Infinite U_d, U_p ground state of the extended Hubbard model

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The renormalization of the extended Hubbard model proposed by Zhang and Rice [Phys. Rev. B **37**, 3759 (1988)] that leads to the (nearest-neighbor-only) t-J model is scrutinized in the infinite correlation limit. We demonstrate that the $U_d, U_p \rightarrow \infty$ limit obtained from the extended Hubbard model does not have the same ground state as the $U \rightarrow \infty$ extrapolation of the t-J model.

A microscopic Hamiltonian for the doped CuO_2 planes is now recognized as one of the essential elements required to describe the high-T_c oxides, and it is still unclear what the correct Hamiltonian is. Essentially, the question has been: How much of the detailed electronic structure of the Cu $3d$ and O $2p$ orbitals needs to be included in the Hamiltonian in order to adequately represent the "low-energy" physics contained in these planes?

It has been established[1] that upon doping La_2CuO_4 with a divalent ion, such as Sr, the holes that are produced on the CuO_2 planes reside in the O $2p$ orbitals. Henceforth we shall assume these to be the σ orbitals. However, Anderson[2] has claimed that only a single-band model, viz. a mixed-valence Cu^{3+}-Cu^{2+} Hamiltonian, is sufficient to describe this system. Anderson's claim was formalized in a recent paper by Zhang and Rice.[3] These authors began with an effective Hamiltonian that explicitly included the occupation of the O $2p$ orbitals by holes upon doping.[4] They then tried to argue that the O holes (more precisely, Wannier functions formed from the O hole states) hybridize with the Cu holes to form a reasonably localized[5] singlet. The most important claim made in this paper was that this singlet was sufficiently separated from higher energy excited states so that its *magnetic interactions* with all the Cu holes could be ignored. Thus Zhang and Rice[3] argued that the two-band model reduces to an effective one-band Hamiltonian, where the singlet behaves like a doubly occupied Cu $3d_{x^2-y^2}$ orbital.

More recently, Zhang[6] has attempted to show that in the limit of the Hubbard energy U_d and the Cu-O promotion energy ε, both going to infinity such that $U_d-\varepsilon>0$ remains finite, the one-band renormalization is exact. His study focused on a completely different part of the Hamiltonian [see Fig. 1(a) of Ref. 7] than our study does, and thus provides a valuable complement.

In this Comment we scrutinize the renormalization performed by Zhang and Rice[3] in the following manner. We begin with the extended Hubbard model proposed by Emery[4(a)] and consider a single O hole. We do not set the Hubbard intrasite repulsion energy U_p equal to zero, as was done by Zhang and Rice. However, the inclusion of this energy does not alter their arguments and only modifies their expressions for some of the effective exchange and hopping energies (also see Ref. 8). Then, in the strong-correlation limit one derives[4(b)] an effective Hamiltonian which describes (i) O hole hopping processes to second order in the p-d hybridization energy t_{pd} (which necessarily includes the Cu-O superexchange), and (ii) the Cu-Cu superexchange which is the lowest-order extensive energy (viz. of order t_{pd}^4) when only one O hole is present. One may then apply the Zhang and Rice procedure to renormalize this effective Hamiltonian into a new one-band effective Hamiltonian. Now, consider taking the limit $U_d, U_p \rightarrow \infty$ both before and after performing the Zhang and Rice renormalization. If the renormalization procedure[3] is correct, these two limiting Hamiltonians should have the same low-energy physics. Our approach is represented in Fig. 1, where the objects of our study are the limiting Hamiltonians denoted by $H_{1,\infty}$ and $H_{2,\infty}$.

We first determine the limiting form of the effective Hamiltonian obtained in Ref. 3 in the $U_d, U_p \rightarrow \infty$ limit, viz. we find $H_{1,\infty}$. Explicitly including U_p in the Zhang-

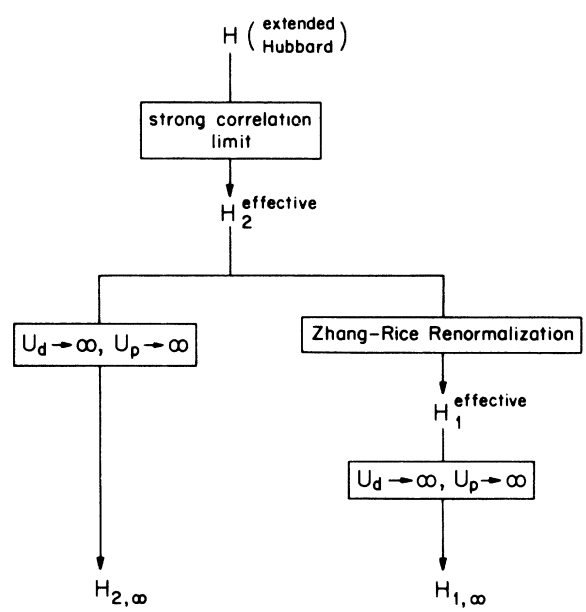

FIG. 1. The various limits applied to the extended Hubbard Hamiltonian. In the strong-correlation limit one obtains $H_2^{(\text{eff})}$ (see Ref. 4). Then, $H_{1,\infty}$ and $H_{2,\infty}$ may be derived from the $U_p \rightarrow \infty$, $U_d \rightarrow \infty$ limits after and before the Zhang and Rice renormalization is applied.

Rice derivation of the Cu-Cu superexchange constant [see Eq. (4) of Ref. 3] one finds

$$J=\frac{4t_{pd}^4}{\varepsilon^2}\left[\frac{1}{U_d}+\frac{2}{U_p+2\varepsilon}\right]. \quad (1)$$

Thus the magnetic interaction in the Zhang and Rice effective Hamiltonian [see Eq. (18) of Ref. 3] vanishes in this infinite-U limit. For the hopping part of the effective Hamiltonian [see Eqs. (15) and (16) of Ref. 3] we shall only consider near-neighboring hopping (e.g., Zhang and Rice estimate that the next-near-neighbor hybridization is an order of magnitude smaller than the near-neighbor hopping frequency). The motivation for this is simple: The benefit of possibly being able to reduce the two-band model to an effective one-band model is the simplicity of the latter, and the inclusion of higher-order hopping processes diminishes the utility of this approach. Thus, one obtains for the infinite-U limit the effective one-band Hamiltonian:

$$H_{1,\infty}=-t^{(1)}\sum_{\langle ij\rangle,\sigma}(d_{i\sigma}^{\dagger}d_{j\sigma}+\text{H.c.}),\qquad t^{(1)}=\alpha\frac{t_{pd}^2}{\varepsilon}, \quad (2)$$

where $\langle ij\rangle$ denotes neighboring Cu sites, the $d_{i\sigma}$ are projected fermionic operators that prohibit double occupancy, and α is a numerical constant. The ground state of Eq. (2), for the d orbitals forming a square (bipartite) lattice, was determined by Nagaoka[9] in the case of one hole and corresponds to a ferromagnetically polarized Cu-spin state.

We next apply the infinite-U limit directly to the effective Hamiltonian derived from the extended Hubbard model in the strong-correlation limit. The effective Hamiltonian is obtained by assuming that the t_{pd} hybridization energy is a small perturbation on the Hubbard-type correlation energies. In the Hamiltonian we consider, the only hopping processes allowed correspond to virtual excitations with a completely unoccupied Cu orbital, and are shown in Fig. 1(b) of Ref. 7. (Note that the spins of the two carriers do not restrict the occurrence of this hopping process.) The Hamiltonian of this system can be written

$$H_{2,\infty}=t^{(2)}\sum_{\langle lil'\rangle\sigma}{}' [p_{l\sigma}^{\dagger}p_{l'\sigma}(1-n_{i,-\sigma})+p_{l\sigma}^{\dagger}d_{i-\sigma}^{\dagger}d_{i\sigma}p_{l'-\sigma}+\text{H.c.}], \quad (3)$$
$$t^{(2)}\cong\frac{t_{pd}^2}{\varepsilon}.$$

In Eq. (3) i labels the Cu sites, and l the O sites, $\langle lil'\rangle$ indicates an O-Cu-O triplet, the primed sum indicates $l\neq l'$, and $n_{i,\sigma}$ is the number operator for site i, spin σ.

Clearly, $H_{2,\infty}$ is manifestly different from $H_{1,\infty}$. To check the possibility that it nevertheless describes the same low-energy physics, we now examine the ground state of $H_{2,\infty}$. For a state with all of the holes' spins parallel, one may solve exactly for the band structure, and find

$$\varepsilon_+(\mathbf{k})=2t^{(2)}(1+\cos k_x+\cos k_y),\qquad \varepsilon_-(\mathbf{k})=-2t^{(2)}. \quad (4)$$

The minimum energy state for the completely polarized state is $-2t^{(2)}$. Now flip a single spin. This is a two-body problem (the location of the O hole and the location of the flipped spin) that can be solved numerically. The ground state has appreciable amplitude only when the flipped spin is within a few lattice constants of the O hole. Its energy is significantly lower than the polarized state, viz. $-4.46562t^{(2)}$, and corresponds to the point $\mathbf{k}=0$.

We have obtained additional results for more flipped spins using the iterative product method[10] on a 4×4 CuO_2 cluster with periodic boundary conditions. The only inputs that are required in this numerical work are (i) the wave vector of the state, and (ii) the total S^z (to be denoted by S_T^z) of the spin system. For example, if $S_T^z=\frac{17}{2}$, we necessarily find the ferromagnetically polarized $(S=\frac{17}{2})$ state whose energy is given by Eq. (4). Then, we flip one spin and look for the minimum energy state in the $S_T^z=\frac{15}{2}$ spin sector. We find that the minimum energy state also corresponds to $S=\frac{15}{2}$ at $\mathbf{k}=0$, indicative of the instability of the fully polarized ferromagnetic state against a spin flip.

The ground state of these clusters may be determined by taking $S_T^z=\frac{1}{2}$, from which all possible total $S=\frac{1}{2},\ldots,S^{\max}(=\frac{17}{2})$ states could be projected out as the ground state. The minimum energy configuration is found to be a $S=\frac{5}{2}$ state, where the wave vector is on the magnetic Brillouin-zone boundary, viz. $|k_x|+|k_y|=\pi$ [the $(\pi/2,\pi/2)$ and $(\pi,0)$ states are degenerate for our 4×4 lattice; this is purely a finite-size effect]. It has an energy of $-4.53187t^{(2)}$. We have shown all $\mathbf{k}=0$ and $\mathbf{k}=(\pi/2,\pi/2)$ minimum energy states, as a function of S_T^z, in Table I.

One focus of our study is a comparison of the ground states of $H_{1,\infty}$ and $H_{2,\infty}$, which we have now calculated. If they represented the same low-energy physics, then the ground state of $H_{2,\infty}$, like the ground state of $H_{1,\infty}$, should have $S=S^{\max}-1(=\frac{15}{2})$ and $\mathbf{k}=0$. Quite simply, since the O hole forms a singlet with the Cu hole, and the resulting ground state of $H_{1,\infty}$ is the completely polarized ferromagnetic state, the total spin of this state corresponds to $S=S^{\max}-1$. From our 4×4 cluster studies with $H_{2,\infty}$ we have shown that this state is unstable with respect to lower spin sectors. At present the $S=\frac{5}{2}$ ground state is not fully understood. Further, this behav-

TABLE I. $\mathbf{k}=0$ and $(\pi/2,\pi/2)$ minimum-energy states as a function of S_T^z.

S_T^z	$E(\mathbf{k}=0)$	S_{tot}	$E(\mathbf{k}=(\pi/2,\pi/2))$	S_{tot}
$\frac{17}{2}$	−2.0	$\frac{17}{2}$	−2.0	$\frac{17}{2}$
$\frac{15}{2}$	−4.46562	$\frac{15}{2}$	−3.43989	$\frac{15}{2}$
$\frac{13}{2}$	−4.46562	$\frac{15}{2}$	−4.46602	$\frac{13}{2}$
$\frac{11}{2}$	−4.47676	$\frac{11}{2}$	−4.46602	$\frac{13}{2}$
$\frac{9}{2}$	−4.47676	$\frac{11}{2}$	−4.48322	$\frac{9}{2}$
$\frac{7}{2}$	−4.51851	$\frac{7}{2}$	−4.49435	$\frac{7}{2}$
$\frac{5}{2}$	−4.51851	$\frac{7}{2}$	−4.53187	$\frac{5}{2}$
$\frac{3}{2}$	−4.52196	$\frac{3}{2}$	−4.53187	$\frac{5}{2}$
$\frac{1}{2}$	−4.52196	$\frac{3}{2}$	−4.53187	$\frac{5}{2}$

ior is not peculiar to 4×4 clusters. We have also examined the following sequence of $\mathbf{k}=0$ minimum energy states for a 5×5 cluster: $S_T^z=13$, 12, 11, 10. Once again, we find

$$E^{S_T^z=13}(=-2.0)>E^{S_T^z=12}(=-4.48346)=E^{S_T^z=11}>E^{S_T^z=10}(=-4.51603)\,,$$

thus displaying the instability of the $S=S^{\max}-1$, $H_{1,\infty}$ ground state with respect to lower total spin states. Again, the lowering of the total spin is identical to the pattern of the 4×4 cluster. To be specific, for $S_T^z=13$, 12, 11, 10, $S=13$, 12, 12, 10, respectively.

One prominent feature of both the 4×4 and 5×5 clusters is the dramatic decrease in energy of the $S=S^{\max}-1$ state relative to the $S=S^{\max}$ state. Also, further lowerings of the spin are accompanied by much smaller energy splittings. It thus seems that the Zhang-Rice renormalization has done well in isolating the most important energy splitting in the infinite-U problem considered here, although their procedure clearly misses some of the lower-energy magnetic interactions important to the ground-state wave function.

An interesting consequence of the failure of $H_{1,\infty}$ to properly represent the low-energy physics comes from comparing this study to that of Zhang.[6] There, he purports that the renormalization is exact when the only virtual excitations involved are those having doubly occupied Cu orbitals [see Fig. 1(a) of Ref. 7]. The other virtual excitation processes [see Fig. 1(b) of Ref. 7] involving completely unoccupied Cu orbitals (considered here) have been shown to disagree with the predictions of the Zhang and Rice effective one-band renormalization.

The terms that we have omitted from our study, viz. the higher-order hopping processes to neighbors more distant than the first, can be expected to aid the Zhang and Rice renormalization in this infinite correlation limit. To be specific, if one includes the so-called t' terms in $H_{1,\infty}$, the Nagaoka state is no longer necessarily the ground state. However, we have not investigated this issue.

In conclusion, *at least* in the infinite-U limit, our study shows that the Zhang and Rice[3] renormalization which only includes near-neighbor hopping processes does not adequately represent the low-energy physics of a single hole in these planes.

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