Ferromagnetism in the one-dimensional Hubbard model with orbital degeneracy: From low to high electron density

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We studied ferromagnetism in the one-dimensional Hubbard model with doubly degenerate atomic orbitals by means of the density-matrix renormalization-group method and obtained the ground-state phase diagrams. It was found that ferromagnetism is stable from low to high ($0<n<1.75$) electron density when the interactions are sufficiently strong. The quasi-long-range order of triplet superconductivity coexists with the ferromagnetic order for a strong Hund coupling region, where the interorbital interaction $U'-J$ is attractive. At quarter-filling ($n=1$), the insulating ferromagnetic state appears, accompanying orbital quasi-long-range order. For low densities ($n<1$), ferromagnetism occurs owing to the ferromagnetic exchange interaction caused by virtual hoppings of electrons, the same as in the quarter-filled system. This comes from separation of the charge and spin-orbital degrees of freedom in the strong-coupling limit. This ferromagnetism is fragile against variation of band structure. For high densities ($n>1$), the phase diagram of the ferromagnetic phase is similar to that obtained in infinite dimensions. In this case, the double exchange mechanism is operative for stabilizing the ferromagnetic order and this long-range order is robust against variation of the band dispersion. A partially polarized state appears in the density region $1.68 \lesssim n \lesssim 1.75$ and phase separation occurs for n just below the half-filling ($n=2$).

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I. INTRODUCTION

The Hubbard model has been employed for a long time as a standard model for metallic ferromagnetism of itinerant electrons.[1–3] It is, however, not easy to show that the Hubbard model simulates a metallic ferromagnet. Many investigations revealed that a simple single-band Hubbard model on a hypercubic lattice may not exhibit ferromagnetism. Some additional features in the model seem to be necessary in order to stabilize ferromagnetism. One such feature is a special lattice or band structure. Lieb first showed that a half-filled flat band induces a net magnetization.[4] Then Mielke and Tasaki introduced other examples of flat-band ferromagnets.[5,6] Tasaki proved, furthermore, that a class of models with half-filled lowest bands with finite band dispersions exhibits ferromagnetism for sufficiently strong intra-atomic repulsions.[7] Müller-Hartmann found ferromagnetism in a one-dimensional system where the band dispersion has two minima.[8] It was also shown by perturbational as well as numerical methods that partially filled bands in such systems can support ferromagnetism.[9–12]

Another important factor realizing ferromagnetism was found to be the degeneracy of atomic orbitals.[13–15] Actually, magnetic carriers of typical metallic ferromagnets originate from the degenerate $3d$ orbitals, though they are mixed with s or p orbitals. In the presence of degenerate orbitals, Hund coupling favors local triplet spin configurations of two electrons occupying different orbitals at the same site. The following mechanisms were proposed to lead to bulk ferromagnetism from intra-atomic Hund coupling.

Zener proposed the so-called *double-exchange* mechanism originally for doped manganites, which works when the electron density per site is not an integer,[14,16] e.g., the density of electrons per site (n) is between I and $I+1$. If electrons are strongly correlated, each lattice site is occupied by either I or $I+1$ electrons, and Hund coupling forces their spins to be parallel in an atom. The magnitude of the formed atomic spin is $I/2$ or $(I+1)/2$ for $I \leqslant N_d-1$, and $N_d-I/2$ or $N_d-(I+1)/2$ for $I \geqslant N_d$, where N_d denotes the degree of degeneracy. An electron can hop from a site occupied by $I+1$ electrons to a site occupied by I electrons. Since the hopping matrix is diagonal with respect to the spin indices, an electron can hardly hop between sites whose spins are directed in antiparallel form, while it can freely propagate among sites with parallel spins. As a result, ferromagnetic spin alignment that lowers the kinetic energy is favored.

Another mechanism leading to ferromagnetism is most effective when the electron density per site is an integer, $n=I$, where I is an integer that satisfies $1 \leqslant I \leqslant N_d-1$ or $N_d+1 \leqslant I \leqslant 2N_d-1$.[17] Each site is occupied by I electrons in the strong-coupling regime and hoppings of electrons occur as virtual processes. The intermediate state of a second-order process has the lowest energy if the spins are aligned parallelly. This leads to an effective ferromagnetic exchange interaction that induces orbital ordering at the same time. Van Vleck argued that the ferromagnetic exchange due to virtual hoppings might be the origin of the metallic ferromagnetism in Ni.[15]

Though the mechanisms favoring ferromagnetism can be qualitatively understood as above, it is far from trivial whether ferromagnetic long-range order occurs in bulk systems. We need to examine whether the models with orbital degeneracy really simulate ferromagnets by reliable methods. For this purpose, we study the simplest model with orbital degeneracy, the Hubbard model with doubly degenerate atomic orbitals. The model is described by the Hamiltonian

$$H=-\sum_{i<j} t_{ij} \sum_{m=A,B} \sum_{\sigma=\uparrow,\downarrow} (c^{\dagger}_{im\sigma}c_{jm\sigma}+\text{H.c.})+U\sum_{i} \sum_{m=A,B} n_{im\uparrow}n_{im\downarrow}+U'\sum_{i} \sum_{\sigma=\uparrow,\downarrow} n_{iA\sigma}n_{iB-\sigma}+(U'-J)\sum_{i} \sum_{\sigma=\uparrow,\downarrow} n_{iA\sigma}n_{iB\sigma}$$

$$-J\sum_{i} (c^{\dagger}_{iA\uparrow}c_{iA\downarrow}c^{\dagger}_{iB\downarrow}c_{iB\uparrow}+\text{H.c.})-J'\sum_{i} (c^{\dagger}_{iA\uparrow}c^{\dagger}_{iA\downarrow}c_{iB\uparrow}c_{iB\downarrow}+\text{H.c.}), \quad (1)$$

where $c^{\dagger}_{im\sigma}$ ($c_{im\sigma}$) creates (annihilates) an electron at site i with spin $\sigma(=\uparrow,\downarrow)$ in the orbital $m(=A,B)$. Here we assumed that only the hoppings between the same orbitals exist, and the Coulomb interaction works only between electrons on a same site. The interaction parameters U, U', J, and J' represent the intra- and the interorbital repulsion, the exchange (Hund-rule) coupling, and the pair hopping, respectively. Particle-hole symmetry allows us to study only the case with $0\leqslant n\leqslant 2$.

Quite a few previous studies exist on the doubly degenerate Hubbard model. One must be careful in comparing them, since different assumptions were employed for the interaction parameters. Many assumed that $J'=0$. In fact, these parameters are dependent on each other if we calculate them from orbital wave functions. The relation

$$J=J' \quad (2)$$

holds when the orbital wave functions are real. In addition, the interaction parameters U, U', and J satisfy the relation

$$U=U'+2J \quad (3)$$

for e_g orbitals, which is relevant for the cubic symmetry. This Hamiltonian has the spin SU(2) and charge U(1) symmetries. In addition, orbital degrees of freedom have U(1) rotational symmetry since

$$\left[H,\sum_{i} \tau^{y}_{i}\right]=0. \quad (4)$$

Here the orbital pseudo-spin-operator is defined as $\tau^{y}_{i}=\frac{1}{2}\Sigma_{\sigma=\uparrow,\downarrow}\mathbf{C}^{\dagger}_{i\sigma}\sigma^{y}_{i}\mathbf{C}_{i\sigma}$, where σ^{y}_{i} denotes the Pauli matrix, and $\mathbf{C}^{\dagger}_{i\sigma}=(c^{\dagger}_{iA\sigma},c^{\dagger}_{iB\sigma})$. The last symmetry holds if the coupling parameters satisfy relations (2) and (3), and it could be easily seen in the effective Hamiltonian derived in the strong-coupling limit.[29] Because of this rotational symmetry, a rigorous argument for one-dimensional systems excludes oscillating orbital long-range order (LRO) corresponding to τ^{z}_{i} correlations.[33] In the limit of $J(=J')=0$, the symmetry of orbital degrees of freedom becomes SU(2) invariant and the whole Hamiltonian has the high symmetry SU(4).

We assume the relations (2) and (3), and assume all interaction parameters to be positive throughout this work. In realistic situations the parameters satisfy $U>U'>J$, but we study the strong Hund-coupling case $J\geqslant U'$ as well, for theoretical interest. Let us explain the level structure of a doubly occupied atomic site since it rules the physics of the model (1). The spin-triplet states, where two electrons occupy different orbitals, have the lowest energy $U'-J$. In one of three spin-singlet states, electrons occupy different orbitals and the energy is $U'+J$. In the other two singlets with the energies $U-J'$ $(=U'+J)$ and $U+J'$ $(=U'+3J)$, electrons occupy the same orbital. In the strongly correlated regime where $U'>J\gg|t_{ij}|$, almost all sites are empty or singly occupied for $n<1$, while they are singly or doubly occupied for $n>1$ and spins in a doubly occupied site form a triplet. Thus the ground-state properties for $U'>J$ strongly depend on whether n is less than, equal to, or more than unity. If J is larger than U', a doubly occupied site has negative interaction energy and hence electrons tend to form bound triplet pairs. In this case, sites are empty or doubly occupied for $0<n<2$ if N_e is even. If N_e is odd, there can be an unpaired electron, which will cause a strong finite-size effect.

Roth examined the model in three dimensions in the quarter-filled case $(n=1)$.[17] She found that the ferromagnetic ground state has an orbital superlattice structure in which two sublattices are occupied by electrons of different orbitals when the interaction is strong. This kind of ground state was studied by using an effective Hamiltonian in the strong-coupling limit[18–20] and by means of the mean-field theory for general electron density.[21] Several exact diagonalization studies were performed for small clusters in one dimension.[22–26] Most of them investigated the quarter-filled case $(n=1)$ and found the ferromagnetic ground state for $U'\gtrsim J$. Hirsch[26] studied the less-than-quarter-filled case and found the ferromagnetic ground state. The results, however, depend strongly on the boundary conditions and the number of lattice sites. There are rigorous proofs for the ferromagnetic ground state in strong-coupling limits in one dimension.[23,27,28] One must be careful in that these proofs are valid in different limits of strong coupling. For the strong Hund-coupling case ($U\to\infty$ and $U'>J\to\infty$), existence of ferromagnetism is proved for $1<n<2$.[23,27] In the special limit $J=U'\to\infty$ and $U\to\infty$, ferromagnetism is stable for $0<n<2$.[23] Shen obtained a rather general result that the ground state is fully spin polarized for any n between 0 and 2 except for 1 if $U=\infty$, and U' (>0) and $J=J'$ (>0) are finite.[28] The present model (1) was also studied in infinite dimensions using the dynamical mean-field theory.[29,30] Under the assumptions (2) and (3), the ferromagnetic ground states with and without orbital order were found for $n=1$ and $n>1$, respectively, while ferromagnetism was not found for $n<1$ up to the interactions of $U=40$ and $J\leqslant U'=20$.[29,31] Bünemann *et al.* studied ferromagnetism in the three-dimensional two-band model with a rather realistic density of states (DOS) for Ni using a Gutzwiller approximation. Their results showed that an increase of the DOS at the Fermi level could stabilize ferromagnetism for electron-doped cases $(2>n>1)$.[32]

In this paper, we studied the ground state of the model (1) in one dimension under open boundary conditions, using the density-matrix renormalization group (DMRG) method.[34] This method enables us to study larger systems than those studied previously. Owing to the open boundary condition, we found remarkably little size dependence. If we apply the periodic boundary condition, electrons can exchange their positions by turning around the chain and it causes very large size dependence of the ground state (e.g., even-odd oscillations). Preliminary results of this study were reported previously in Ref. 35.

This paper is constructed as follows: In Sec. II, we briefly review the DMRG method. In Sec. III, we study the present model with only nearest-neighbor hoppings and report our numerical results, such as magnetic phase diagrams. Ferromagnetic phases appear for a wide parameter region and for all electron densities ($0<n<2$). In most of the density region, the ferromagnetic states are fully polarized, whereas partially polarized ferromagnetic states are found in a small region ($1.68 \leqslant n \leqslant 1.75$). We also found coexistence of metallic ferromagnetism and quasi-long-range order of triplet superconductivity when the Hund coupling is stronger than the interorbital Coulomb repulsion ($J>U'$). Near the half-filling case ($1.75<n<2$), phase separation occurs, and the paramagnetic (Haldane) phase and ferromagnetic one coexist. In Sec. IV, we examine the stability of the ferromagnetic states obtained in Sec. III, adding perturbation to the density of states. The metallic ferromagnetic order for more than quarter-filling ($n>1$) is stable against this perturbation, but, for less than quarter-filling ($n<1$), it easily becomes unstable by this variation. Finally, we give a summary and discussion in Sec. V. The Appendixes contain rigorous results in the strong-coupling limit. Using charge and spin-orbital separation, we show that the ferromagnetic spin state for less than quarter-filling is the same as that at quarter-filling. The ferromagnetism at less than quarter-filling is created by the exchange interaction produced by a virtual second-order hopping processes.

II. METHOD

We obtained the ground state of the model (1) with up to 62 sites using the DMRG method.[34] The method is standard and we will not describe it in detail. Readers should refer to White's paper[34] for the DMRG method. We note only several points particular to this study. We employed the open boundary condition throughout this paper. In the DMRG calculations, we always kept rotational symmetry in the spin space so that the obtained ground state is an eigenstate of the total spin.[10]

We used the finite-system method of DMRG to obtain the ground-state phase diagrams of the model with up to 16 sites. This method is superior to the infinite-system method in terms of accuracy of the ground-state quantities of finite systems. Another merit of this method is that the final result does not depend so strongly on the ground state of the initial small system and on the path of the renormalization process as in the infinite-system method. Repeated sweeps of the renormalization processes in the finite-system method can usually remedy the failure due to a wrong initial state. Near the phase boundary between a paramagnetic phase and a ferromagnetic one with saturated magnetization, however, the final results sometimes depend on the choice of the renormalization paths. For example, two different choices of the paths $(N,N_e)=(4,2)(6,3)(8,4)(10,5)(12,6)(14,7)(16,8)$ and $(N,N_e)=(4,2)(6,4)(8,4)(10,6)(12,6)(14,8)(16,8)$ give a perfect ferromagnetic ground state and a paramagnetic one, respectively, at $(N,N_e)=(16,8)$ for $U'=J=2|t|$, where N_e and N are the number of electrons and lattice sites, respectively. Since the transition is of first order, the energy levels of a paramagnetic state and a ferromagnetic one naturally exist very close to each other near the phase boundary. To study the phase diagram carefully, we searched the ground state through many renormalization paths. Finally, we regard the lowest-energy state as the ground state. Hence, we need to try several paths and initial states and compare their results in order to obtain a reliable phase diagram as long as the number m_D of reserved eigenstates of the density matrix is finite. The maximum number of m_D was chosen to be 200 in this study for technical reasons.

In order to calculate longer correlations we also studied the systems with up to 62 sites using the infinite-system DMRG method. Results of short chains were obtained by using the exact diagonalization method.

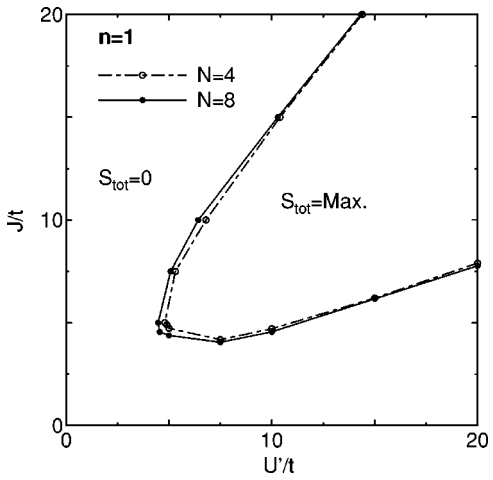

FIG. 1. Ground-state phase diagram at quarter-filling ($n=1$) of the model with nearest-neighbor hoppings. Interaction parameters are set as $U=U'+2J$ and $J=J'$. The label "S_{tot}=Max." denotes the perfect ferromagnetic phase, and "$S_{tot}=0$" the paramagnetic one.

III. RESULTS FOR THE NEAREST-NEIGHBOR MODEL

In this section, we present the results for the model with only nearest-neighbor hoppings ($t_{ij}=t\delta_{i,j\pm1}$).

A. Quarter-filled system

We first exhibit the results in the quarter-filled case ($n=1$). Figure 1 shows the $(U'/t, J/t)$ phase diagram of the ground state of the quarter-filled system obtained for $N=4$ and 8. The difference between the results for $N=4$ and N

$=8$ is amazingly small. We hence believe that the present results are representing the phase diagram of an infinite system, and did not study larger systems at this electron density. A ferromagnetic ground state with full spin polarization appears around $J \simeq U'$ for $U'/t \gtrsim 5$. The parameter regions $J/U' \gg 1$ and $J/U' \ll 1$ are paramagnetic. No partially polarized state was found at this filling. The present result is similar to those by previous studies with open boundary conditions though different assumptions for parameters were employed.[22,23] In previous studies employing periodic or antiperiodic boundary conditions, the phase boundaries of their ferromagnetic phases depend on the system size greatly.[22,24,26]

The appearance of the ferromagnetism in the region $U' > J$ can be well understood in terms of the effective Hamiltonian in the strong-coupling limit ($U' - J \gg t$). At quarter-filling, every site is singly occupied in this limit, and only the spin and orbital degrees of freedom remain. The second-order effects of virtual hoppings between singly occupied sites lead to an effective Hamiltonian $\mathcal{H}_{\rm eff}$ for the spin and orbital degrees of freedom:[18–20,29]

$$\mathcal{H}_{\rm eff} = \sum_{i=1}^{N-1} h(i,i+1), \tag{5}$$

$$h(i,j) \equiv -2t^2 \left\{ \frac{4U}{U^2 - J'^2} \left(\frac{1}{4} + \tau_i^z \tau_j^z \right) \left(\frac{1}{4} - \boldsymbol{S}_i \cdot \boldsymbol{S}_j \right) - \frac{2J'}{U^2 - J'^2} (\tau_i^- \tau_j^- + \tau_i^+ \tau_j^+) \left(\frac{1}{4} - \boldsymbol{S}_i \cdot \boldsymbol{S}_j \right) + \frac{2U'}{U'^2 - J^2} \left[\frac{1}{4} - \tau_i^z \tau_j^z - 2(\boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j - \tau_i^z \tau_j^z) \right.\right.$$
$$\left.\left. \times \left(\frac{1}{4} + \boldsymbol{S}_i \cdot \boldsymbol{S}_j \right) \right] + \frac{2J}{U'^2 - J^2} \left[\tau_i^z \tau_j^z - \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j + 2 \left(\frac{1}{4} - \tau_i^z \tau_j^z \right) \left(\frac{1}{4} + \boldsymbol{S}_i \cdot \boldsymbol{S}_j \right) \right] \right\}. \tag{6}$$

Here $\boldsymbol{S}_i$ is a spin operator and $\boldsymbol{\tau}_i = (\tau_i^x, \tau_i^y, \tau_i^z)$ is a pseudo-spin-operator representing the orbital degrees of freedom, e.g., τ_i^+ is defined as $\Sigma_\sigma c_{iA\sigma}^\dagger c_{iB\sigma}$. According to Eq. (6) the exchange energy between sites i and $i+1$ is $-2t^2/(U' - J)$, $-2t^2/(U' + J)$, and $-2Ut^2/(U^2 - J^2)$ for the states $|m,\sigma\rangle_i |\overline{m},\sigma\rangle_{i+1}$, $|m,\sigma\rangle_i |\overline{m},-\sigma\rangle_{i+1}$, and $|m,\sigma\rangle_i |m,-\sigma\rangle_{i+1}$, respectively, where $|m,\sigma\rangle_i$ denotes the state of the site i occupied by an electron of orbital m with spin σ, and $\overline{m}$ labels the complement of m, e.g., $\overline{A} = B$. As a result, $\mathcal{H}_{\rm eff}$ favors ferromagnetism with an orbital antiferromagnetic superlattice structure, where electrons on two sublattices occupy different orbitals. Numerical results of the four-site system described by $\mathcal{H}_{\rm eff}$ exhibited that the ground state of $\mathcal{H}_{\rm eff}$ is ferromagnetic for $J > 0.35U'$. This agrees with our observation that the lower boundary of the ferromagnetic phase in Fig. 1 approaches the line $J = 0.35U'$ for large U'/t. We may consider that the system is well described by $\mathcal{H}_{\rm eff}$ for $U'/t \gtrsim 10$ and $U' > J$. A numerical study by two of the present authors in infinite dimensions showed that the ferromagnetism with antiferromagnetic pseudo-spin-order is stable for $J > 0$ in the strong-coupling limit,[29] which agrees with the result in the classical limit of $\mathcal{H}_{\rm eff}$. The ferromagnetic phase is smaller in one dimension than that in infinite dimensions due to stronger quantum fluctuations. In one dimension, the antiferromagnetic orbital correlations, which support the ferromagnetism, do not grow to a real long-range order but remains as a quasi-long-range order (QLRO), since orbital degrees of freedom have U(1) rotational symmetry and a rigorous argument excludes oscillating orbital LRO in one dimension.[33]

In the ferromagnetic phase at $n = 1$, we found only fully polarized states. Note that the charge and orbital degrees of freedom of fully polarized states can be described by a single-band Hubbard model with intra-atomic repulsion $U' - J$, where the conventional spin degrees of freedom are replaced with the orbital ones.[28] Hence, we can conclude that this ferromagnetic state has orbital antiferromagnetic QLRO for $U' - J > 0$. In addition, for general filling n, one can write down the asymptotic form of the orbital correlation function in the fully polarized ferromagnetic phase in the form

$$\langle \tau_0^z \tau_l^z \rangle \sim \cos(n\pi l) |l|^{-\alpha_S} \tag{7}$$

for $U' - J > 0$. The exponent $\alpha_S (= 1 + K_\rho)$ is obtained from the single-band Hubbard model with coupling $U' - J$ at filling n.[36,37] We also checked the orbital ordering by the DMRG method and presented the results in Fig. 2.

Also, from the above mapping, we can see that a metal-insulator transition occurs in the ferromagnetic phase on the line $U' = J$, i.e., the ferromagnetic state is insulating for $U' > J$ and metallic for $U' \leqslant J$. (Figure 3 shows chemical potential dependence of the electron density for $U'/t = 15$ and $J/t = 10$ with $N = 16$.) On the other hand, in the paramagnetic phase, since each band is quarter-filled and the perfect nesting no longer exists, a metal-insulator transition may not occur with an infinitesimal repulsion $U' - J$, which works between electrons with the same spin in different orbitals. Indeed, for paramagnetic states at $J = 0$, Assaraf *et al.* numerically showed that a metal-insulator transition occurs at $U_c/t \sim 2.8$.[38] We expect that, in the paramagnetic phase with finite $J (> 0)$, a metal-insulator transition may occur at a finite positive value of $U' - J$. Figure 4 shows numerical results of the electron density as a function of the chemical potential in the paramagnetic phase with $J/t = 3$ and U'/t

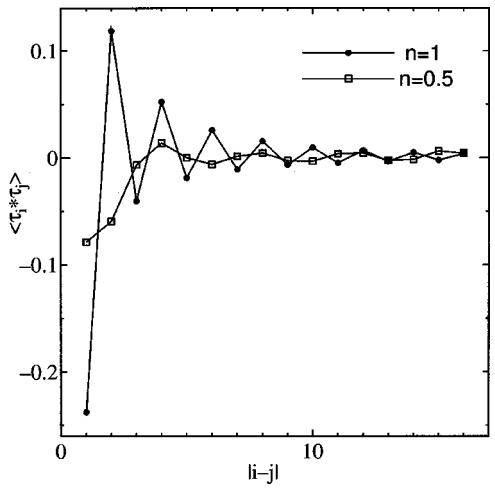

FIG. 2. Correlation functions of orbital ordering $\langle \tau_i \tau_j \rangle$ in the ferromagnetic ground state for $J/t=15$ and $U'/t=20$ at filling $n=1$ and $n=0.5$. The system size is 34 and i is fixed at $N/2=17$.

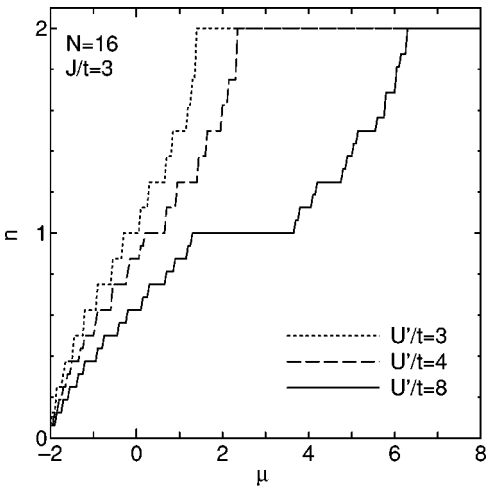

FIG. 4. Electron density (n) per site as a function of the chemical potential (μ) for $U'/t=3$, 4, and 8, and $J/t=3$ for $N=16$. The flat parts indicate insulating states. All states are paramagnetic.

$=3$, 4, and 8. The data for $U'/t=8$ clearly show that the quarter-filled state is insulating. The data for $U'/t=3$ and 4 seem to indicate that the systems are metallic at quarter filling, though it is hard to estimate the critical point from the present calculation because of finite-size effects.

For $J=0$, the effective Hamiltonian (5) reduces to a model with SU(4) symmetry. It is known that the ground state of this model is a spin-singlet state ($S=\tau=0$) in one dimension.[39] The paramagnetic state obtained for $0.35U' > J > 0$ in Fig. 1 may be interpreted as an extension of this SU(4) symmetric state.

We find that, for the $U'=J$ case, the ferromagnetic phase extends down to a weak-coupling region. At $U'=J$, double occupation of a site does not cost energy and the ferromagnetic ground state is metallic. The ferromagnetism in the strong-coupling region is stabilized by a kind of the double-exchange mechanism as was discussed rigorously for $U'=J=\infty$.[23]

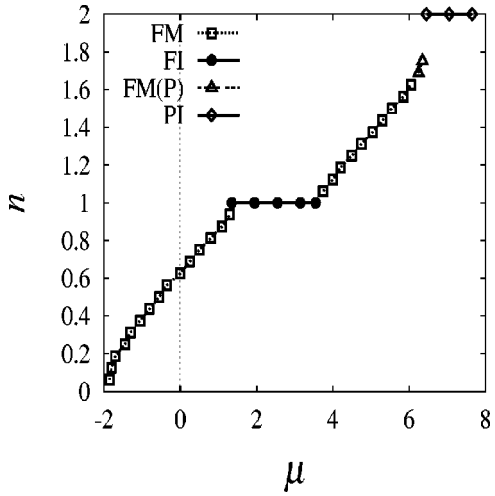

FIG. 3. Electron density n per site as a function of the chemical potential μ for $U'/t=15$ and $J/t=10$ for $N=16$. The flat parts indicate insulating states. Abbreviations indicate the characters of the ground states: FM, ferromagnetic metal; FI, ferromagnetic insulator; FM(P), partially ferromagnetic metal; PI, paramagnetic insulator.

The ferromagnetic phase extends to the parameter region $J>U'$. In this region, the fully polarized states can be described by the attractive single-band Hubbard model,[28] whose ground state is known to have QLRO of the pairing correlations.[40] Hence the ferromagnetic ground state for $J>U'$ has a QLRO of triplet superconductivity as well. For strong attraction ($J-U' \gg t$), all electrons are coupled into triplet pairs if N_e is even and the system is described by an effective Hamiltonian $\mathcal{H}_b$ in terms of hard-core bosons with spin unity:

$$\mathcal{H}_b = -\sum_{i=1}^{N-1} \tilde{t} P \left[\sum_{s=0,\pm 1} (b_{is}^\dagger b_{i+1s} + \text{H.c.}) + n_i^b + n_{i+1}^b \right] P + \sum_{i=1}^{N-1} P[\tilde{J} \boldsymbol{S}_i^b \cdot \boldsymbol{S}_{i+1}^b + (2\tilde{t} - \tilde{J}) n_i^b n_{i+1}^b] P, \tag{8}$$

where $\tilde{t}=2t^2/(J-U')$ and $\tilde{J}=2t^2/(J+U)$. The summation in $\mathcal{H}_b$ runs over all the nearest-neighbor sites. The creation and spin operators of a boson at a site i are defined as

$$b_{i1}^\dagger = c_{iA\uparrow}^\dagger c_{iB\uparrow}^\dagger,$$

$$b_{i0}^\dagger = \frac{1}{\sqrt{2}} (c_{iA\uparrow}^\dagger c_{iB\downarrow}^\dagger + c_{iA\downarrow}^\dagger c_{iB\uparrow}^\dagger),$$

$$b_{i-1}^\dagger = c_{iA\downarrow}^\dagger c_{iB\downarrow}^\dagger, \tag{9}$$

and

$$(S_i^b)^z = b_{i1}^\dagger b_{i1} - b_{i-1}^\dagger b_{i-1}, \tag{10}$$

$$(S_i^b)^- = \sqrt{2}(b_{i-1}^\dagger b_{i0} + b_{i0}^\dagger b_{i1}), \tag{11}$$

$$(S_i^b)^+ = \sqrt{2}(b_{i1}^\dagger b_{i0} + b_{i0}^\dagger b_{i-1}), \tag{12}$$

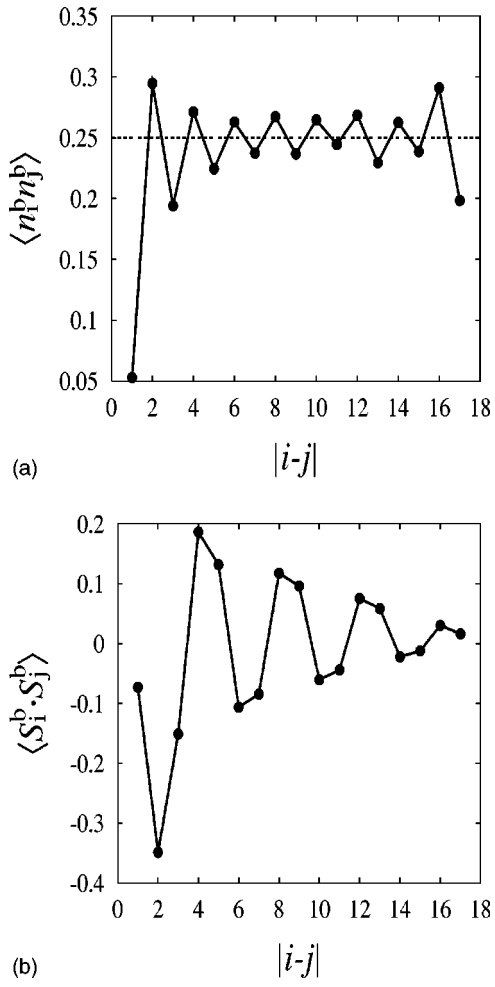

FIG. 5. Correlation functions $\langle n_i^b n_j^b \rangle$ and $\langle \mathbf{S}_i^b \cdot \mathbf{S}_j^b \rangle$ in the paramagnetic ground state for $J/t=50$ and $U'/t=10$ at quarter-filling. The system size is 36 and i is fixed at $N/2=18$.

respectively. The number operator n_i^b is defined as $\Sigma_{s=0,\pm 1} b_{is}^\dagger b_{is}$ and P projects out states in which sites are occupied by more than one boson. Since $\tilde{J}$ is positive, $\mathcal{H}_\mathrm{b}$ does not favor ferromagnetism and the ferromagnetic phase should not extend to this region. We examined the phase boundary in the small system with $N=4$ and found that the slope of the phase boundary approaches unity for large U'/t. The appearance of ferromagnetism in the region $J \gtrsim U'$ is thus interpreted as a smearing out of the ferromagnetic ground state at $J=U'$ to this region. Namely, this ferromagnetism is also caused by the double-exchange mechanism at least in the strong-coupling region. The above arguments should hold not only for the quarter-filled case but also for the hole-doped and electron-doped cases. Actually the slope of the phase boundary for $J>U'$ approaches unity for large U'/t also in the systems with $(N,N_\mathrm{e})=(6,4)$ and $(4,6)$. Shen showed coexistence of ferromagnetism and triplet pairing correlations in the whole region where $U=\infty$ and $1<J/U'<\infty$.[28] On the other hand, the present result shows that such a phase appears only in a small region close to the line $J=U'$. This discrepancy comes from the difference in the assumed relations between parameters.

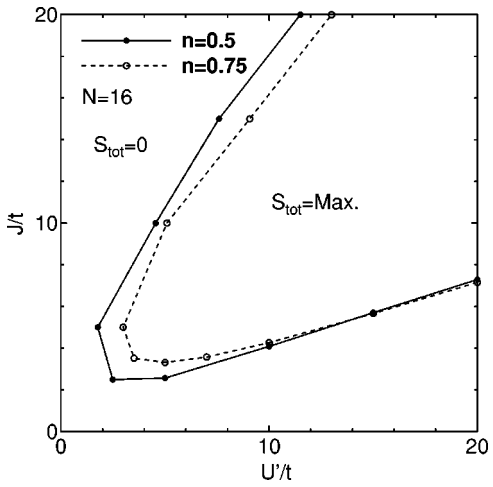

FIG. 6. Ground-state phase diagram for densities $n=0.5$ and 0.75 in the $N=16$ system. Interaction parameters satisfy $U=U'+2J$ and $J=J'$.

Next, we consider the spin-singlet ground state for $J \gg U'$ where the system is described by $\mathcal{H}_\mathrm{b}$. Figure 5 shows the density correlation function $\langle n_i^b n_j^b \rangle$ of bosons and the spin correlation function $\langle \boldsymbol{S}_i^b \cdot \boldsymbol{S}_j^b \rangle$ in the ground state of the system with 36 sites obtained by the infinite-system DMRG method. The correlations were measured from the center, i.e. i is fixed to be $N/2$. We observe an even-odd oscillation in the density correlations. This oscillation is due to repulsive interactions between bosons. Actually the second term in $\mathcal{H}_\mathrm{b}$ works as repulsions since $||\tilde{J}\boldsymbol{S}_i^b \cdot \boldsymbol{S}_{i+1}^b + 2\tilde{t} - \tilde{J}|| > 0$ holds when $n_i^b n_{i+1}^b = 1$. On the other hand, $\langle \boldsymbol{S}_i^b \cdot \boldsymbol{S}_j^b \rangle$ shows an oscillation with the period four with slow decay. This oscillation is understood as a superposition of the density correlation with period two and the antiferromagnetic spin correlations caused by the exchange coupling $\tilde{J}$.

B. Hole- and electron-doped systems

Next we study the hole-doped case ($n<1$), where holes are doped into the quarter-filled system. Figure 6 shows the $(U'/t, J/t)$ phase diagram of the ground states for $n=0.5$ and 0.75 in the system with $N=16$. A ferromagnetic phase appears for a wide parameter region and the magnetization is saturated in the whole phase. Size dependence among the results for $N=8$, 12, and 16 was very weak, as in the case of quarter-filling. Comparing with the result for $n=1$ we note that the ferromagnetic phase has expanded in the weak-coupling region down to $U'/t \simeq 3$ as well as to a region where $J \gtrsim U'$.

We note that the lower boundary of the ferromagnetic phase for large U'/t $(>J/t)$ almost agrees with that for quarter-filling. This result is a manifestation of the separation of the charge and spin-orbital degrees of freedom in one dimension. We can derive this result by using the same argument as that employed by Ogata and Shiba for the single-band Hubbard model.[41] In the limit $U'-J=\infty$, the motion of electrons is described by that of spinless fermions on a single chain, and the ground-state wave function is decomposed

into a spinless fermion (charge) part and a spin-orbital part. The spin-orbital part is described in terms of spins and pseudospins in a *squeezed* system with N_e sites where empty sites are omitted. Interactions among the spins and pseudospins are caused by virtual hopping processes and described by the following Hamiltonian (see Appendix A):

$$\mathcal{H}'_{\rm eff} = n\left(1 - \frac{\sin 2n\pi}{2n\pi}\right)\mathcal{H}_{\rm eff}, \tag{13}$$

where $\mathcal{H}_{\rm eff}$ is the Hamiltonian given by Eq. (5) where the site labels of the spin-orbital quantities are those of the squeezed system. Since $\mathcal{H}'_{\rm eff}$ differs from $\mathcal{H}_{\rm eff}$ only by a multiplicative factor, it leads to the $(U'/t, J/t)$ phase diagram identical to that for quarter-filling in the strong-coupling limit. This argument explains the present result that the lower boundaries of the ferromagnetic phases for $n=0.5$, 0.75, and 1 agree very well for $U'/t \gtrsim 10$. We may conclude that the origin of the ferromagnetism in this region is the effective exchange coupling due to virtual hoppings. Orbital degrees of freedom are also similar to those at quarter-filling except for the difference of the characteristic wavelength. This behavior can be seen in the orbital correlation function in the ferromagnetic phase obtained by the DMRG method (Fig. 2) and the asymptotic form given by Eq. (7). Note that the exponent α_S in Eq. (7) does not depend on the filling n in the strong-coupling limit.

The above result greatly depends on the fact that the wave function is decoupled to the charge and spin-orbital parts in the limit $U'-J=\infty$, and that the ground-state energy is independent of the spin-orbital degrees of freedom in the first order of t. It should be noted that this is not the case in either higher dimensions or one-dimensional models with far-neighbor hoppings. In these cases the motion of electrons leads to effective spin-orbital interactions in the first order of t, as in the case of Nagaoka's ferromagnetism. In fact, ferromagnetism was not found for $n<1$ in infinite dimensions.[29,31] We will discuss the effects of far-neighbor hoppings in Sec. IV.

It is remarkable that the ferromagnetism appears for rather weak Hund-rule coupling, that is, $J/t \simeq 3$ for $U'/t \simeq 5$. Hirsch argued, based on a diagonalization study of finite-size systems, that the Hund-rule coupling is not effective enough to realize ferromagnetism in systems with low density ($n<1$) and that ferromagnetic exchange interaction between different sites are necessary to explain ferromagnetism in systems such as Ni.[26] The present result, however, shows that a moderate Hund-rule coupling is sufficient to support ferromagnetism in the one-dimensional model with nearest-neighbor hoppings.

Finally we examined the electron-doped case where $n>1$. The phase diagram for $n=1.25$ in the systems with $N=8$ and 16 is shown in Fig. 7. Size dependence was very weak, as in the case of quarter-filling. In the systems with $N_e=4m+2$, where m is an integer, ground states in the weak-coupling region show small magnetization $S_{\rm tot}=1$ instead of $S_{\rm tot}=0$. This weak spin polarization occurs when one-electron states at the Fermi level are half-filled, i.e., $N_e=4m+2$, under the open-boundary condition. The Hund

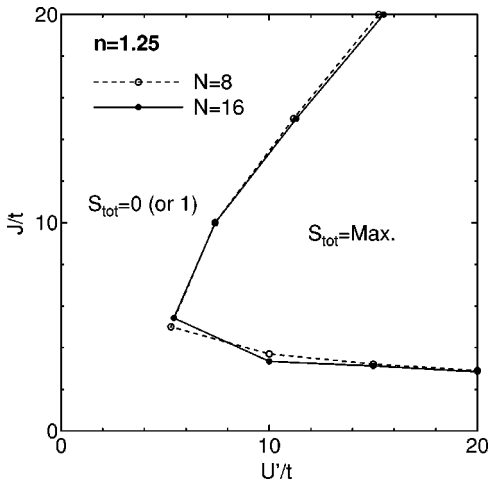

FIG. 7. Ground-state phase diagram at density $n=1.25$ for the system with 8 and 16 sites. Interaction parameters satisfy $U=U'+2J$ and $J=J'$. In the case of $N=8$, paramagnetic states show small magnetization $S_{\rm tot}=1$ because of a finite-size effect under open boundary condition (see text).

coupling aligns the two electrons at the Fermi level parallel and produces the $S_{\rm tot}=1$ ground state. We regard the appearance of $S_{\rm tot}=1$ weak polarization as a finite-size effect and not as evidence of unsaturated ferromagnetism in bulk systems. In the ferromagnetic phase, the magnetization is always saturated at this electron density. The ferromagnetism appears in a larger region than that in the quarter-filled case in particular for small J/t and large U'/t. This enhancement of the stable ferromagnetic state is a result of the double-exchange mechanism, which works effectively for $1<n<2$. The appearance of ferromagnetism for $U>U'>J \gg t$ is expected from a rigorous proof that holds in the limit where $U>U'>J\to\infty$.[27] Our numerical results agree with this argument and ensure that the ferromagnetism extends to a finite parameter region.

We show the electron density n as a function of the chemical potential μ for $U'/t=15$ and $J/t=10$ in Fig. 3 for the system with 16 sites. For $n>1$ and $n<1$, the ferromagnetic ground state is metallic, since the compressibility $dn/d\mu$ is finite. For $n=1$ and 2, the value of $dn/d\mu$ is vanishing and hence the ground state is insulating. The system is a fully polarized ferromagnetic insulator for the quarter-filling case. On the other hand, the ground state is paramagnetic at the half-filling ($n=2$), where triplet electron pairs occupy all the lattice sites. Triplet pairs on nearest-neighbor sites are interacting antiferromagnetically due to the second-order effect of virtual hoppings. As a result the ground state at $n=2$ should be a Haldane singlet with an excitation gap. There is a jump in the density between $n=1.75$ and 2 in Fig. 3, which implies the occurrence of phase separation. The occurrence of phase separation was found also in infinite dimensions.[35]

We found partially polarized ground states in a small region of density where $1.6875 \leqslant n \leqslant 1.75$. As the density increases and approaches the half-filling, the antiferromagnetic interactions between the triplet pairs become operative and suppress the ferromagnetism due to the double exchange

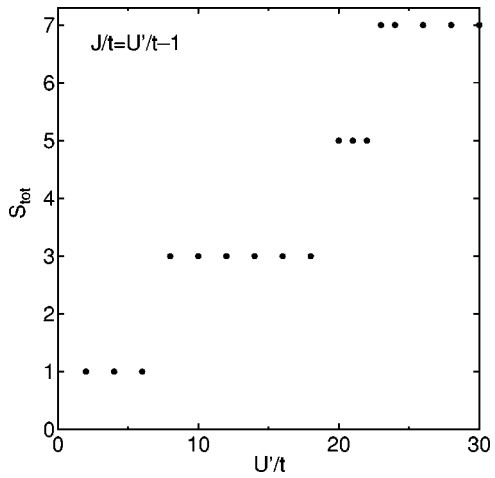

FIG. 8. Total spin of the ground state as a function of U'/t in the system where $J/t=U'/t-1$ and $(N,N_e)=(8,14)$.

mechanism. This may cause the appearance of the partially polarized states. We show the magnetization of a small system where $(N,N_e)=(8,14)$ as a function of J in Fig. 8. The figure shows that the partially polarized state appears in a finite range of the parameter, i.e., $8<U'/t<23$ with $J/t=U'/t-1$. This result may imply that the transition from a paramagnetic to ferromagnetic ground state is of the second order for $n\lesssim 2$ in contrast to the discontinuous change to a fully polarized state observed in other lower density region.

IV. EFFECT OF THE BAND DISPERSION

It is widely known that the profile of the density of states (DOS) of the band plays an important role in the realization of itinerant ferromagnetism. In the Hartree-Fock theory of the Hubbard model, for example, the ferromagnetism is stabilized if $UD_F>1$, where D_F denotes the DOS at the Fermi level. In fact, the whole profile of the DOS affects the stability of the ferromagnetism.[1,42] The DOS of the nearest-neighbor model in one dimension, which we have studied above, has a minimum at the center of the band and diverges at the band edges. These features are quite different from those of DOS in higher dimensions. In this section, we examine the effect of the band dispersion (or DOS) on ferromagnetism, studying a one-dimensional model with far-neighbor hoppings. The model we employ has a linear dispersion of the band as

$$\epsilon_k=\begin{cases}-2t+(4tk/\pi) & (0<k<\pi)\\ -2t-(4tk/\pi) & (-\pi<k<0)\end{cases} \tag{14}$$

instead of $-2t\cos k$ of the nearest-neighbor model, and hence its DOS is independent of the band energy (see Fig. 9). For this model, the hopping integrals are calculated from the dispersion (14) by

$$t_{ij}=\frac{2}{N+1}\sum_k \epsilon_k \sin(ki)\sin(kj), \tag{15}$$

where the Fourier transform of $c^\dagger_{im\sigma}$ is given by

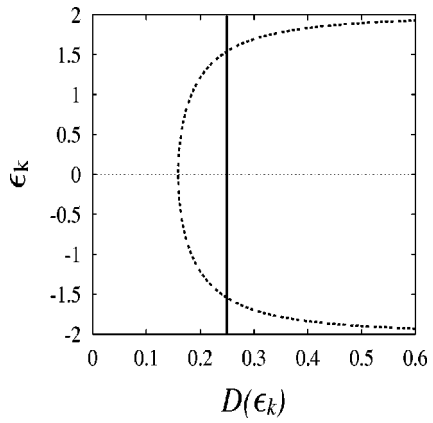

FIG. 9. Density of states per site and spin in the nearest-neighbor model (dotted line) and in the linear-band model (solid line).

$$c^\dagger_{km\sigma}=\sqrt{\frac{2}{N+1}}\sum_{i=1}^{N}\sin(ki)c^\dagger_{im\sigma} \tag{16}$$

and $k=l\pi/(N+1)$ with $l=1,2,\ldots,N$. Due to the electron-hole symmetry of the dispersion (14) the system is bipartite, i.e., the hopping integrals t_{ij} vanish for $|i-j|=2l$ with integer l, and are always negative for $|i-j|=2l+1$ for positive t. The hopping integral t_{ij} is given by $-t[1-(-1)^{i-j}]/\pi(i-j)^2$ in the limit $N\to\infty$. We call this model *linear-band* model in the following. We study small clusters with $N=4$, 5, and 6 under the open boundary conditions, exactly diagonalizing them, and compare the results with those of the nearest-neighbor model.

We show the ground-state phase diagram for the quarter-filling obtained from the systems with $(N,N_e)=(4,4)$ in Fig. 10. The phase boundaries for two models are in good agreement in the strong-coupling region where $U'>J$, while the ferromagnetism is slightly suppressed in the linear-band model in the weak-coupling region where $J\geqslant U'$. The ferromagnetism is assisted by antiferromagnetic orbital QLRO when $U'>J$. The long-range hoppings in the linear-band model do not destroy the orbital correlations since t_{ij} satis-

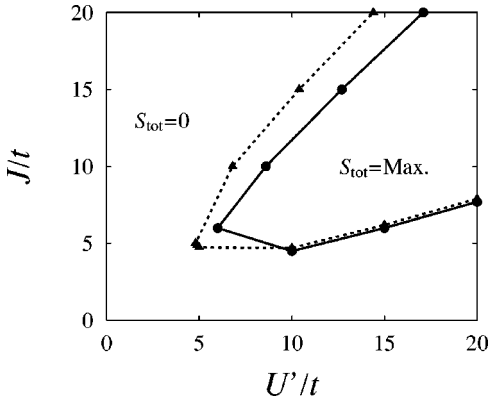

FIG. 10. Ground-state phase diagram at quarter-filling obtained by the exact diagonalization of the system with $N=N_e=4$. Filled circles and filled triangles display the phase boundary for the linear-band model and the nearest-neighbor model, respectively.

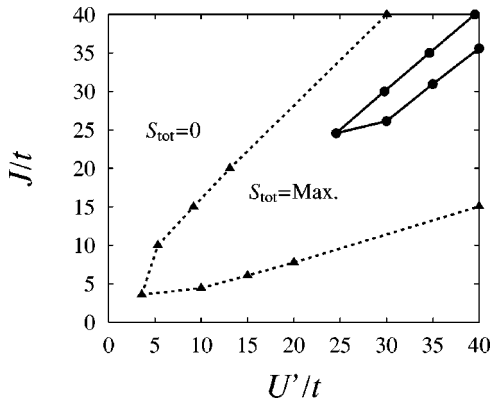

FIG. 11. Ground-state phase diagram for the system with $(N,N_e)=(6,4)$. Filled circles and filled triangles display the phase boundary for the linear-band model and the nearest-neighbor model, respectively.

fies the bipartite condition. The present result suggests that the phase boundary between the ferromagnetic and paramagnetic phases does not depend strongly on the spatial dependence of the effective exchange interactions.

Next we show the phase diagram for $(N,N_e)=(6,4)$ in Fig. 11 as an example of the hole-doped case. It is striking that the ferromagnetic region for the linear-band model is strongly suppressed compared to that for the nearest-neighbor model. The ferromagnetic phase appears only for $U'/t \geqslant 25$ and exists in a very narrow region along the line $J/U'=1$. This strong reduction of the ferromagnetic phase for $U'>J$ is interpreted as a result of the breakdown of the separation of the charge and spin-orbital degrees of freedom. An electron can pass the other electrons by far-neighbor hoppings, and they lead to effective interactions among the spin and orbital degrees of freedom in the first order of t_{ij}. The effective Hamiltonian in the limit $U'>J\rightarrow\infty$, which contains only hopping terms and prohibits double occupancy, leads to a unique paramagnetic ground state $(S=0)$ in the linear-band model for $(N,N_e)=(6,4)$. Consequently, the ferromagnetic phase does not appear for $U'>J \gg t$ in this model and occurs only in the region $J \simeq U'$ and $U'/t \gtrsim 25$.

Figure 12 displays the phase diagram for $(N,N_e)=(5,6)$ as an example of the electron-doped case. In this case, the phase boundary for the linear-band model is similar to that for the nearest-neighbor model. The ferromagnetism for $U'>J \gg t$ is caused by the double-exchange mechanism. Far-neighbor hoppings are expected to favor ferromagnetism as well as nearest-neighbor ones. We note that rigorous proofs[23,27,28] for ferromagnetism in the strong-coupling limit do not hold for the linear-band model. The present result implies that the ferromagnetic state for $n>1$ is robust against the variation of the DOS and would survive in higher dimensions. Actually, the ferromagnetic state was found to be stable for a wide range of interaction parameters for $n>1$ in infinite dimensions.[29]

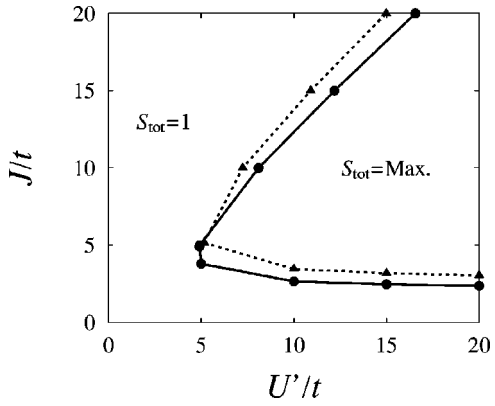

FIG. 12. Ground-state phase diagram for $(N,N_e)=(5,6)$. Filled circles and filled triangles display the phase boundary for the linear-band model and the nearest-neighbor model, respectively.

Though we have studied only small systems, the above results clearly show that the band dispersion has a strong effect on the stability of ferromagnetism for the hole-doped system. On the other hand, it gives only a minor effect on the ferromagnetism for the quarter-filled and the electron-doped systems.

V. SUMMARY AND DISCUSSION

We studied ferromagnetism in the one-dimensional Hubbard model with orbital degeneracy by numerical methods. We first studied the model with only nearest-neighbor hoppings by the DMRG calculations of clusters with up to 16 sites and obtained the following results:

(1) In the case of the quarter-filling $(n=1)$, a fully polarized ferromagnetic phase appears in a region $U'/t \geqslant 4$ and $J/t \geqslant 4$. The ferromagnetic state is insulating for $U'>J$ and metallic for $J \geqslant U'$. The ferromagnetism for $U'-J \gg t$ is caused mainly by the second-order hopping processes. The phase boundary between the ferromagnetic and paramagnetic phases approaches the asymptote $J=0.35U'$ for large U' $(>J)$. The ferromagnetic phase extends considerably to a region with $J>U'$ for the intermediate-coupling regime, but the phase boundary on this side becomes parallel to the line $J=U'$ for large U'/t.

(2) In the hole-doped cases $(n=0.5$ and $0.75)$, metallic ferromagnetism appears in a similar parameter region to that of insulating ferromagnetism at the quarter-filling. The phase boundary between the ferromagnetic and paramagnetic phases for large U' $(>J)$ agrees with that for $n=1$, which results from decoupling of the ground-state wave function into the charge and spin-orbital parts in the limit $U'-J=\infty$. The ferromagnetic phase expands to the weak-coupling region more than the quarter-filled case.

(3) In the electron-doped case $(n=1.25)$, the ferromagnetic phase dominates the region with $U'>J$. This ferromagnetism is metallic and caused mainly by the double-exchange mechanism. Near the half-filled case $(1.6875 \leqslant n \leqslant 1.75)$, this ferromagnetic order becomes partially saturated.

(4) In a large-Hund-coupling region, $J>U'$, QLRO of triplet superconductivity coexists with the metallic ferromagnetism, which appears for all electron densities, i.e., $0<n<1.75$.

It is important to note that the present results for the phase diagram showed little system-size dependence. We hence

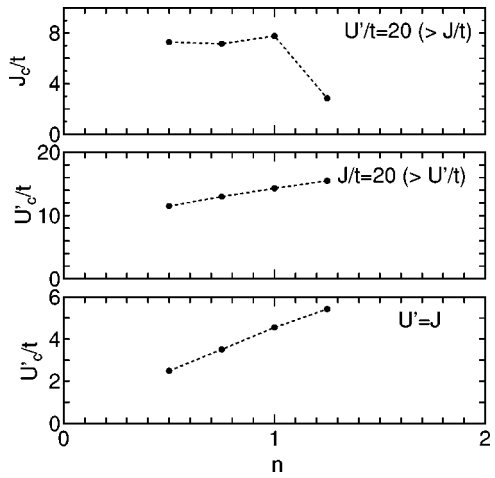

FIG. 13. Critical values of the interaction parameters for the appearance of ferromagnetism as functions of the density: J_c/t for $U'/t=20$ (top), U'_c/t for $J/t=20$ (middle), and U'_c/t $(=J_c/t)$ for $U'=J$ (bottom).

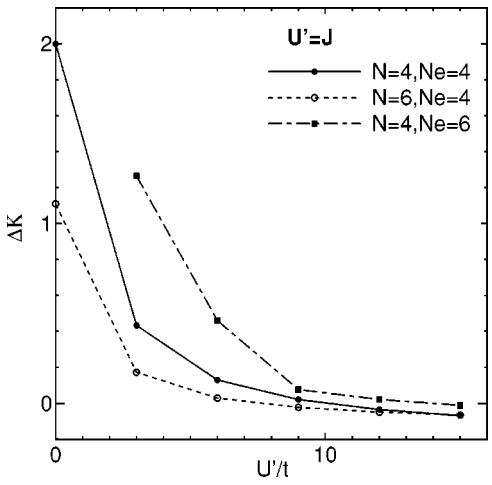

FIG. 14. Difference ΔK of the kinetic energy in ferromagnetic states K_F from that in paramagnetic states K_P, i.e., $\Delta K=K_F-K_P$. The numbers of system sizes and electrons are set as $(N,N_e)=(6,4)$, (4,4), and (4,6).

claim that the present results represent the properties in the thermodynamic limit.

The critical values of the interaction parameters for the appearance of ferromagnetism are shown in Fig. 13. In the case of $U'>J$, the critical Hund coupling J_c/t is almost constant for $n\leqslant 1$, while it suddenly drops for $n=1.25$. Though we have not examined for other n values for $n>1$, the data suggest a clear discrepancy between $n>1$ and $n\leqslant 1$. For $U'=J$ and $U'<J$, the critical interorbital repulsion U'_c/t is apparently a smooth function of the density. For the case $U'=J$, U'_c/t seems to vanish for decreasing n. It would be interesting to examine whether the system exhibits ferromagnetism with infinitesimal interactions in the low-density limit.

The double-exchange mechanism causes ferromagnetism by lowering the kinetic energy, and hence the strength of the double-exchange mechanism may be measured by the difference ΔK of the kinetic energy in the ferromagnetic state K_F from that in the paramagnetic one K_P, i.e., $\Delta K=K_F-K_P$. Largely negative ΔK implies that the double-exchange mechanism is effective. We show ΔK for $U'=J$ in the small systems with $(N,N_e)=(6,4)$, (4,4), and (4,6) in Fig. 14. We see that ΔK is a decreasing function of U'/t in all the cases and becomes negative for large U'/t. The value U'_0/t where $\Delta K=0$ decreases with decreasing n, which implies that the double-exchange mechanism is more effective in the system with lower density for $U'=J$. The values of U'_0/t themselves are, however, much larger than the critical value U'_c/t for the appearance of the ferromagnetism. For example, $U'_0/t\simeq 8$ and $U'_c/t\simeq 4$ for $(N,N_e)=(6,4)$. This result shows that the ferromagnetism in the weak-coupling region is not caused by the double-exchange mechanism. The ferromagnetism occurs for a gain of the interaction energy. The situation is similar in the system with $(N,N_e)=(4,6)$ for $U'>J$ as well. The value J_0/t where $\Delta K=0$ is much larger than the critical value J_c/t. For example, $J_0/t\simeq 7$ and $J_c/t\simeq 3$ for $U'/t=20$. The system-size dependence of U'_0/t (and J_0/t) is left for a future study, in particular, whether it agrees with U'_c/t (and J_c/t) or not in the thermodynamic limit.

We found a partially polarized ferromagnetic state for a density region adjoining the phase-separation region just below half-filling, where the magnetization gradually changes depending on the strength of interactions. In these states, ferromagnetic spin correlation decays especially near edges of open systems. We may need further study in order to confirm that this partial ferromagnetism remains in the thermodynamic limit. There is also another possibility that a partially polarized state might apparently appear because of phase separation into a perfectly polarized part and a paramagnetic part. Recently phase separation is found in other systems and is thought to be a common feature of strong correlations.[35,43]

Next, we examined the effect of band dispersion on ferromagnetism using diagonalization of small clusters for a model with far-neighbor hoppings. The ferromagnetism is greatly destabilized at less than quarter-filling $n<1$. In this case, the second-order effects of hoppings, which are dominating in the nearest-neighbor hopping model, are overwhelmed by the first-order effect. The phase diagram for the quarter-filling does not change greatly by far-neighbor hoppings that satisfy the bipartite condition. This result will be modified if the frustration is introduced by nonbipartite hopping integrals. Ferromagnetism for the electron-doped case is quite robust against variation of the DOS shape.

We may extract some presumptions on the ferromagnetism due to the orbital degeneracy in two and three dimensions both from the present results and those in infinite dimensions.[29,31] At quarter-filling $(n=1)$ ferromagnetism is supported by the orbital antiferromagnetic correlations for $U'>J$. This mechanism is common in all dimensions and robust if the hopping integrals satisfy the bipartite condition. We hence expect that the insulating ferromagnetic phase occurs in a similar parameter region in all dimensions. The lower phase boundary will approach the line $J=\alpha U'$ $(0.35>\alpha>0)$ for large U'/t, and α will decrease with increasing

dimensionality. For the electron-doped system ($n>1$), it is natural to expect that the double-exchange mechanism works in any dimension. The metallic ferromagnetism for $U'>J$ will appear in a similar parameter region in any dimension for $2>n>1$, since this ferromagnetic order is insensitive to the variation of the band dispersion. The situation is subtle in the case of the hole-doped system ($n<1$). The double-exchange mechanism hardly works for $n<1$ because of interorbital Coulomb repulsion. In this density region, indeed, variation of the band dispersion strongly destabilizes ferromagnetism in one dimension, and no ferromagnetic phase was found in infinite dimensions, though only sparse parameter points were examined.[29,31] In three (and two) dimensions, hence, the ferromagnetism might not appear in the simple nearest-neighbor hopping model on hypercubic lattices for $n<1$. To confirm this argument, we need to take account of the interplay between the electron correlations and the band dispersion and need to accomplish strenuous calculations for two- and three-dimensional systems.

For $J>U'$, QLRO of triplet superconductivity appears, which is supported by ferromagnetic order. In this region, a ferromagnetic state is stabilized by the double-exchange mechanism. However, this ferromagnetic state is affected by far-neighbor hoppings and, in infinite dimensions, the boundary of the ferromagnetic phase does not extend beyond the $J=U'$ line up to the coupling $U'=10$,[29] though we (T.M. and K.K.) did not study the $J>U'$ region. The coexistence of ferromagnetism and triplet superconductivity for $J\geqslant U'$ might not appear in higher dimensions. We expect that a two-dimensional system may be a plausible candidate for showing ferromagnetic triplet superconductivity.

Properties of paramagnetic ground states are of theoretical interest as well, though we did not study them in detail. The model has SU(4) symmetry for $J=0$ and is solved exactly in one dimension.[39] Recent numerical works clarified the properties of the quarter-filled system.[44,45] It will be an interesting problem to investigate the spin and orbital correlations for general n and $J\geqslant 0$. From the charge and spin-orbital separation as shown in Appendix A, we can say that the spin degrees of freedom for $n<1$ are equal to those at $n=1$ in the strong-coupling limit. In the other paramagnetic region for $J\gg U'$, electrons are bound to form triplet pairs. We found strong charge correlations for the quarter-filling but did not find LRO of charge density. It is an interesting problem to study whether a charge ordering occurs and coexists with antiferromagnetic LRO in higher dimensions.

ACKNOWLEDGMENTS

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APPENDIX A: THE EFFECTIVE HAMILTONIAN FOR $n<1$ IN THE STRONG-COUPLING LIMIT

In this appendix, we derive the effective exchange Hamiltonian for $n<1$ in the limit $U'-J\gg t$ in the nearest-neighbor hopping model. We treat the hopping term in Eq. (1) as a perturbation. In the unperturbed ground state, every site is singly occupied or empty. As the first-order effect of the hopping term, electrons hop from singly occupied sites to empty ones. The effective Hamiltonian in the first order of t is written as

$$H_{\rm eff}^{(1)}=-t\sum_{i=1}^{N}\sum_{m,\sigma}(\tilde{c}_{im\sigma}^{\dagger}\tilde{c}_{i+1m\sigma}+\text{H.c.}), \tag{A1}$$

where $\tilde{c}_{jm\sigma}\equiv c_{jm\sigma}(1-n_{jm-\sigma})(1-n_{j\bar{m}\sigma})(1-n_{j\bar{m}-\sigma})$ is the Gutzwiller-projected annihilation operator and $\tilde{n}_j$ is defined as $\Sigma_{m,\sigma}\tilde{c}_{jm\sigma}^{\dagger}\tilde{c}_{jm\sigma}$. In the unperturbed ground-state subspace $\tilde{n}_j$ is 0 or 1. Since the electrons cannot exchange their positions under the open boundary conditions, the matrix elements of $H_{\rm eff}^{(1)}$ are independent of the spin-orbital degrees of freedom. Hence $H_{\rm eff}^{(1)}$ is equivalent to a Hamiltonian for free spinless fermions, i.e.,

$$H_{\rm eff}^{(1)}=-t\sum_{i=1}^{N}(a_{i+1}^{\dagger}a_i+\text{H.c.}), \tag{A2}$$

where $a_i^{\dagger}$ is the creation operator of a spinless fermion. Then the number operator $\tilde{n}_i$ is equivalent to $a_i^{\dagger}a_i$. We may write down the ground-state wave function $|\Psi_{\rm g}\rangle$ as a direct product of the ground state of spinless fermions, $|\Phi_{\rm SF}\rangle$, and a spin-orbital wave function $|\Omega\rangle$ as[41]

$$|\Psi_{\rm g}\rangle=|\Phi_{\rm SF}\rangle\otimes|\Omega\rangle. \tag{A3}$$

Here $|\Phi_{\rm SF}\rangle$ is a simple Slater determinant for spinless fermions and describes only the charge degrees of freedom. The ground-state energy is degenerate for any spin-orbital wave function $|\Omega\rangle$ up to the first order in terms of t. The second-order terms due to virtual hoppings determine $|\Omega\rangle$. The effective Hamiltonian in the second order is given by

$$H_{\rm eff}^{(2)}=H_{\rm eff}^{(2a)}+H_{\rm eff}^{(2b)}, \tag{A4}$$

where

$$H_{\rm eff}^{(2a)}=\sum_{i=1}^{N}\tilde{n}_i\tilde{n}_{i+1}h(i,i+1) \tag{A5}$$

and

$$H_{\rm eff}^{(2b)}=\sum_{i=1}^{N}\sum_{\sigma}\sum_{m}\Bigg[-\frac{t^2}{U'-J}(\tilde{c}^{\dagger}_{i-1m\sigma}n_{i\bar{m}\sigma}\tilde{c}_{i+1m\sigma}+\text{H.c.})+\frac{t^2}{U'-J}(\tilde{c}^{\dagger}_{i-1\bar{m}\sigma}\tilde{c}^{\dagger}_{im\sigma}\tilde{c}_{i\bar{m}\sigma}\tilde{c}_{i+1m\sigma}+\text{H.c.})$$
$$-\frac{U't^2}{(U')^2-J^2}(\tilde{c}^{\dagger}_{i-1m\sigma}n_{i\bar{m}-\sigma}\tilde{c}_{i+1m\sigma}+\text{H.c.})+\frac{U't^2}{(U')^2-J^2}(\tilde{c}^{\dagger}_{i-1\bar{m}\sigma}\tilde{c}^{\dagger}_{im-\sigma}\tilde{c}_{i\bar{m}\sigma}\tilde{c}_{i+1m-\sigma}+\text{H.c.})$$
$$-\frac{Jt^2}{(U')^2-J^2}(\tilde{c}^{\dagger}_{i-1m\sigma}\tilde{c}^{\dagger}_{i\bar{m}-\sigma}\tilde{c}_{i\bar{m}\sigma}\tilde{c}_{i+1m-\sigma}+\text{H.c.})+\frac{Jt^2}{(U')^2-J^2}(\tilde{c}^{\dagger}_{i-1\bar{m}\sigma}\tilde{c}^{\dagger}_{im-\sigma}\tilde{c}_{i\bar{m}-\sigma}\tilde{c}_{i+1m\sigma}+\text{H.c.})$$
$$-\frac{Ut^2}{U^2-(J')^2}(\tilde{c}^{\dagger}_{i-1m\sigma}n_{im-\sigma}\tilde{c}_{i+1m\sigma}+\text{H.c.})+\frac{Ut^2}{U^2-(J')^2}(\tilde{c}^{\dagger}_{i-1m\sigma}\tilde{c}^{\dagger}_{im-\sigma}\tilde{c}_{im\sigma}\tilde{c}_{i+1m-\sigma}+\text{H.c.})$$
$$-\frac{J't^2}{U^2-(J')^2}(\tilde{c}^{\dagger}_{i-1m\sigma}\tilde{c}^{\dagger}_{im-\sigma}\tilde{c}_{im\sigma}\tilde{c}_{i+1\bar{m}-\sigma}+\text{H.c.})+\frac{J't^2}{U^2-(J')^2}(\tilde{c}^{\dagger}_{i-1m\sigma}\tilde{c}^{\dagger}_{im-\sigma}\tilde{c}_{i\bar{m}-\sigma}\tilde{c}_{i+1\bar{m}\sigma}+\text{H.c.})\Bigg]. \tag{A6}$$

The first term $H_{\rm eff}^{(2a)}$ represents the exchange interactions between electrons occupying nearest-neighbor sites, where $h(i,i+1)$ is defined in the effective Hamiltonian (6) for the quarter-filling. The second term $H_{\rm eff}^{(2b)}$ represents correlated hoppings between next-nearest-neighbor sites. The effective Hamiltonian $H_{\rm eff}^{(2)}$ contains both the charge and spin-orbital degrees of freedom. We may average charge degrees of freedom in $H_{\rm eff}^{(2)}$ out since $|\Phi_{\rm SF}\rangle$ is fixed to minimize $H_{\rm eff}^{(1)}$. In order to accomplish the averaging we introduce the *squeezed* system where the empty sites are omitted from the original system. Hence it is a chain with $N_{\rm e}$ sites with spin and orbital degrees of freedom on each site. We label the sites in the squeezed system by η. Employing the notation j_η for the position in the original system of the ηth electron in the squeezed system, we rewrite $H_{\rm eff}^{(2)}$ as

$$H_{\rm eff}^{(2a)}=\sum_{\eta=1}^{N_{\rm e}}\sum_{i=1}^{N}\tilde{n}_i\tilde{n}_{i+1}\delta_{ij_\eta}h(\eta,\eta+1) \tag{A7}$$

and

$$H_{\rm eff}^{(2b)}=\sum_{\eta=1}^{N_{\rm e}}\sum_{i=1}^{N}\sum_{\sigma_0=\pm}\sum_{m_0=\pm}(\tilde{n}_i a^{\dagger}_{i-1}a_{i+1}+\text{H.c.})\,\delta_{ij_\eta}\Theta(\eta,\sigma_0,m_0), \tag{A8}$$

where

$$\Theta(\eta,\sigma_0,m_0)\equiv\Bigg\{-\frac{t^2}{U'-J}(\tfrac{1}{2}+\sigma_0 S^z_\eta)\tau^{m_0}_\eta(\tfrac{1}{2}+\sigma_0 S^z_{\eta+1})\tau^{-m_0}_{\eta+1}+\frac{t^2}{U'-J}(\tfrac{1}{2}+\sigma_0 S^z_\eta)(\tfrac{1}{2}-m_0\tau^z_\eta)(\tfrac{1}{2}+\sigma_0 S^z_{\eta+1})(\tfrac{1}{2}+m_0\tau^z_{\eta+1})$$
$$-\frac{U't^2}{(U')^2-J^2}S^{\sigma_0}_\eta\tau^{m_0}_\eta S^{-\sigma_0}_{\eta+1}\tau^{-m_0}_{\eta+1}+\frac{U't^2}{(U')^2-J^2}(\tfrac{1}{2}+\sigma_0 S^z_\eta)(\tfrac{1}{2}-m_0\tau^z_\eta)(\tfrac{1}{2}-\sigma_0 S^z_{\eta+1})(\tfrac{1}{2}+m_0\tau^z_{\eta+1})$$
$$-\frac{Jt^2}{(U')^2-J^2}(\tfrac{1}{2}+\sigma_0 S^z_\eta)\tau^{m_0}_\eta(\tfrac{1}{2}-\sigma_0 S^z_{\eta+1})\tau^{-m_0}_{\eta+1}+\frac{Jt^2}{(U')^2-J^2}S^{\sigma_0}_\eta(\tfrac{1}{2}-m_0\tau^z_\eta)S^{-\sigma_0}_{\eta+1}(\tfrac{1}{2}+m_0\tau^z_{\eta+1})$$
$$-\frac{Ut^2}{U^2-(J')^2}S^{\sigma_0}_\eta(\tfrac{1}{2}+m_0\tau^z_\eta)S^{-\sigma_0}_{\eta+1}(\tfrac{1}{2}+m_0\tau^z_{\eta+1})+\frac{Ut^2}{U^2-(J')^2}(\tfrac{1}{2}+\sigma_0 S^z_\eta)(\tfrac{1}{2}+m_0\tau^z_\eta)(\tfrac{1}{2}-\sigma_0 S^z_{\eta+1})$$
$$\times(\tfrac{1}{2}+m_0\tau^z_{\eta+1})-\frac{J't^2}{U^2-(J')^2}(\tfrac{1}{2}+\sigma_0 S^z_\eta)\tau^{m_0}_\eta(\tfrac{1}{2}-\sigma_0 S^z_{\eta+1})\tau^{m_0}_{\eta+1}+\frac{J't^2}{U^2-(J')^2}S^{\sigma_0}_\eta\tau^{m_0}_\eta S^{-\sigma_0}_{\eta+1}\tau^{m_0}_{\eta+1}\Bigg\}. \tag{A9}$$

The symbols $\sigma_0=+,-$ and $m_0=+,-$ correspond to the spin $\uparrow,\downarrow$ and the orbital A,B, respectively. The correlated hopping processes in the original system are mapped to the spin-orbital exchange processes in the squeezed system as illustrated in Fig. 15.

In the limit where $N\to\infty$ with n kept constant, the expectation values of $\tilde{n}_i\tilde{n}_{i+1}\delta_{ij_\eta}$ and $(\tilde{n}_i a^{\dagger}_{i-1}a_{i+1}+\text{H.c.})\,\delta_{ij_\eta}$ in the state $|\Phi_{\rm SF}\rangle$ are independent of both η and i. Then we obtain

$$\langle H_{\rm eff}^{(2a)}\rangle_{\rm SF}=\frac{N}{N_{\rm e}}\langle \tilde{n}_i\tilde{n}_{i+1}\rangle_{\rm SF}\sum_{\eta=1}^{N_{\rm e}} h(\eta,\eta+1), \qquad \text{(A10)}$$

$$\langle H_{\rm eff}^{(2b)}\rangle_{\rm SF} =\frac{2N}{N_{\rm e}}\langle \tilde{n}_i a_{i-1}^{\dagger}a_{i+1}\rangle_{\rm SF}\sum_{\eta=1}^{N_{\rm e}}\sum_{\sigma_0=\pm}\sum_{m_0=\pm}\Theta(\eta,\sigma_0,m_0). \qquad \text{(A11)}$$

Here the notation $\langle\cdots\rangle_{\rm SF}$ means the expectation value in the state $|\Phi_{\rm SF}\rangle$. We note that the matrix elements of $\Theta(\eta,\sigma_0,m_0)$ are equal to those of $-h(\eta,\eta+1)/2$. We estimate the expectation values as

$$\langle \tilde{n}_i\tilde{n}_{i+1}\rangle_{\rm SF}=n^2-\left(\frac{\sin n\pi}{\pi}\right)^2 \qquad \text{(A12)}$$

and

$$\langle \tilde{n}_i a_{i-1}^{\dagger}a_{i+1}\rangle_{\rm SF}=n\frac{\sin 2n\pi}{2\pi}-\left(\frac{\sin n\pi}{\pi}\right)^2, \qquad \text{(A13)}$$

by using Wick's theorem.

Finally, we obtain the effective Hamiltonian for the spin-orbital degrees of freedom as

$$\langle H_{\rm eff}\rangle_{\rm SF}=n\left(1-\frac{\sin 2n\pi}{2n\pi}\right)\mathcal{H}_{\rm eff}. \qquad \text{(A14)}$$

Here $\mathcal{H}_{\rm eff}$ is equal to the effective Hamiltonian (5) for quarter-filling, where the summation over lattice sites are taken over those in the squeezed system. The factor $n(1-\sin 2n\pi/2n\pi)$ is positive for all densities $(0<n<1)$. Hence, the effective spin-orbital exchange interactions in the hole-doped system are same as those for the quarter-filled system except for a single multiplicative factor. The present result suggests that the same fact holds quite generally for one-dimensional systems with any number of internal degrees of freedom.

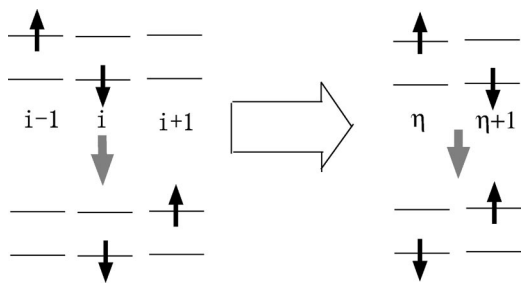

FIG. 15. An example of mapping from labeling of electrons by sites to labeling by counting only electrons from the left (ηth electron). A second-order term $\tilde{n}_{iB\downarrow}\tilde{c}_{i+1A\uparrow}^{\dagger}\tilde{c}_{i-1A\uparrow}$ is mapped to the term $S_{\eta}^{-}\tau_{\eta}^{-}S_{\eta+1}^{+}\tau_{\eta+1}^{+}$.

APPENDIX B: FERROMAGNETISM DUE TO A SINGLE UNPAIRED ELECTRON IN THE LIMIT WHERE $J-U'=\infty$

In finite-size calculations with an odd number of electrons we find that the ferromagnetic state is stable in a large parameter region where $J>U'$ as shown in Fig. 16. This ferromagnetism is caused by the motion of a single unpaired electron among bound triplet pairs. We consider a system with an odd-$N_{\rm e}$ system in the strong-coupling limit where $J\to\infty$ with J/U' (>1) kept constant under the open boundary conditions. We prove, in the following, that the ground state of this system is fully polarized. Only nearest-neighbor hoppings are assumed to exist.

In this limit two electrons on a site are bound to form a triplet pair. As a result $M=(N_{\rm e}-1)/2$ sites are doubly occupied and a single unpaired electron exits. In this limit, only allowed processes in the Hamiltonian are hoppings of an electron from a doubly occupied site to a singly occupied one and those from a singly occupied to a vacant one. The effective Hamiltonian $H_{\rm eff}$ is written as

$$H_{\rm eff}=-t\sum_{i=1}^{N}\{P_i^D c_{im\sigma}^{\dagger}P_i^S P_{i+1}^S c_{i+1m\sigma}P_{i+1}^D + P_i^S c_{im\sigma}^{\dagger}P_i^V P_{i+1}^V c_{i+1m\sigma}P_{i+1}^S+\text{H.c.}\}, \qquad \text{(B1)}$$

where P_i^D, P_i^S, and P_i^V are the projection operators for the doubly occupied triplet, the singly occupied, and vacant states, respectively. We can divide the whole phase space into subspaces with fixed N_A, N_B, and S^z. Here N_A and N_B denote the number of electrons in the orbitals A and B, respectively $(|N_A-N_B|=1)$, which are conserved. Each subspace is further divided into ${}_{N-1}C_M$ sectors according to the configuration of doubly occupied and vacant sites. States in each sector have the same configuration of doubly occupied and empty sites if we neglect the singly occupied site. Different sectors are disconnected with respect to $H_{\rm eff}$. We call the sectors as $\Gamma_j(N_A,N_B,S^z)$, where $j=1,2,\ldots,{}_{N-1}C_M$.

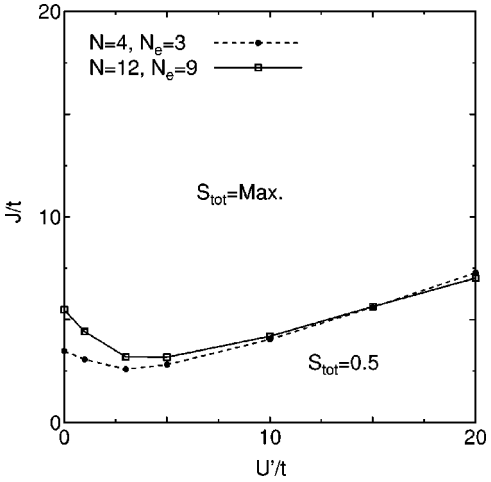

FIG. 16. Ground-state phase diagram for $(N,N_{\rm e})=(4,3)$ and (12,9) as examples of the odd-$N_{\rm e}$ cases.

We can show for any two configurations α and β of spins and electrons belonging to the same sector $\Gamma_j(N_A,N_B,S^z)$ that

(I) there exists $n \geqslant 1$ such that $\langle \Phi_\alpha | H_{\rm eff}^n | \Phi_\beta \rangle \neq 0$,

(II) $\langle \Phi_\alpha | H_{\rm eff} | \Phi_\beta \rangle \leqslant 0$. Here $|\Phi_\alpha\rangle$ denotes a basis vector chosen as

$$|\Phi_\alpha\rangle = \left[\prod_{l=1}^{M} (-1)^{j_l} \right] A_{\alpha_1} A_{\alpha_2} \cdots A_{\alpha_N} |0\rangle, \qquad \text{(B2)}$$

where α_i denotes the atomic state of the ith site and A_{α_i} is the corresponding operator, i.e., $c_{iA\uparrow}^\dagger c_{iB\uparrow}^\dagger$, $c_{iA\downarrow}^\dagger c_{iB\downarrow}^\dagger$, and $(1/\sqrt{2})(c_{iA\uparrow}^\dagger c_{iB\downarrow}^\dagger + c_{iA\downarrow}^\dagger c_{iB\uparrow}^\dagger)$ for doubly occupied triplet states, $c_{im\sigma}^\dagger$ for singly occupied states, and unity for a vacant state. The number j_l denotes the position of the lth doubly occupied site counted from an end. Here $|0\rangle$ is vacuum state. The proof of conditions (I) and (II) is straightforward.[27]

Now that the two conditions (I) and (II) on the matrix elements of $H_{\rm eff}$ are satisfied, the Perron-Frobenius theorem ensures that the ground state in the sector $\Gamma_j(N_A,N_B,S^z)$ is unique and can be written as a linear combination of all the basis vectors with strictly positive (or negative) coefficients. The positive (or negative) definiteness of the coefficients leads to the finding that the ground state is an eigenstate of the maximum value of the total spin.[27]

We thus proved that the ground state in each sector is fully polarized. As a result the ground state for subspace with fixed N_A and N_B is fully polarized. We understand that the large ferromagnetic region in the phase diagram in the case of odd N_e for $J-U' \gg t$ is caused by the motion of a single unpaired electron and is a finite-size effect.

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[1] J. Kanamori, Prog. Theor. Phys. **30**, 275 (1963).

[2] M. C. Gutzwiller, Phys. Rev. Lett. **10**, 159 (1963).

[3] J. Hubbard, Proc. R. Soc. London, Ser. A **276**, 238 (1993).

[4] E. H. Lieb, Phys. Rev. Lett. **62**, 1201 (1989); **62**, 1927(E) (1989).

[5] A. Mielke, J. Phys. A **24**, L73 (1991); **24**, 3311 (1991); **25**, 4335 (1992); Phys. Lett. **A174**, 443 (1993); A. Mielke and H. Tasaki, Commun. Math. Phys. **158**, 341 (1993).

[6] H. Tasaki, Phys. Rev. Lett. **69**, 1608 (1992).

[7] H. Tasaki, Phys. Rev. Lett. **75**, 4678 (1995).

[8] E. Müller-Hartmann, J. Low Temp. Phys. **99**, 349 (1995).

[9] K. Penc, H. Shiba, F. Mila, and T. Tsukagoshi, Phys. Rev. B **54**, 4056 (1996).

[10] H. Sakamoto and K. Kubo, J. Phys. Soc. Jpn. **65**, 4056 (1996).

[11] P. Pieri, S. Daul, D. Baeriswyl, M. Dzierzawa, and P. Fazekas, Phys. Rev. B **54**, 9250 (1996).

[12] S. Daul and R. M. Noack, Z. Phys. B: Condens. Matter **103**, 293 (1997).

[13] J. C. Slater, Phys. Rev. **49**, 537 (1936); **49**, 931 (1936).

[14] C. Zener, Phys. Rev. **81**, 440 (1951); **82**, 403 (1951).

[15] J. H. Van Vleck, Rev. Mod. Phys. **25**, 220 (1953).

[16] P. W. Anderson and H. Hasegawa, Phys. Rev. **100**, 675 (1955).

[17] L. M. Roth, Phys. Rev. **149**, 306 (1966).

[18] K. I. Kugel and D. I. Khomskii, Zh. Éksp. Teor. Fiz. **64**, 1429 (1973) [Sov. Phys. JETP **37**, 725 (1973)].

[19] M. Cyrot and C. Lyon-Caen, J. Phys. C **36**, 253 (1975).

[20] S. Inagaki, J. Phys. Soc. Jpn. **39**, 596 (1975).

[21] S. Inagaki and R. Kubo, Int. J. Magn. **4**, 139 (1973).

[22] K. Kusakabe and H. Aoki, Mol. Cryst. Liq. Cryst. **232**, 431 (1993).

[23] K. Kusakabe and H. Aoki, Physica B **194-196**, 217 (1994).

[24] W. Gill and D. J. Scalapino, Phys. Rev. B **35**, 215 (1987).

[25] J. Kuei and R. T. Scaletter, Phys. Rev. B **55**, 14 968 (1997).

[26] J. E. Hirsch, Phys. Rev. B **56**, 11 022 (1997).

[27] K. Kubo, J. Phys. Soc. Jpn. **51**, 782 (1982).

[28] S. Q. Shen, Phys. Rev. B **57**, 6474 (1998).

[29] T. Momoi and K. Kubo, Phys. Rev. B **58**, R567 (1998).

[30] K. Held and D. Vollhardt, Eur. Phys. J. B **5**, 473 (1998).

[31] In the dynamical mean-field theory, Held and Vollhardt (HV) found ferromagnetism for the hole-doped region (Ref. 30) ($n<1$) at $U=8$, $U'=6$, and $J=2$, but two of us [Momoi and Kubo (MK)] did not discover it (Ref. 29) in the region up to $U \leqslant 40$ and $U' \leqslant 20$. One possibility of this discrepancy may be that ferromagnetic phase appears in a very narrow region for the hole-doped case and MK could not discover it. As another possibility, note that the systems studied are different in these two cases. In Ref. 30, HV adopted a semielliptic DOS. On the other hand, in Ref. 29, MK used a Gaussian DOS, which is the exact one for the hypercubic lattice in infinite dimensions. As we showed in the present paper, the shape of DOS can greatly affect the appearance of ferromagnetism for $n<1$. Since the long tail of the Gaussian DOS is disadvantageous to ferromagnetism at low densities, the discrepancy of the phase diagrams presumably comes from the choice of DOS. Also, HV took an Ising anisotropic limit of the Hund coupling and neglected pair-hopping terms, but MK treated all terms correctly.

[32] J. Bünemann, W. Weber, and F. Gebhard, Phys. Rev. B **57**, 6896 (1998).

[33] T. Momoi, J. Stat. Phys. **85**, 193 (1996).

[34] S. R. White, Phys. Rev. Lett. **69**, 2863 (1992); Phys. Rev. B **48**, 10 345 (1993).

[35] K. Kubo, D. M. Edwards, A. C. M. Green, T. Momoi, and H. Sakamoto, in *Physics of Manganites*, edited by T. A. Kaplan and S. D. Mahanti (Kluwer Academic/Plenum, New York, 1999), p. 71.

[36] H. J. Schulz, Phys. Rev. Lett. **64**, 2831 (1990).

[37] N. Kawakami and S.-K. Yang, Phys. Lett. A **148**, 359 (1990).

[38] R. Assaraf, P. Azaria, M. Caffarel, and P. Lecheminant, Phys. Rev. B **60**, 2299 (1999).

[39] B. Sutherland, Phys. Rev. B **12**, 3795 (1975).

[40] N. M. Bogoliubov and V. E. Korepin, Int. J. Mod. Phys. B **3**, 427 (1989).

[41] M. Ogata and H. Shiba, Phys. Rev. B **41**, 2326 (1990); H. Shiba and M. Ogata, Int. J. Mod. Phys. B **5**, 31 (1991).

[42] A. Sakurai, Prog. Theor. Phys. **39**, 312 (1968).

[43] S. Yunoki, J. Hu, A. L. Malvezzi, A. Moreo, N. Furukawa, and E. Dagotto, Phys. Rev. Lett. **80**, 845 (1998).

[44] Y. Yamashita, N. Shibata, and K. Ueda, Phys. Rev. B **58**, 9114 (1998).

[45] B. Frischmuth, F. Mila, and M. Troyer, Phys. Rev. Lett. **82**, 835 (1999).