Itinerant ferromagnetism in strongly correlated electron systems

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We exactly show that the ground state of the Anderson lattice with $U=\infty$ is ferromagnetic at quarter filling if the level of localized electrons ε_f is deep enough: $\varepsilon_f<\varepsilon_{fc}$, where ε_{fc} is of the order of the bandwidth. Rigorous arguments show that if $\varepsilon_f<\varepsilon_{fc}$, the ground state has the total spin $S=(N-1)/2$ for $N_e=N+1$, where N is the number of lattice sites and N_e is that of electrons. This indicates that a transition to a (incompletely) magnetically ordered ground state will occur for a value of ε_f less than ε_{fc}. We observe this transition for finite U if $-\varepsilon_f$ is sufficiently large. An extension to more generalized models is discussed. The exact diagonalization technique is applied to a cluster cut out of the CuO_2 plane. Our analysis shows that the system with one-hole doping has a ferromagnetic phase in the ground state, indicating that a doped hole in the O p orbital is moving around in the ferromagnetic background of Cu spins.

I. INTRODUCTION

Heavy fermions and oxide superconductors are typical strongly correlated fermion systems.[1,2] The undoped oxide compounds exhibit rich magnetic structures with strong antiferromagnetic correlations. Heavy fermions also show fruitful ground-state properties including superconductivity, magnetic ordering, and paramagnetism with a largely enhanced specific-heat coefficient.[1] Many of heavy-fermion compounds show strong antiferromagnetic correlations and undergo antiferromagnetic transitions at low temperatures. A certain class of materials has been reported to develop tiny ordered magnetic moments of order 0.02–0.04 μB.[3] Furthermore, a few ferromagnetic heavy-fermion compounds were found to indicate a new class of magnetic materials.[4]

Since one of interesting elements of heavy fermions and oxide superconductors lies in an interplay between magnetism and itinerancy,[3,5] we consider the Anderson lattice model (periodic Anderson model) in order to gain insight into the physical properties of these systems:

$$H=-t\sum_{\langle ij\rangle\sigma}c_{i\sigma}^{\dagger}c_{j\sigma}+V\frac{1}{\sqrt{N}}\sum_{ki\sigma}(e^{ik\cdot R_i}c_{k\sigma}^{\dagger}f_{i\sigma}+\mathrm{H.c.})+\varepsilon_f\sum_{i\sigma}f_{i\sigma}^{\dagger}f_{i\sigma}+U\sum_i n_{fi\uparrow}n_{fi\downarrow}\ , \tag{1.1}$$

where $n_{fi\sigma}=f_{i\sigma}^{\dagger}f_{i\sigma}$ and $c_{k\sigma}=(1/\sqrt{N})\sum_j e^{-ik\cdot R_j}c_{j\sigma}$. The conduction-electron operators are represented by $c_{i\sigma}$ ($c_{i\sigma}^{\dagger}$) and local f electrons are denoted by $f_{i\sigma}$ ($f_{i\sigma}^{\dagger}$). U is the on-site Coulomb repulsion between f electrons.

The purpose of this paper is to investigate ferromagnetism of the Anderson lattice Hamiltonian at quarter filling by rigorous methods. Recently there have been interesting works on the ferromagnetism of the Kondo lattice. Our work has a close relation to recent interest on the ferromagnetism of the Kondo lattice.[6,7] We assume that the on-site Coulomb repulsion of localized electrons is large. We denote the number of lattice sites by N and that of electrons by N_e. At quarter filling there is one electron per site: $N_e=N$. First we show rigorously that for $N_e=N+1$, the ground state is (incompletely) ferromagnetic with the total spin $S=(N-1)/2$ if the level of localized electrons ε_f is sufficiently deep: $\varepsilon_f<\varepsilon_{fc}$. ε_{fc} is a critical value which we cannot know precisely only by rigorous arguments. The above statement holds also for the finite U case if U is large enough, where ε_f is dependent on U and the system forms a ferromagnetic order for $U>U_c$ and $\varepsilon_f<\varepsilon_{fc}(U)$. For less than or equal to quarter filling, the ferromagnetic state is described by spinless fermions occupying the lower band. At quarter filling $N_e=N+1$, our exact arguments predict a metal-insulator transition as well as a ferromagnetic one at $U=U_c$ if $\varepsilon_f<\varepsilon_{fc}(U)$, or at $\varepsilon_f=\varepsilon_{fc}(U)$ if $U>U_c$. Second, we determine critical values of ε_{fc} by the exact diagonalization method in small systems. We can safely extrapolate ε_{fc} to the infinite limit $N\to\infty$ and we show a phase diagram to indicate ferromagnetic regions. When U is very small or $U=0$, we can clearly apply the Fermi-liquid theory to describe the ground state and lower excited states properly. However, we find ferromagnetic regions for sufficiently large U. This indicates a breakdown of Fermi-liquid descriptions of heavy fermions at quarter filling with the increase of U.

The CuO_2 plane in the oxide superconductors is also within the scope of our study. We adopt the three-band Hubbard model given as

$$H=\sum_{\langle ij\rangle\sigma}[-t_{pd}(p_{i\sigma}^{\dagger}d_{j\sigma}+\mathrm{H.c.})-t_{pp}(p_{i\sigma}^{\dagger}p_{j\sigma}+\mathrm{H.c.})]+\sum_{i\sigma}(-\Delta)n_{di\sigma}+U\sum_i n_{di\uparrow}n_{di\downarrow}\ . \tag{1.2}$$

Here $p_{i\sigma}$ and $d_{i\sigma}$ are the annihilation operators of holes with spin σ on the O p and Cu d orbitals at site i, respectively. $-\Delta$ is the energy of a hole in the Cu orbital and U is the on-site Coulomb repulsion. We consider a Cu_4O_8 cluster with one-hole doping by the exact diagonalization method. This system also contains the phase with high-

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spin state, indicating that a doped hole is moving in the ferromagnetic background.

This paper is arranged as follows. In Sec. II, we show some rigorous statements on the ferromagnetism of the Anderson lattice for $N_e=N+1$. Our proposition suggests an existence of a critical value of ε_{fc} below which the ground state is ferromagnetic. We give a remark about frustration effects for the Anderson model. In Sec. III, the numerical diagonalization method is applied to show a phase diagram for small N. It is shown that ε_{fc}'s in the limit $N\to\infty$ are finite, which indicates that localized spins are ferromagnetically ordered even in the thermodynamic limit. A phase diagram of the ground state in the case of one-hole doped into a Cu_4O_8 cluster is shown in the t_{pd}-t_{pp} parameter space. Concluding remarks follow in Sec. IV.

II. RIGOROUS STATEMENTS

A. Rigorous statements for the Anderson lattice model

In this section we present some rigorous arguments to show that the ground state is ferromagnetic for $N_e=N+1$, if U and $-\varepsilon_f$ are sufficiently large. In the following we show a theorem below.

Theorem 1

Let us assume that $N_e=N+1$ and $U=\infty$. If ε_f is negative and $-\varepsilon_f$ is sufficiently large, then the ground state of the 1D Anderson lattice Hamiltonian (1.1) with open boundary condition has the total spin $S=(N-1)/2$ and is unique, apart from S_z degeneracy.

Proof

We set $N_e=N+1$. If $-\varepsilon_f \gg V$, we can restrict ourselves to truncated basis sets which contain at most two conduction electrons. We consider the following basis states:

$$\psi_{i\sigma;\{\sigma_n\}}=\sigma c_{i\sigma}^\dagger f_{1\sigma_1}^\dagger f_{2\sigma_2}^\dagger \cdots f_{N\sigma_N}^\dagger|0\rangle , \tag{2.1}$$

where $\{\sigma_n\}$ $(n=1,2,\ldots,N)$ denotes a set of spin configurations of f electrons. Applying the Hamiltonian to $\psi_{i\sigma;\{\sigma_n\}}$, we obtain

$$\begin{aligned} H\psi_{i\sigma;\{\sigma_n\}} &= -t\sigma(c_{i+1\sigma}^\dagger+c_{i-1\sigma}^\dagger)f_{1\sigma_1}^\dagger f_{2\sigma_2}^\dagger\cdots f_{N\sigma_N}^\dagger|0\rangle \\ &\quad +V\sigma c_{i\sigma}^\dagger\sum_j(-1)^{j-1}c_{j\sigma_j}^\dagger f_{1\sigma_1}^\dagger\cdots \\ &\qquad\qquad \times f_{j-1\sigma_{j-1}}^\dagger f_{j+1\sigma_{j+1}}^\dagger\cdots f_{N\sigma_N}^\dagger|0\rangle \\ &\quad +N\varepsilon_f\psi_{i\sigma;\{\sigma_n\}} . \end{aligned} \tag{2.2}$$

Off-diagonal elements due to the kinetic part of the Hamiltonian are always negative if $(-t)<0$ for the periodic boundary condition. $H\psi_{i\sigma;\{\sigma_n\}}$ has nonzero matrix elements with the following basis sets:

$$\psi_{i\sigma,j\sigma';\{\sigma_n\}} =(-1)^j\sigma c_{i\sigma}^\dagger c_{j\sigma'}^\dagger f_{1\sigma_1}^\dagger\cdots f_{j-1\sigma_{j-1}}^\dagger f_{j+1\sigma_{j+1}}^\dagger\cdots f_{N\sigma_N}^\dagger|0\rangle , \tag{2.3}$$

which contain two conduction electrons. When $i=j$, from Eq. (2.3) we obtain

$$\psi_{i\uparrow,i\downarrow;\{\sigma_n\}}=\psi_{i\downarrow,i\uparrow;\{\sigma_n\}} =-(-1)^i c_{i\downarrow}^\dagger c_{i\uparrow}^\dagger f_{1\sigma_1}^\dagger\cdots f_{i-1\sigma_{i-1}}^\dagger f_{i+1\sigma_{i+1}}^\dagger\cdots f_{N\sigma_N}^\dagger|0\rangle . \tag{2.4}$$

Then we easily obtain

$$\langle\psi_{i\sigma,j\sigma';\{\sigma_n\}}|H|\psi_{i\sigma;\{\sigma_n\}}\rangle=-V\delta_{\sigma'\sigma_j}, \text{ for } i\neq j , \tag{2.5a}$$

and

$$\langle\psi_{i\uparrow,i\downarrow;\{\sigma_n\}}|H|\psi_{i\sigma;\{\sigma_n\}}\rangle=-V\delta_{-\sigma,\sigma_i} , \tag{2.5b}$$

which are negative if $V>0$. The action of H on $H\psi_{i\sigma;\{\sigma_n\}}$ leads to third vectors,

$$\psi_{i\sigma,j+1\sigma';\{\sigma_n\}}=A_{i\sigma,j+1\sigma'}c_{i\sigma}^\dagger c_{j+1\sigma'}^\dagger f_{1\sigma_1}^\dagger\cdots f_{j-1\sigma_{j-1}}^\dagger f_{j+1\sigma_{j+1}}^\dagger\cdots f_{N\sigma_N}^\dagger|0\rangle , \tag{2.6a}$$

$$\psi_{i\sigma,j-1\sigma';\{\sigma_n\}}=A_{i\sigma,j-1\sigma'}c_{i\sigma}^\dagger c_{j-1\sigma'}^\dagger f_{1\sigma_1}^\dagger\cdots f_{j-1\sigma_{j-1}}^\dagger f_{j+1\sigma_{j+1}}^\dagger\cdots f_{N\sigma_N}^\dagger|0\rangle , \tag{2.6b}$$

$$\psi_{i+1\sigma,j\sigma';\{\sigma_n\}}=A_{1+1\sigma,j\sigma'}c_{i+1\sigma}^\dagger c_{j\sigma'}^\dagger f_{1\sigma_1}^\dagger\cdots f_{j-1\sigma_{j-1}}^\dagger f_{j+1\sigma_{j+1}}^\dagger\cdots f_{N\sigma_N}^\dagger|0\rangle , \tag{2.6c}$$

and

$$\psi_{i-1\sigma,j\sigma';\{\sigma_n\}}=A_{i-1\sigma,j\sigma'}c_{i-1\sigma}^\dagger c_{j\sigma'}^\dagger f_{1\sigma_1}^\dagger\cdots f_{j-1\sigma_{j-1}}^\dagger f_{j+1\sigma_{j+1}}^\dagger\cdots f_{N\sigma_N}^\dagger|0\rangle . \tag{2.6d}$$

We can arrange phase factors $A_{i\sigma,j+1\sigma'},\ldots$, so that matrix elements are negative $(-t)<0$. Thus we have shown that all the off-diagonal elements are nonpositive for $-\varepsilon_f\gg V$. According to the Perron-Frobenius theorem,[8,9] the lowest eigenvalue state Ψ_σ is unique and is a linear combination of basis states with positive coefficients. We can easily show that such a state has the total spin $S=(N-1)/2$.[7] In the subspace $S^z=(N-1)/2$, we define a state $\Psi_{\max}$ with $S=(N-1)/2$. $\Psi_{\max}$ is given by

$$\Psi_{\max}=\sum_i(-1)^{i-1}(c_{i\uparrow}^\dagger f_{i\downarrow}^\dagger-c_{i\downarrow}^\dagger f_{i\uparrow}^\dagger)\prod_{j\neq i}f_{j\uparrow}^\dagger|0\rangle . \tag{2.7}$$

Applying the total spin lowering operator S^-, we obtain a state with $S=(N-1)/2$ and lower S^z:

$$(S^-)^n\Psi_{\max}=\sum_i(-1)^{i-1}(c_{i\uparrow}^\dagger f_{i\downarrow}^\dagger-c_{i\downarrow}^\dagger f_{i\uparrow}^\dagger)(S^-)^n\prod_{j\neq i}f_{j\uparrow}^\dagger|0\rangle . \tag{2.8}$$

Since this state is a linear combination of basis states with non-negative coefficients, it has a nonzero inner product: $\langle\Psi_g|(S^-)^n\Psi_{\max}\rangle\neq 0$. Note that a trial state with $S=(N+1)/2$,

$$\psi_{\mathrm{tr}}=\sum_i(-1)^{i-1}(S^-)^n(c_{i\uparrow}^\dagger f_{i\downarrow}^\dagger+c_{i\downarrow}^\dagger f_{i\uparrow}^\dagger)\prod_{j\neq i}f_{j\uparrow}^\dagger|0\rangle , \tag{2.9}$$

and Ψ_g are orthogonal $\langle\psi_{\mathrm{tr}}|\Psi_g\rangle=0$ due to a factor σ in (2.1). Thus we can conclude that the ground state Ψ_g has the total spin $S=(N-1)/2$.

For $N_e=N+1$, we obtain the quarter-filled model in the limit $N\to\infty$. The ferromagnetism of the ground state indicates that we can describe it by spinless fermion model of the Anderson lattice. It is then easily followed that the lower band is completely filled by spinless fermions and thus we have an insulating ground state.

From the theorem above we know the existence of ε_{fc}; for $\varepsilon_f<\varepsilon_{fc}$ the ground state is ferromagnetic. However, we should refer to other methods to know exact values of ε_{fc}. Note that we have a possibility that $|\varepsilon_{fc}|$ is infinite. Numerical calculations in small systems provide us one way to obtain ε_{fc}. Thus, we have performed exact diagonalizations for the Anderson lattice Hamiltonian in Eq. (1.1) to determine ε_{fc}, which is the subject of Sec. III.

Before proceeding further, we discuss that the above theorem holds for finite U if U is large enough. Since the large U allows us to truncate the basis space, similar discussions prove the following theorem.

Theorem 2

Let us assume that $N_e=N+1$. If U is large and ε_f is deep enough, the ground state of the 1D Anderson lattice Hamiltonian with open boundary condition has the total spin $S=(N-1)/2$ and is unique apart from S^z degeneracy. The finite U case will be investigated by numerical methods in Sec. III.

B. Anderson lattice with frustrations

Here we consider the following one-dimensional (1D) Hamiltonian:

$$H=-t\sum_{\langle ij\rangle\sigma}c_{i\sigma}^\dagger c_{j\sigma}+V\sum_{i\sigma}[(c_{i\sigma}^\dagger+c_{i+1\sigma}^\dagger)f_{i\sigma}+\mathrm{H.c.}]$$
$$+\varepsilon_f\sum_{i\sigma}f_{i\sigma}^\dagger f_{i\sigma}+U\sum_i n_{fi\uparrow}n_{fi\downarrow} , \tag{2.10}$$

which we illustrate in Fig. 1. Frustration effects are contained in the mixing term of Eq. (2.10). The model for

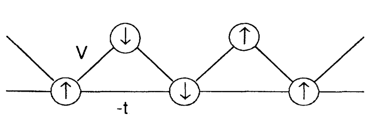

FIG. 1. Lattice structure of the one-dimensional Anderson lattice with frustrations.

CuO_2 plane in the oxide superconductor is considered to be a variant of the 2D Anderson lattice with frustrations, which we will discuss in Sec. III. We investigate now whether we can apply the Perron-Frobenius theorem to this model. We consider a set of truncated basis states as for the original Anderson lattice,

$$\psi_{i\sigma;\{\sigma_n\}}=\sigma c_{i\sigma}^\dagger f_{1\sigma_1}^\dagger f_{2\sigma_2}^\dagger\cdots f_{N\sigma_N}^\dagger|0\rangle , \tag{2.11a}$$

$$\psi_{i\sigma,j\sigma';\{\sigma_n\}}=(-1)^j\sigma c_{i\sigma}^\dagger c_{j\sigma'}^\dagger f_{1\sigma_1}^\dagger\cdots f_{j-1\sigma_{j-1}}^\dagger f_{j+1\sigma_{j+1}}^\dagger$$
$$\times\cdots f_{N\sigma_N}^\dagger|0\rangle , \tag{2.11b}$$

$$\tilde{\psi}_{i\sigma,j\sigma';\{\sigma_n\}}=(-1)^j\sigma c_{i\sigma}^\dagger c_{j+1\sigma'}^\dagger f_{1\sigma_1}^\dagger\cdots f_{j-1\sigma_{j-1}}^\dagger f_{j+1\sigma_{j+1}}^\dagger$$
$$\times\cdots f_{N\sigma_N}^\dagger|0\rangle . \tag{2.11c}$$

It easily appears that matrix elements are not always negative in this space because one obtains

$$\langle\psi_{i\sigma,j\sigma';\{\sigma_n\}}|H|\psi_{i\sigma;\{\sigma_n\}}\rangle=-V\delta_{\sigma'\sigma_j} , \tag{2.12a}$$

$$\langle\tilde{\psi}_{i\sigma,j\sigma';\{\sigma_n\}}|H|\psi_{i\sigma;\{\sigma_n\}}\rangle=-V\delta_{\sigma'\sigma_j} , \tag{2.12b}$$

and

$$\langle\tilde{\psi}_{i\sigma,i\sigma';\{\sigma_n\}}|H|\psi_{i+1\sigma';\{\sigma_n\}}\rangle=V\delta_{\sigma\sigma_i} . \tag{2.12c}$$

Therefore we cannot know only by exact arguments whether the ground state can be ferromagnetic or not for $N_e=N+1$ when effects of frustrations are taken into account. We show, however, in Sec. III that numerical calculations reveal the ferromagnetic ground state for $N_e=N+1$, if ε_f is well below the Fermi level. In other words we are allowed to say that very small frustrations are not enough to destroy ferromagnetic ordering.

III. NUMERICAL RESULTS

A. 1D Anderson lattice

We use the Lanczos method to obtain eigenvalues of the ground state in the subspace with $S^z=M\,(0\le M\le S)$. We show in Figs. 2(a) and 2(b) the ground-state energy versus ε_f for $N_e=N+1$, where $V=0.2$ and $N=4$ and 6. We observe that the ferromagnetic state with $S=(N-1)/2$ is the ground state for large $-\varepsilon_f$. In Fig. 3 we show ε_{f_c} vs $1/N$ for several values of V in the limit $U=\infty$, where $N=4$, 5, 6, 7, and 8, and $N_e=N+1$. Extrapolated values of ε_{fc} are presented in Fig. 4, where the solid line denotes ε_{fc} in the limit $N=\infty$, below which the ground state is ferromagnetic. As easily known, ε_{fc} is of the order of the bandwidth over the wide range of V.

Here we estimate the ground-state energy by simple calculations. When $U=0$, the dispersions of the mixed band are given by

$$E_k^{\pm}=(\varepsilon_k+\varepsilon_f)/2\pm\sqrt{(\varepsilon_k-\varepsilon_f)^2/4+V^2} .$$

We evaluate ground-state energy in two ways and compare them with exact values as shown in Table I. In column A we show the ground-state energies for $U=0$.

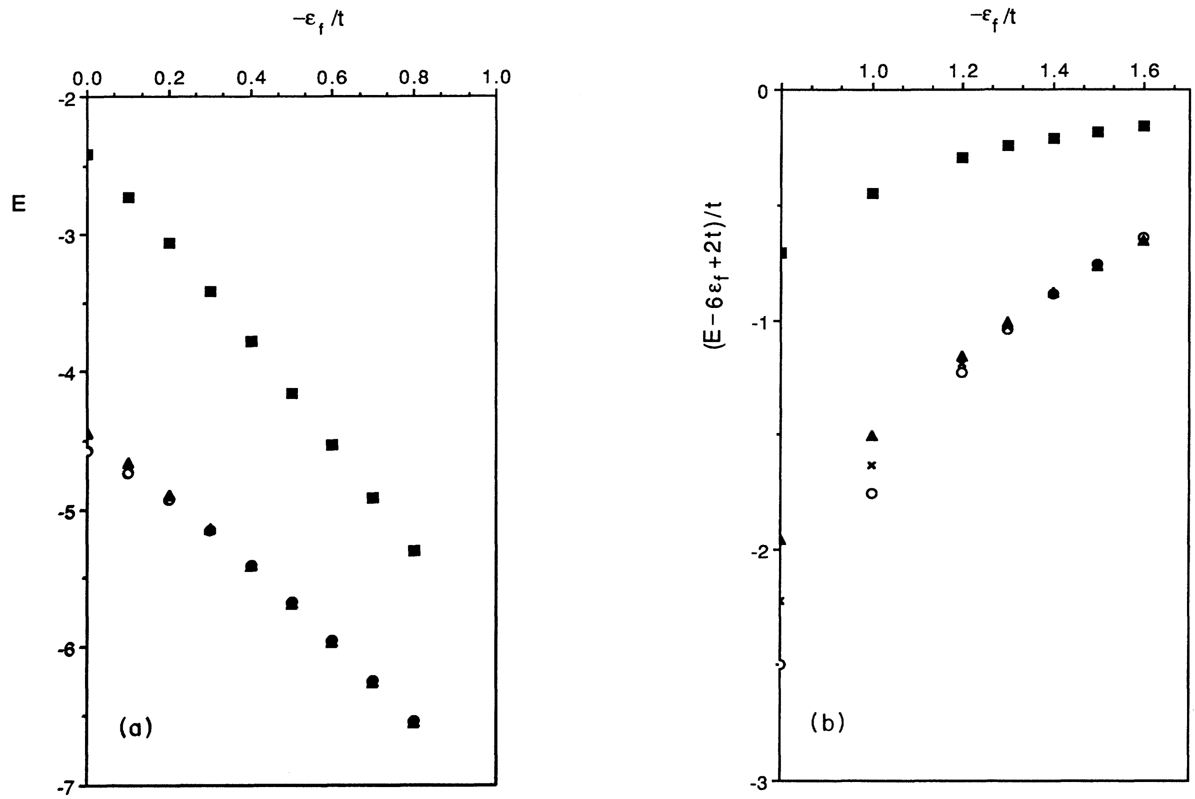

FIG. 2. Ground-state energy vs ε_f for $N_e = N+1$. Parameters are $V = 0.2$ and $N =$ (a) 4 and (b) 6. (a) Circles, triangles, and squares are for $S = 1/2$, $3/2$, and $5/2$, respectively. (b) Circles, crosses, triangles, and squares are for $S = 1/2$, $3/2$, $5/2$, and $7/2$, respectively.

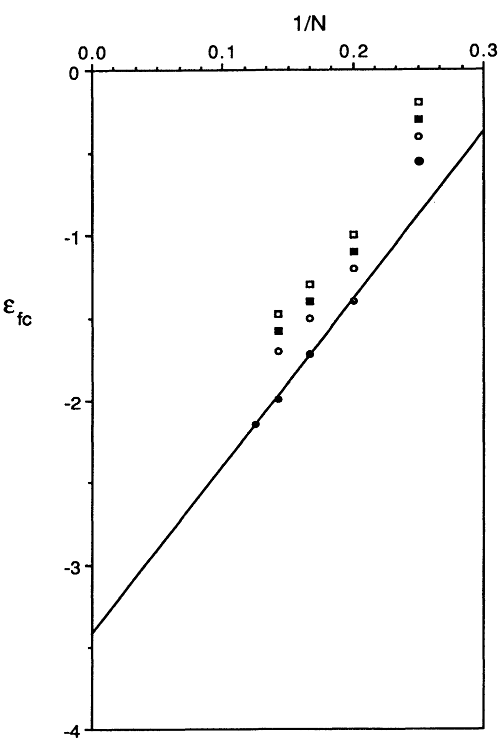

FIG. 3. Critical values ε_{fc} vs $1/N$ for $N_e = N+1$. Parameters are $V = 0.5$, 0.2, 0.1, and 0.02 from the bottom ($t = 1$).

Column B indicates the case where the lower band is filled completely by up spins and we add one down spin at the bottom of the conduction band as illustrated in Fig. 5. This picture reminds us of the band structure of the Hubbard gap. Clearly, when ε_f is deep, the ground-state energy is well approximated by the ferromagnetic model in column B. We also point out that if the position of ε_f is well above ε_{fc}, the ground state is degenerate with respect to its momentum for $U = 0$.

In Fig. 6 we have plotted U_c vs $1/N$ for $\varepsilon_f = -4$ and -3. We obtain finite values of U_c for $\varepsilon_f < \varepsilon_{fc}$ in the limit $N = \infty$. We denote the critical value of ε_f by $\varepsilon_{fc}(U)$ for finite U cases. In Fig. 7 we show ferromagnetic regions in

TABLE I. Comparison of the ground-state energy for $N_e = N+1$, $V = 0.2$, and $U = \infty$. In column A we show energies for $U = 0$ and in column B we show those obtained by the ferromagnetic model where the lower bands is filled with up-spin electrons and we add one down spin at the bottom of conduction band ε_k.

N	ε_f	Exact	A ($U=0$)	B (ferro.)
4	0.0	−4.579	−4.6396	−4.4396
	−1.0	−7.139	−7.1926	−7.1288
	−2.0	−10.2736	−10.4594	−10.2496
6	0.0	−8.214	−8.2322	−6.1937
	−2.0	−14.330	−14.5673	−14.3136

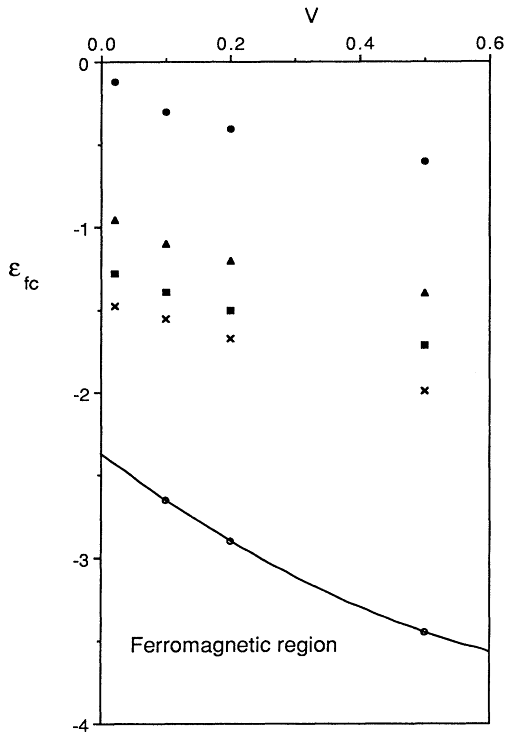

FIG. 4. Ferromagnetic regions in the ε_f-V plane for $N_e = N+1$ and $t=1$. ε_{fc}'s are plotted for $N=4$, 5, 6, and 7 (from the top) with the periodic boundary condition. Solid line shows the critical line in the limit $N=\infty$, below which the ground state is ferromagnetic.

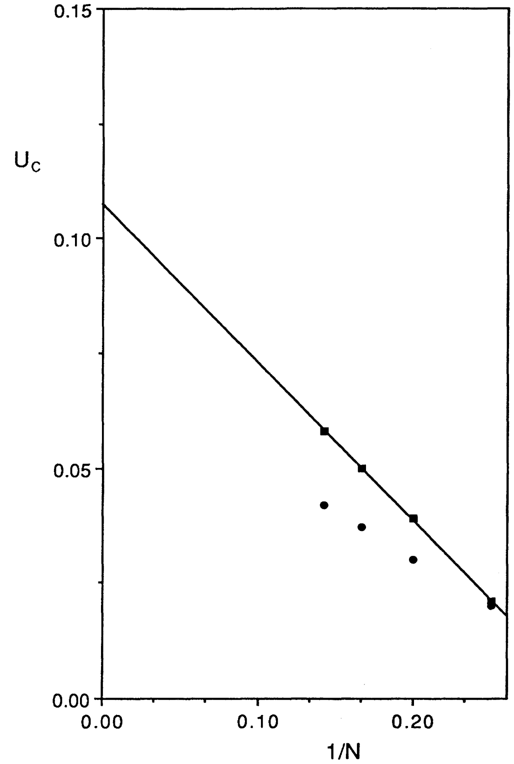

FIG. 6. Critical values U_c vs $1/N$ for $N_e = N+1$. Parameters are $\varepsilon_f = -4$ (circles) and -3 (squares), and $V=0.2$ ($t=1$).

the $\varepsilon_f - U$ plane for $N_e = N+1$. We observe the phase transition at $U=U_c$ if $-\varepsilon_f$ is large enough to be comparable to the order of the bandwidth.

Let us turn to the 1D frustrated Anderson lattice shown in Fig. 1. We present ε_{fc} for several values of V in Fig. 8. Extrapolated values of ε_{fc} in the limit $N=\infty$ are finite as shown in Fig. 9, leading to an existence of the ferromagnetic ground state. This ground state is described in a manner similar to the original Anderson lattice; localized electrons are aligned ferromagnetically and one electron is at the bottom of the upper band $E_k^+ \approx \varepsilon_k$.

Our theorems are valid even if there are ferromagnetic intersite Ruderman-Kittel-Kasuya-Yosida (RKKY) interactions because off-diagonal elements are still negative. However, antiferromagnetic RKKY interactions violate the negativity and thus the condition of the theorem is not satisfied.

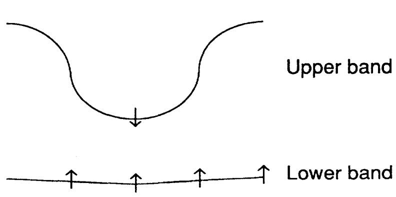

FIG. 5. Schematic illustration of the band structure in the ferromagnetic region.

B. 2D CuO_2 plane with one-hole doping

Let us turn to investigate the three-band Hubbard model in Eq. (1.2). This model can be regarded as a variant of the 2D frustrated Anderson lattice model. In this

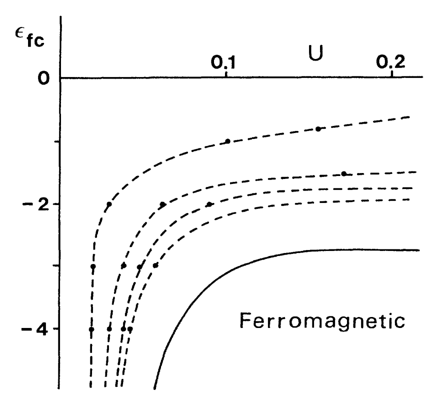

FIG. 7. Ferromagnetic regions in the ε_f-U plane for $N_e = N+1$ and $V=0.2$ ($t=1$). Dashed lines show critical lines for $N=4$, 5, 6, and 7 (from the top) and the solid line represents that in the limit $N=\infty$.

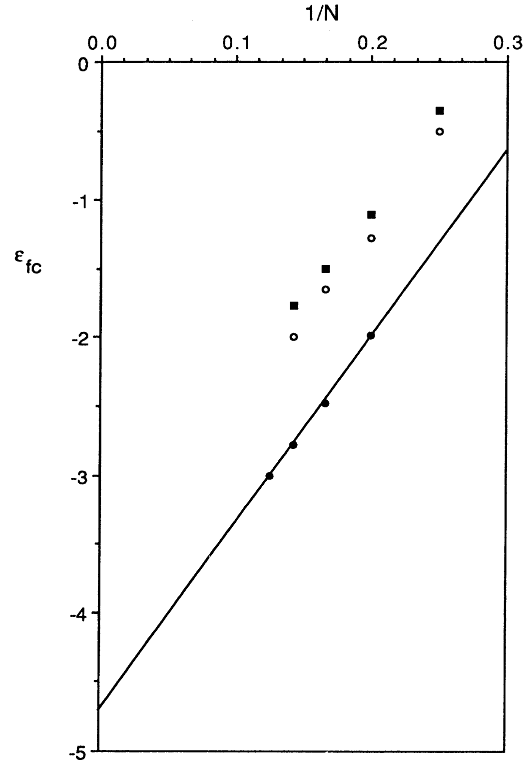

FIG. 8. Critical values of ε_{fc} vs $1/N$ for the frustrated Anderson lattice and $N_e = N+1$. Parameters are as follows: $V=0.5$, 0.2, and 0.1 (from the bottom) in units of t.

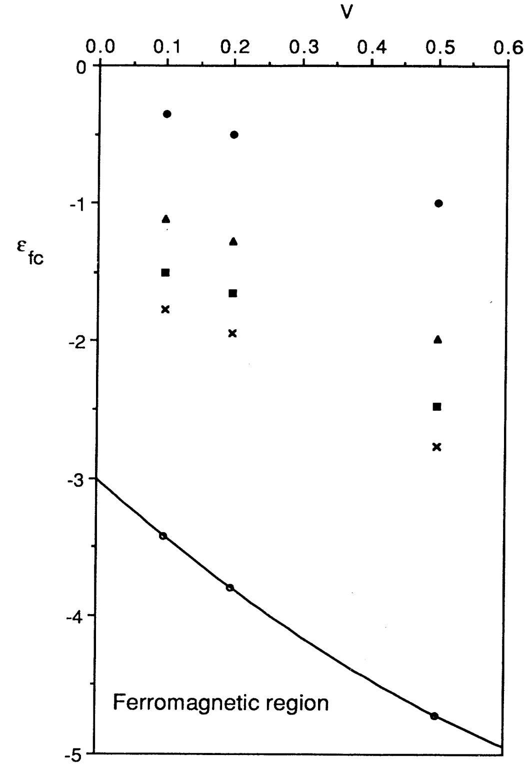

FIG. 9. Ferromagnetic region in the ε_{fc}-V plane for the frustrated Anderson lattice where $N_e = N+1$ for N=4, 5, 6, and 7 (from the top).

section we use the usual hole notation found in the literature.[2] The undoped system has an intrinsic hole at each Cu orbital, exhibiting a strong antiferromagnetic correlation. An extra hole, doped mainly at the O p_σ orbital, is considered to couple strongly with the intrinsic hole at the Cu d orbital.

In Fig. 10 we show the phase diagram of the ground state with one hole doped into the Cu_4O_8 cluster in the t_{pd} vs t_{pp} plane. Parameters are $\Delta = 3.6$ and $U = 10$. We have found two types of states depending on parameters for the periodic boundary conditions. As long as t_{pp}/t_{pd} is small, the one-hole ground state becomes $S = 1/2$ because Cu spins and O holes are strongly mixed due to the hybridization term. In this region, the ground state is degenerate with respect to its total momentum as $(\pi, 0)$ and $(0, \pi)$.[10] Now let us discuss the effect of t_{pp}. If t_{pp}/t_{pd} increases beyond a threshold, the ground state turns out to be a new state with the spin eigenvalue $S = 3/2$ and the total momentum (0,0). This state can be regarded as the (incomplete) ferromagnetic state discussed previously in this paper. We can easily imagine a picture where a doped hole is moving in the ferromagnetic background of Cu spins. If one of the boundary conditions is changed into an antiperiodic one, the total energy is stabilized for the periodic boundary condition at the region with the large values of t_{pd} and t_{pp}, giving the ground state with $S = 1/2$ and the momentum of $(\pi, \pi/2)$.

Figure 11 represents schematically the electronic structure of the high-spin state. The doped hole forms a local singlet with an intrinsic hole at the Cu site and other holes at Cu sites couple ferromagnetically among them. The ground-state wave function is a superposition of configurations with various locations of the local singlet. In each configuration the wave function of the doped hole is isotropic around the localized center at the Cu site. We may call this singlet the Zhang-Rice singlet[11] although the background is ferromagnetic. Our local singlet has a tail delocalized to neighboring O orbitals.

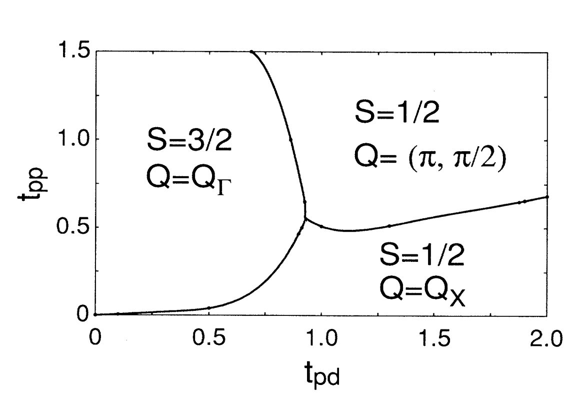

FIG. 10. Phase diagram of the ground state in the case of one-hole doped into the Cu_4O_8 cluster in the t_{pd}-t_{pp} plane. The ground state has three regions with different total momentum Q and spin S. Q_Γ and Q_X denote (0,0) and $(\pi, 0)$, respectively.

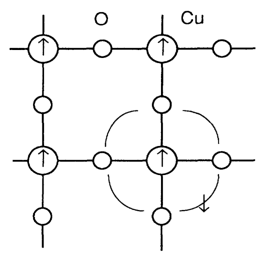

FIG. 11. Schematic representation of a doped hole at p_σ orbital in the weak-hybridization case.

IV. DISCUSSION

In summary, by exact methods we have shown that the ground state of the Anderson lattice model is incompletely ferromagnetic with $S=(N-1)/2$ when $N_e=N+1$, if the level of f electrons is deep enough, i.e., $\varepsilon_f<\varepsilon_{fc}$. The critical level ε_{fc} appears to be of the order of the bandwidth. Our discussions essentially depend on the Perron-Frobenius theorem of the matrix analysis. We have obtained exact values of ε_{fc} by numerical diagonalizations in small clusters and extrapolating them to infinite systems $N\rightarrow\infty$. If $\varepsilon_f\gg\varepsilon_{fc}$, the ground state is degenerate, as we would expect for the noninteracting case. Our theory predicts a ferromagnetic transition as the intra-atomic Coulomb interaction is increased or the localized level ε_f is decreased. This indicates that a transition to an insulating magnetically ordered ground state will occur for $\varepsilon_f<\varepsilon_{fc}$ or $U>U_c$ at quarter filling in the limit of infinite N. Thus, the ferromagnetic region exists near the insulating phase. Please note that our results indicate an example of itinerant electron ferromagnetism.[12] We have also shown that frustrated systems form an incomplete ferromagnetic order although the Perron-Frobenius theorem never applies to such systems.

In the 2D CuO_2 model with one-hole doping, the high-spin state shows up as the ground state in the t_{pd}-t_{pp} plane. In our opinion this state can be recognized as the ferromagnetic state discussed throughout the paper. In the case where the hybridization t_{pd} dominates over direct p-p hopping, t_{pp}, the ground state with $S=1/2$ is degenerate with respect to its momentum, which agrees with the predictions of the noninteracting band picture. If t_{pd} is not so large, the ground state turns out to be ferromagnetic with the spin quantum number $S=(N-1)/2$ and the momentum (0,0).

Our ferromagnetism has the same origin as that of the Nagaoka theorem[13] for the single-band Hubbard model. The ferromagnetic state is the most favorable to gain kinetic and hybridization energy. Our results discussed here are valid for finite U although the Nagaoka theorem is rigorously applicable only in the limit $U\rightarrow\infty$. Here let us comment that several ferromagnetic rare-earth compounds have been reported in a long history of study on the dense Kondo system,[4] for example U_3As_4 (Ref. 14), $CeSi_{2-x}$, and $CeRh_3B_2$. There may be a possibility that ferromagnetic transitions occur based on our program.

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