Validity of the t-J model

F. C. Zhang*
Theoretische Physik, ETH-Hönggerberg, 8093 Zürich, Switzerland
and University of Cincinnati, Cincinnati, Ohio 45221

T. M. Rice†
Theoretische Physik, ETH-Hönggerberg, 8093 Zurich, Switzerland
and Center for Material Science, Los Alamos National Laboratory, Los Alamos, New Mexico 87545
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Emery and Reiter [Phys. Rev. B **38**, 11938 (1988)] have questioned the validity of a single-band t-J model to describe the low-energy properties of CuO_2 planes. Their criticisms are based on an examination of the exact solution in a ferromagnetic background. In this Comment we present several arguments which lead us to conclude that this ferromagnetic limit, however, is compatible with the t-J model.

I. INTRODUCTION

The form of the effective Hamiltonian that describes the low-energy properties of the CuO_2 planes in the high-T_c superconductors is controversial. The aim must be to find the simplest Hamiltonian, eliminating all terms which are not relevant to the determination of the superconducting fixed point. Such simplified Hamiltonians have in the past played a central role in solid-state physics, e.g., the reduced BCS Hamiltonian or the several Anderson Hamiltonians. Shortly after the original discovery, Anderson[1] proposed an effective Hamiltonian, which we shall call the t-J model, that has the form that applies in large-U limit of a single-band Hubbard model. The proposal remains controversial and the relation of the t-J model to a more general Hamiltonian containing Cu and O bands and intra- and interatomic Coulomb interactions continues to be debated.

Earlier we presented a derivation[2] of the t-J model starting from a two-band Hamiltonian but ignoring the onsite Coulomb interaction on the O atoms, the intersite Cu-O Coulomb interaction and direct O-O hopping terms. Some authors[3,4] have criticized our derivation because of the omissions but others, Mila[5] and Eskes and Sawatzky,[6] obtained similar forms from a more general starting point. Our purpose in this Comment is not to examine this point further but to discuss the objections recently raised by Emery and Reiter.[7] These authors have the same starting Hamiltonian as Ref. 2. They point out that in the limit, where virtual transitions of two holes onto the Cu atoms dominate, the model is exactly soluble for a ferromagnetic (FM) spin configuration. However, they interpret their results in this limit as essentially different to the t-J model. In this Comment we will present a series of arguments which lead us to conclude that the limiting case they consider is compatible with the t-J model and supports rather than refutes the conclusions of Ref. 2.

II. TWO-BAND MODEL IN A FERROMAGNETIC STATE

The starting Hamiltonian for a single CuO_2 layer is

$$H=\sum_{i,\sigma}\varepsilon_d d_{i\sigma}^{\dagger}d_{i\sigma}+\sum_{l,\sigma}\varepsilon_p p_{l\sigma}^{\dagger}p_{l\sigma}+U\sum_i d_{i\uparrow}^{\dagger}d_{i\uparrow}d_{i\downarrow}^{\dagger}d_{i\downarrow}+H', \tag{1}$$

where $d_{i\sigma}^{\dagger}$ creates a $Cu(3d_{x^2-y^2})$ hole, and $p_{l\sigma}^{\dagger}$ creates a $O(2p_x,2p_y)$ hole. U is the on-site Coulomb repulsion at a Cu site. The atomic energy ε_d is set equal to zero, and $\varepsilon_p>0$. The Cu-O hybridization is given by

$$H'=t\sum_{i,\sigma}\sum_{l\in\{i\}}d_{i\sigma}^{\dagger}p_{l\sigma}+\text{H.c.}, \tag{2}$$

in which sum over l runs over the four O sites around Cu site i. In Eq. (2), we assume the O hole to be in the antibonding state, and the phase factor in the hybridization has been absorbed[7] in the operators $p_{l\sigma}^{\dagger}$.

There is an important symmetry in Hamiltonian (1), primarily due to the symmetry of the Cu and O atomic wave functions. To see this clearly, let us define a symmetric combination of four O-hole states around a Cu site

$$P_{i\sigma}=\tfrac{1}{2}\sum_{l\in\{i\}}p_{l\sigma} \tag{3}$$

whose anticommunication relations are given by

$$\{P_{i\sigma},P_{j\sigma'}^{\dagger}\}=\delta_{\sigma\sigma'}(\delta_{ij}+\tfrac{1}{4}\delta_{\langle ij\rangle,0}), \tag{4}$$

where $\delta_{\langle i,j\rangle,0}=1$ if i and j are nearest neighbors, and 0 otherwise. The hybridization term, Eq. (2), can then be written as

$$H'=2t\sum_{i,\sigma}d_{i\sigma}^{\dagger}P_{i\sigma}+\text{H.c.}; \tag{5}$$

therefore, only the symmetric O states, which is one half the number of the total O states, couple to the Cu ions. The other half of the O states are nonbonding; hence they are irrelevant to the low-energy physics. This symmetry should be preserved in approximate treatments of the Hamiltonian (1).

Treating t as a small parameter so that we need only keep the leading fourth-order term (1), with one hole/Cu atom, it reduces to a spin-$\frac{1}{2}$ Heisenberg model

$$H_S=J\sum_{\langle ij\rangle}\mathbf{S}_i\cdot\mathbf{S}_j, \tag{6}$$

with

$$J=4t_0^4\varepsilon_p^{-2}(\varepsilon_p^{-1}+U^{-1}), \tag{7}$$

where $\mathbf{S}_i$ are spin-$\frac{1}{2}$ operators for Cu holes. This corresponds to undoped La_2CuO_4.

Upon doping, an additional hole will sit primarily on the symmetric O state if $U > \varepsilon_p$, rather than on the individual atomic O states. This hole is mobile in the Cu spin background. Up to the second order, the effective Hamiltonian in the subspace with one hole at every Cu site, and an additional O hole is given by

$$H_2 = -4t_1 \sum_{i\sigma\sigma'} d^\dagger_{i\sigma} P_{i\sigma} P^\dagger_{i\sigma'} d_{i\sigma'} - 4t_2 \sum_{i\sigma\sigma'} P^\dagger_{i\sigma} d_{i\sigma} d^\dagger_{i\sigma'} P_{i\sigma'} , \quad (8)$$

with $t_1 = t^2/\varepsilon_p$; and $t_2 = t^2/(U-\varepsilon_p)$. Equation (8) can be obtained by using degenerate perturbation theory, or by a canonical transformation. We would like to point out that after the canonical transformation the operators $d^\dagger_{i\sigma}$ and $P^\dagger_{i\sigma}$ no longer refer to atomic states confined to Cu and O ions but each describes a hybridized mixture of Cu- and O-atomic states. Nonetheless, below we shall refer to them simply as Cu or O states.

The first term arises from intermediate states containing two O holes, and the second from a doubly occupied Cu-hole state. If we use the atomic representation for the O hole, Eq. (8) is identical to the Hamiltonian recently studied by Emery and Reiter.[7]

The total spin **S** commutes with Hamiltonian (1) and can be used to classify the eigenstates of (1). Emery and Reiter[7] have pointed out that certain eigenstates, namely, those with very large values for S, can be exactly solved in the limit $|t_1/t_2| \to 0$. They obtained the eigenstates at a total of $N+1$ holes, which have eigenvalue of $S_z = -(N-1)/2$. Such states are highly excited states since the Heisenberg term (7) favors antiferromagnetic order and therefore a value of $S = \frac{1}{2}$. However, the latter problem is not simple at all. The situation is similar to the case of the one-band Hubbard model in the large-U limit which as Nagaoka[8] emphasized, is exactly soluble for ferromagnetic but not for antiferromagnetic spin configurations. We will return to this point later but for now we follow Emery and Reiter[7] and discuss the ferromagnetic state ignoring the Heisenberg term so that the Hamiltonian reduces to (8).

They have found in the limit $|t_1/t_2| \to 0$ eigenfunctions for (8) of the form

$$|\Phi_k\rangle = \left(P^\dagger_{k\uparrow} - \beta_{\mathbf{k}} \sum_{\mathbf{q}} \beta_{\mathbf{q}}^{-1} P^\dagger_{\mathbf{q}\downarrow} S^\dagger_{\mathbf{k}-\mathbf{q}}\right) |\mathrm{FM}\downarrow\rangle , \quad (9)$$

where

$$P_{\mathbf{k}\uparrow} = N^{-1/2} \beta_{\mathbf{k}} \sum_i P_{i\sigma} \exp(-i\mathbf{k}\cdot\mathbf{R}_i) , \quad (10)$$

$$\beta_{\mathbf{k}} = [1 + 1/2(\cos k_x + \cos k_y)]^{-1/2} , \quad (11)$$

and $S^\dagger_{\mathbf{k}}$ is a Cu-spin-raising operator. $|\mathrm{FM}\downarrow\rangle$ denotes a FM background with all Cu spin terms. The corresponding energy eigenvalues are

$$\lambda_{\mathbf{k}} = -8t_2 - 2t_2(\cos k_x + \cos k_y) . \quad (12)$$

We can rewrite the eigenfunctions (9) in the following form:

$$|\Phi_{\mathbf{k}}\rangle = (2/N)^{1/2} \beta_{\mathbf{k}} \sum_i \psi^\dagger_i d_{i\downarrow} \exp(-i\mathbf{k}\cdot\mathbf{R}_i) |\mathrm{FM}\downarrow\rangle , \quad (13)$$

where

$$\psi^\dagger_i = \frac{1}{\sqrt{2}} (P^\dagger_{i\uparrow} d^\dagger_{i\downarrow} - P^\dagger_{i\downarrow} d^\dagger_{i\uparrow}) , \quad (14)$$

is a spin singlet composed of a Cu hole at site i and a hole on the four neighboring O sites.

In Ref. (2), we constructed spin singlets based on the *orthogonal* symmetric O states with its central Cu hole

$$\tilde{\psi}^\dagger_i = \frac{1}{\sqrt{2}} (\phi^\dagger_{i\uparrow} d^\dagger_{i\downarrow} - \phi^\dagger_{i\downarrow} d^\dagger_{i\uparrow}) , \quad (15)$$

with $\phi_{i\sigma}$ the orthogonal symmetric O state given by

$$\phi_{i\sigma} = N^{-1/2} \sum_k P_{\mathbf{k}\sigma} \exp(i\mathbf{k}\cdot\mathbf{R}_i) . \quad (16)$$

Although the detailed forms of the two singlets ψ_i and $\tilde{\psi}_i$ are not identical, they both describe a local spin singlet with the square symmetry. It turns out to be more convenient to use $\tilde{\psi}_i$ to estimate the effective hopping matrix between a singlet and Cu-hole doublet in the general parameter region where $t_1 \neq 0$. In the special case $t_1 = 0$ the nonorthogonal ψ_i given an exact description, while the orthogonalized $\tilde{\psi}_i$ give a very good approximate description. We illustrate this in Fig. 1 where we plot the overlap between the exact eigenstates (13) and those defined by substituting $\tilde{\psi}^\dagger_i$ for $\psi^\dagger_i$ in (13). The overlap is everywhere large (≥ 0.95 in the lower energy half of the Brillouin zone). Similarly the energy spectrum is slightly different (by a few percent) as discussed in Ref. 2.

Emery and Reiter[7] propose that the correct basis to describe the results is composed of a hole on a single O atom coupled to its two neighboring Cu atoms, i.e., basis states of the form $6^{-1/2}[2|\downarrow\uparrow\downarrow\rangle - |\uparrow\downarrow\downarrow\rangle - |\downarrow\downarrow\uparrow\rangle]$. The lowest

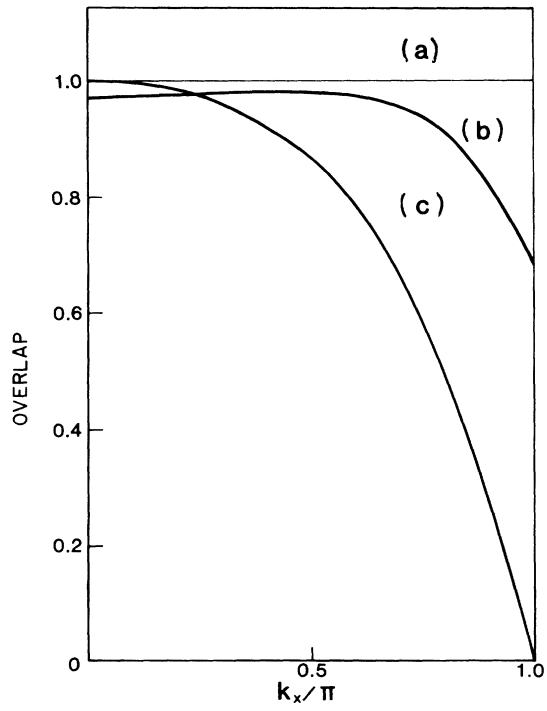

FIG. 1. The overlap between the exact eigenfunction (13) of H_2 and two approximate eigenfunctions, (b) is the form (13) with $\tilde{\psi}_i$ substitute for ψ_i, and (c) is the result when we are restricted to combinations of Emery-Reiter basis functions only. Curve (a) is the exact form (13). In all curves $\mathbf{k} = (k_x, k_x)$, i.e., from the Γ point to the M corner of the Brillouin zone.

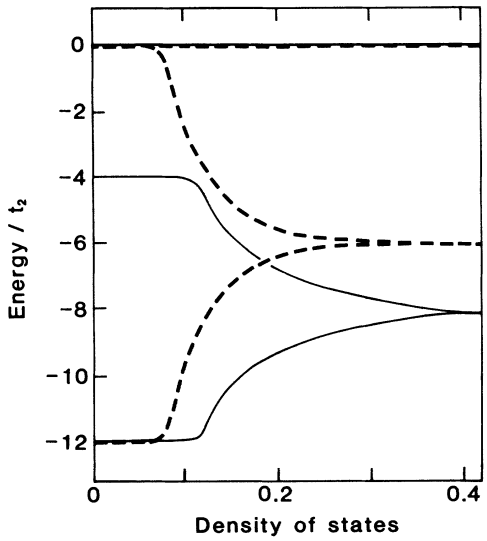

FIG. 2. The density of states as a function of energy of the Hamiltonian H_2. The solid curve is the exact value obtained from (12). Note that there is an energy gap of magnitude $4t_2$ separating the split off band from the remainder of the spectrum at energy 0. The dashed curve is obtained from (17) when the basis states proposed by Emery and Reiter are used.

energy state of the band (12) ($\mathbf{k}=0$ state) is exactly expressed as a superposition of these basis states. Higher energy states are not, however, and as one moves further away in $\mathbf{k}$ space the overlap drops until at $\mathbf{k}=(\pi,\pi)$ it vanishes completely. The overlap between the exact states and the states derived within the restricted Emery-Reiter basis set is also illustrated in Fig. 1. The corresponding eigenvalues are also markedly different to the exact values (12), namely

$$\lambda_{\mathbf{k}}^{\mathrm{ER}} = -6t_2 - 3t_2(\cos k_x + \cos k_y)\,. \tag{17}$$

These values stretch from $-12t_2$ to 0, as compared to the exact values which go from $-12t_2$ to $-4t_2$. In Fig. 2, the density of states deduced from (17) is compared to the exact density of states.

III. DISCUSSION

Emery and Reiter[7] base their claim that the low-energy physics of the t-J model is not the same as the two-band model (1), on the existence of a finite spin density in O orbitals in the exact states (13), whereas the approximate states obtained by using the orthogonalized basis $\{\tilde{\psi}_i\}$ have strictly zero spin density in the O orbitals. However, we would like to make the following points.

(i) The spin density on the O atoms is not a conserved quantity, i.e., not a good quantum number of the Hamiltonians (1) or (8).

(ii) The exact solution for quantum number $S_z=-(N-1)/2$ has a band of N states split off in energy from the remaining N^2 states with energy 0. This feature is correctly reproduced by using the basis of $\{\tilde{\psi}_i\}$ whereas the Emery-Reiter Cu-O-Cu basis does not lead to an energy splitting.

(iii) The Emery-Reiter basis is O centered and contains $2N$ states. The $\{\tilde{\psi}_i\}$ basis is Cu centered containing N states. The form of the dispersion (12) is that of a Cu-centered tight-binding band and it contains one state/Cu atom or N states total.

(iv) The overlap when we restrict to Cu-O-Cu states becomes poor away from the zone center. The Cu-O-Cu basis inherently mixes the symmetric bonding O states with the nonbonding O states away from $\mathbf{k}=0$, although there is no such mixing in the Hamiltonian (1).

We turn now to the extension to the case $t_1\neq 0$. In this case the exact analytic approach fails but the numerical results of Emery and Reiter[7] show that there is not a drastic change. Again the low-energy states are those of a single nearest-neighbor tight-binding band centered on Cu sites with one state/Cu atom for which the description in terms of the orthogonalized singlets, $\tilde{\psi}_i$ is an excellent approximation.

As we remarked previously, the limit $S=\frac{1}{2}$, not ferromagnetism, is the physically interesting one. This limit is not exactly soluble in the one-band model either. The nature of the low-energy quasiparticles for the one-band model in this limit is not clear, with various possibilities, i.e., separate spin and charge excitations, spinons and holons being fermions, bosons or fractional statistics particles actively discussed at present.[9] Therefore, the mapping of the two-band model into a one-band model has nothing to say about the true quasiparticles.

The question is whether the two-band to one-band mapping can be extended to a general spin configuration. Again the limit $|t_1/t_2|\rightarrow 0$ simplifies matters and recently one of us (F.C.Z.) has obtained a proof of this mapping for general spin configurations. Details of this proof will be published separately.[10] In this proof all the low-energy spectrum of a mobile O hole in a Cu spin system, whose Hamiltonian is described by H_2 of Eq. (8), has been shown to be identical to the spectrum of a vacancy in a single-band model. In general, a state in the single-band model with one vacancy can be written in terms of the linear combination of states $\sum_{\sigma_i} d_{i,\sigma_i}\prod_j d^{\dagger}_{j,\sigma_j}|0\rangle$, where $|0\rangle$ represents the vacuum. If

$$\Psi_{\mathrm{SBM}} = \sum_{i,\{\sigma\}} a_{i,\{\sigma\}} \sum_{\sigma_i} d_{i,\sigma_i} \prod_{j=1}^{N} d^{\dagger}_{j,\sigma_j}|0\rangle\,, \tag{18}$$

is an eigenstate of the single-band Hamiltonian

$$H_{\mathrm{SBM}} = -t_2 \sum_{\langle ij\rangle,\sigma}{}' (1-d^{\dagger}_{i,-\sigma}d_{i,-\sigma}) \times d^{\dagger}_{i\sigma}d_{j\sigma}(1-d^{\dagger}_{j,-\sigma}d_{j,-\sigma}) + \mathrm{H.c.}\,, \tag{19}$$

with $a_{i,\{\sigma\}}$ the coefficients of the linear combination, then

$$\Psi = \sum_{i,\{\sigma\}} a_{i,\{\sigma\}} \psi^{\dagger}_i \sum_{\sigma_i} d_{i,\sigma_i} \prod_j d^{\dagger}_{j,\sigma_j}|0\rangle\,, \tag{20}$$

is an eigenstate of H_2, and has the same energy eigenvalue as Ψ_{SBM} in H_{SBM} except for an overall constant. Furthermore, all other eigenstates of the two-band model can be shown to correspond to the higher energies.[10] The singlet state $\psi^{\dagger}_i$ in the two-band model plays exactly the same role as a vacancy in the singlet-band model. Further, the number of states is the same as the singlet-band model $N(2^{N-1})$. A description in terms of the Cu-O-Cu doublet

basis leads to a large number of states, $N(2^N)$. Note the orthogonalized singlet set of basis states formed by the $\tilde{\psi}_i^\dagger$ operators is completely equivalent to the single-band states defined in (18).

Recently Schüttler and Fedro[11] have examined the form of spin correlations in small clusters (4 Cu sites), induced by the introduction of extra holes. They find results that agree with the local singlet or t-J model. Specifically in a $S=\frac{1}{2}$ ground state, the spin on the O sites is small and the deviations from the singlet model are small also.

IV. CONCLUSION

In this Comment we have examined the case of single hole introduced into an O band in a two-band model with one hole/Cu atom and a ferromagnetic spin alignment. There is a band of states which is split off to lower energies. If we use as criteria the number of states in this band, the form of the dispersion, and the form of the eigenfunction in this band we find an equivalence between the two-band and one-band models. This leads us to conclude, in contrast to Emery and Reiter,[7] that this limit supports rather than refutes the use of a t-J effective Hamiltonian for the low-energy properties of CuO_2 planes.

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*Present address: University of Cincinnati, Cincinnati, OH 45221.

†Present address: Theoretische Physik, Eidenössische Technische Hochschule Hönggerberg, 8093 Zürich, Switzerland.

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