensions.

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