PHYSICAL REVIEW B VOLUME 39, NUMBER 10 1 APRIL 1989

# Exact mapping from a two-band model for Cu oxides to the single-band Hubbard model

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(Received 10 November 1988)

The energy spectrum of a mobile hole in a two-band model for Cu oxides, in the limit where the virtual transitions of two holes on the Cu atoms dominate, is shown by using an exact mapping to be identical to that of an effective Hamiltonian of the strongly correlated single-band Hubbard model.

One of the central theoretical issues in high-temperature superconductors is the choice of the appropriate microscopic model. Soon after the discovery of superconducting Cu oxides, Anderson[1] proposed that a two-dimensional (2D) single-band Hubbard model should be the starting point for studying these materials. Since then this model has been studied extensively. Some other physicists, on the other hand, have proposed that O holes introduced in the superconductors generate an essential difference.[2] In a recent article,[3] Rice and I derived an effective Hamiltonian starting from a two-band model including Cu spin degree of freedom and O charge degree of freedom. We showed that a local singlet of square of O atomic holes and the central $Cu^{2+}$ ion is formed due to the Cu-O hybridization. The singlet moves through the lattice in a similar way as a vacancy in the single-band effective Hamiltonian of the strongly interacting Hubbard model. Based on this, we suggested that the essential physics of a two-band model is equivalent to the single-band model, in agreement with Anderson.[1] There have been various works closely related to the issue of the appropriate model Hamiltonian.[4] Recently Emery and Reiter[5] studied one O mobile hole in ferromagnetic spin configuration, and interpreted their result as essentially different from the single-band model. Rice and I[6] have presented a series of arguments which lead us to conclude that the ferromagnetic case they considered fully supports rather than refutes the single-band model.

In this paper I shall examine this issue by studying a special limiting case where the mapping between the two models becomes mathematically exact. I shall show that in the limit $\varepsilon_p$ and $U\rightarrow\infty$, but $U-\varepsilon_p$ finite, with $\varepsilon_p$ the atomic energy difference between O and Cu holes, and $U$ the Cu on-site Coulomb repulsion, the energy spectrum of a two-band model for a mobile hole is identical to that of a single-band model. There is an exact one-to-one correspondence between a local singlet in Cu oxides and a vacancy in the single-band effective Hamiltonian. The method I adopt involves using a set of non-orthogonal basis states.

The two-band model to be studied is

$$H_2=-4t_1\sum_{i,\sigma,\sigma'}d_{i\sigma}^{\dagger}P_{i\sigma}P_{i\sigma'}^{\dagger}d_{i\sigma'}-4t_2\sum_{i,\sigma,\sigma'}P_{i\sigma}^{\dagger}d_{i\sigma}d_{i\sigma'}^{\dagger}P_{i\sigma'}\,, \tag{1}$$

where

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

In the above equations, $d_{i\sigma}^{\dagger}$ and $p_{l\sigma}^{\dagger}$ are the creation operators of Cu and O holes at sites $i$ and $l$ in Cu-O plane, respectively, and summation over $l$ in Eq. (2) runs over four neighboring O sites around a given Cu site $i$. $P_{i\sigma}$ is the symmetric combination of the O hole, and the phase factor discussed in Ref. 3 has been absorbed in operators $p_{l\sigma}$ for simplicity. And $t_1=t^2/\varepsilon_p$, $t_2=t^2/(U-\varepsilon_p)$, with $t$ the neighboring Cu-O hopping amplitude. Equation (1) can be obtained from an extended Hubbard model[2,3] by applying second-order degenerate perturbation theory in $t$. This was implicitly used in Ref. 3, and explicitly used by Emery and Reiter.[5] In Ref. 5 the Hamiltonian was expressed in terms of the atomic O-hole operators $p_{l\sigma}$ instead of the symmetric combinations $P_{i\sigma}$, but these two expressions are identical.

In Eq. (1) Cu spin-spin correlations have not been included. The spin-spin interaction of each pair is of fourth order in $t$. In the case where the hole concentration is exactly 1 hole per unit cell, the Hamiltonian for Cu oxides is described by a spin-$\frac{1}{2}$ Heisenberg model,[1-3] which is the same as the effective Hamiltonian of the single-band Hubbard model in the large-$U$ limit. With one additional hole, the change in the total spin-spin correlation energy is order of $t^4$, much smaller than the contribution from $H_2$. Therefore, we may approximately use $H_2$ to describe the system, and regard Cu spins as providing a spin-configuration background.

In the following I shall consider a limiting case $t_1=0$. Namely, the virtual transitions of two holes on the Cu-atoms dominate. At $t_1=0$, Eq. (1) can be rewritten as

$$H_2=-8t_2\sum_i\psi_i^{\dagger}\psi_i \tag{3}$$

with $\psi_i$ a spin singlet state[7] given by

$$\psi_i=\frac{1}{\sqrt{2}}(P_{i\uparrow}d_{i\downarrow}-P_{i\downarrow}d_{i\uparrow})\,. \tag{4}$$

Note from Eq. (2) that $P_i$ are normalized but not orthogonal. They obey the following anticommutation relations:

$$\{P_{i\sigma},P_{j\sigma'}^{\dagger}\}=\delta_{\sigma\sigma'}(\delta_{ij}+\tfrac{1}{4}\,\delta\langle ij\rangle)\,, \tag{5a}$$

$$\{P_{i\sigma},P_{j\sigma'}\}=\{P_{i\sigma}^{\dagger},P_{j\sigma'}^{\dagger}\}=0\,, \tag{5b}$$

where $\delta\langle ij\rangle=1$ if $i$ and $j$ are nearest neighbors (NN), and vanishes otherwise. Using Eq. (5), we have commutation

 

relations for $\psi_i$,

$$[\psi_i,\psi_j^\dagger]=\delta_{ij}\left(1-\tfrac{1}{2}\sum_\sigma(d_{i\sigma}^\dagger d_{i\sigma}+P_{i\sigma}^\dagger P_{i\sigma})\right)-\tfrac{1}{8}\delta\langle ij\rangle\sum_\sigma d_{j\sigma}^\dagger d_{i\sigma}\,, \tag{6a}$$

$$[\psi_i,\psi_j]=[\psi_i^\dagger,\psi_j^\dagger]=0\,. \tag{6b}$$

Because of these commutation relations, Hamiltonian (3) is not diagonal in the $\psi_i$ representation.

We now consider one O hole in the Cu-spin background (every Cu site singly occupied). The complete Hilbert space of the system can be constructed from $2N2^N$ bases ($N$ is the number of Cu sites), each of which is of the form

$$P_{i\sigma}^\dagger\prod_{j=1}^N d_{j\sigma_j}^\dagger|0\rangle\,, \tag{7}$$

with $|0>$ the vacuum. These states are all independent, but not orthogonal because of Eq. (5). Consider a subspace of the system, whose basis state consists of a singlet given by Eq. (4) at one site (for instance, $i$) and Cu-hole doublet elsewhere:

$$\psi_i^\dagger\sum_\sigma d_{i\sigma}\prod_{j=1}^N d_{j\sigma_j}^\dagger|0\rangle\,. \tag{8}$$

The total number of such singlet-doublet states is $M=N2^{N-1}$, a quarter of the total degrees of freedom in the whole Hilbert space. We denote a state of Eq. (8) by $|A_n\rangle$, with $n=1,2,...,M$. These states are independent of each other, but not orthogonal. To find the relation to the single-band model, let us consider a system of Cu holes in a square lattice of $N$ sites, whose Hamiltonian is given by a single-band Hubbard model in the large $U$ limit,

$$H_t=t_2\sum_{\langle ij\rangle,\sigma}(1-d_{i,-\sigma}^\dagger d_{i,-\sigma})d_{i\sigma}^\dagger d_{j\sigma}\times(1-d_{j,-\sigma}^\dagger d_{j,-\sigma})+\text{H.c.} \tag{9}$$

The Hilbert space of this system with a vacancy at one site and every singly occupied Cu hole elsewhere, can be constructed from $N2^{N-1}$ basis states,

$$\sum_\sigma d_{i\sigma}\prod_{j=1}^N d_{j\sigma_j}^\dagger|0\rangle\,. \tag{10}$$

The states of Eq. (10) are all orthonormal. By comparison with Eq. (8), there is a one-to-one correspondence on the expression of the singlet-doublet state [Eq. (8)] and of the vacancy-doublet state [Eq. (10)]. Therefore, we may denote Eq. (10) by $|B_n\rangle$ in the same sequence as for $|A_n\rangle$, with $n$ running from 1 to $M$.

It then can be shown that (a)

$$(H_2+8t_2)|A_n\rangle=\sum_{m=1}^M\alpha_{nm}|A_m\rangle\,, \tag{11}$$

with

$$\alpha_{nm}=\langle B_n|H_t|B_m\rangle\,; \tag{12}$$

(b) it follows from (a) that $H_2+8t_2$ contains the full spectrum of $H_t$; (c) the rest of the spectrum of $H_2$, besides that in (b), is a degenerate zero-energy level. Thus, the low-energy physics of a mobile hole in the two-band model is identical to that in the single-band model.

We now prove (a) to (c). To justify (a), we evaluate the left-hand side of Eq. (11). Using Eqs. (3) and (6), one obtains

$$(H_2+8t_2)\psi_i^\dagger\sum_\sigma d_{i\sigma}\prod_{j=1}^N d_{j\sigma_j}^\dagger|0\rangle=-t_2\sum_{k\in\text{NN of }i}\psi_k^\dagger\sum_{\sigma,\sigma'}d_{k\sigma'}d_{i\sigma'}^\dagger d_{i\sigma}\prod_{j=1}^N d_{j\sigma_j}^\dagger|0\rangle\,. \tag{13}$$

The resulting state in the right-hand side is also within the singlet-doublet subspace. Therefore, this subspace forms a closed set under $H_2$. From Eq. (13), besides a self-energy $-8t_2$, $H_2$ describes a hopping process of a local singlet to its NN sites. Applying $H_t$ of Eq. (9) on the corresponding state in the single-band model, one has

$$H_t\sum_\sigma d_{i\sigma}\prod_{j=1}^N d_{j\sigma_j}^\dagger|0\rangle=-t_2\sum_{k\in\text{NN of }i}\sum_{\sigma,\sigma'}d_{k\sigma'}d_{i\sigma'}^\dagger d_{i\sigma}\prod_{j=1}^N d_{j\sigma_j}^\dagger|0\rangle\,. \tag{14}$$

By comparison of Eqs. (13) and (14), we find that the one-to-one correspondence of $|A_n\rangle$ and $|B_n\rangle$ remains valid under Hamiltonian operators $H_2+8t_2$ and $H_t$, respectively. Therefore, if $H_t|B_n\rangle=\sum_m\alpha_{nm}|B_m\rangle$, then $(H_2+8t_2)|A_n\rangle=\sum_m\alpha_{nm}|A_m\rangle$. Since $B_m$ are orthonormal, $\alpha_{nm}$ is given by Eq. (12).

We now prove (b). Let $E$ be an eigenvalue of $H_t$, and $\sum_n\beta_n|B_n\rangle$ be its eigenstate

$$H_t\sum_n\beta_n|B_n\rangle=E\sum_n\beta_n|B_n\rangle\,,$$

we then have

$$\sum_n\beta_n\alpha_{nm}=E\beta_m\,. \tag{15}$$

Using Eqs. (11), (12), and (15),

$$(H_2+8t_2)\sum_n\beta_n|A_n\rangle=\sum_{m,n}\alpha_{nm}\beta_n|A_m\rangle=E\sum_n\beta_n|A_n\rangle\,. \tag{16}$$

From Eq. (16), $\sum_n\beta_n|A_n\rangle$ is an eigenstate of $H_2+8t_2$, corresponding to energy $E$. (b) is justified. Note that the orthogonality is not required to prove (b) from (a).

To show (c), we act $H_2$ on an arbitrary state Eq. (7), in the complete Hilbert space of the two-band model, and find that

$$H_2P_{i\sigma}^\dagger\prod_{j=1}^N d_{j\sigma_j}^\dagger|0\rangle=4\sqrt{2}\sigma t_2\left(\psi_i^\dagger d_{i,-\sigma}+\tfrac{1}{4}\sum_{k\in\text{NN of }i}\psi_k^\dagger d_{k,-\sigma}\right)\prod_{j=1}^N d_{j\sigma_j}^\dagger|0\rangle\,. \tag{17}$$

The state in the right-hand side of Eq. (17) is within the singlet-doublet subspace. It follows that if a state $|\phi\rangle$ is orthogonal to the singlet-doublet subspace, then $\langle\phi|H_2|\text{ any state }\rangle=0$, or $H_2|\phi\rangle=0$. There are $3N2^{N-1}$ states orthogonal to the singlet-doublet subspace in the complete Hilbert space of the two-band model, they are all degenerate with energy eigenvalue zero, higher than the energy levels in the singlet-doublet subspace.

The derivation given above leads to the conclusion that the relevant spectrum of a mobile hole in the two-band model of Eq. (1) in the limit $t_1 \rightarrow 0$ is identical to that of the single-band model.

As an example, we discuss the solution of the model in the ferromagnetic (FM) spin configuration. The eigenenergies and eigenstates of $H_t$ of the single-band model in the FM case with all Cu spin down are trivially given by

$$E_S(\mathbf{k}) = -2t_2[\cos(k_x)+\cos(k_y)] , \tag{18a}$$

$$\Phi_S(\mathbf{k}) = N^{-1/2}\sum_i \exp(i\mathbf{k}\cdot\mathbf{R}_i) d_{i\downarrow} \prod_{j=1}^{N} d_{j\downarrow}^{\dagger} |0\rangle . \tag{18b}$$

By using the mapping discussed above, the eigenenergies and the eigenstates of $H_2$ of the two-band model in the Cu spin FM configuration, with total-spin $z$ component $S_Z = -\frac{1}{2}(N-1)$, are given by

$$E(\mathbf{k}) = -8t_2 - 2t_2[\cos(k_x)+\cos(k_y)] , \tag{19a}$$

$$\Phi(\mathbf{k}) = N^{-1/2}\sum_i \exp(i\mathbf{k}\cdot\mathbf{R}_i) \psi_i^{\dagger} d_{i\downarrow} \prod_{j=1}^{N} d_{j\downarrow}^{\dagger} |0\rangle . \tag{19b}$$

The results for the two-band model are the same as the results obtained by Emery and Reiter,[5] who have studied the same Hamiltonian in FM configuration. They argued, however, based on these results, that the physics of the two-band model is different from the single-band model. Since the solution of Eqs. (19a) and (19b) can be obtained from an exact mapping between the two models, these results in fact fully support the single-band picture.

In summary, I have shown rigorously that the low-energy physics of the two-band model in a limiting case is identical to that of the single-band model. The Hamiltonians for the two-band model and for the single-band Hubbard model are related by a unitary transformation. This limiting case provides an example in which the theoretical proposal by Rice and me[3] on the effective Hamiltonian for superconducting Cu oxides becomes mathematically exact. At $t_1 \neq 0$, the mapping between the two models is approximate from the mathematics point of view. In a separate paper[6] Rice and I have argued that the essential physics of the two models in that general case should still be the same.

I wish to thank T. M. Rice for many useful discussions.

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[7] If we define an operator $\mathbf{S}(i) = \mathbf{S}_{\mathrm{Cu}}(i) + \mathbf{S}_{\mathrm{O}}(i)$, with $\mathbf{S}_{\mathrm{Cu}}(i)$ the Cu-spin $\frac{1}{2}$ operator at site $i$, and $S_{\mathrm{O}}^{z}(i) = \frac{1}{2}(P_{i\uparrow}^{\dagger}P_{i\uparrow} - P_{i\downarrow}^{\dagger}P_{i\downarrow})$, $S_{\mathrm{O}}^{+}(i) = P_{i\uparrow}^{\dagger}P_{i\downarrow}$, $S_{\mathrm{O}}^{-}(i) = P_{i\downarrow}^{\dagger}P_{i\downarrow}$, then $S^2(i)\psi_i^{\dagger}|0\rangle = 0$, implying $\psi_i^{\dagger}$ to be a local spin singlet. Note that $S^2(i)\psi_j^{\dagger}|0\rangle \neq 0$ for NN of $i$ and $j$, because of Eq. (5).