Criterion for the validity of the t-J model based upon a two-band model for copper oxides

J. L. Shen* and C. S. Ting
Department of Physics and Texas Center for Superconductivity, University of Houston, Houston, Texas 77204
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The second-order effective Hamiltonian in the representation of a set of orthogonal operators is derived from a two-band model for Cu oxides. The contribution from the local Cu^{2+} and surrounding O^- spin triplet state to various hopping processes has been included. From the fourth-order perturbation we study doping effects on the background spin-spin interaction and obtain the expression for the ferromagnetic superexchange interaction between two neighboring Cu^{2+} spins with an O^- hole in the middle. The condition for the equivalence between the t-J model and the two-band model for Cu oxides is discussed. In terms of nonorthogonal operators for a single O^- hole, the condition for the exact mapping of a two-band model to a single-band model has also been derived.

A critical problem, which may be relevant to the understanding of the superconductivity mechanism in high-T_c oxide materials, is related to whether the equivalence between the t-J model[1] and two-band Hubbard model[2] can be established. The t-J model has been used to describe the motion of the holes in the $3d$ orbital of the Cu ions. In the undoped case, each of the Cu ions is in the $3d^9$ state that effectively carries a spin $s=\frac{1}{2}$. In the presence of hole doping, a hole goes to one of the Cu sites. In the two-band model the Cu ions always stay in the $3d^9$ states and the doped hole will go to the $2p$ orbital of an oxygen site. The doped hole with $s=\frac{1}{2}$ on an O site may form a singlet or a triplet state with the spin carried by one of its neighboring Cu ($3d^9$) ions. If the effect due to the higher-energy triplet spin state is completely neglected, Zhang and Rice,[3] by examining only the hopping-energy term of the two-band model and under the condition $t_1=t_2$, showed that these two models are approximately equivalent. Here $t_1=t_0^2/\Delta$ and $t_2=t_0^2/(U_d-\Delta)$ with t_0 as the hopping matrix between neighboring $2p$ (O site) and $3d$ (Cu site) orbitals, U_d as the Coulomb repulsive interaction between electrons on Cu site, and $\Delta=\varepsilon_p-\varepsilon_d(<U_d)$ as the energy difference between $2p$ (O) and $3d$ (Cu) levels.

In this paper the relationship between the t-J model and the two-band model will be reexamined by including the contribution of the triplet spin state and for general values of t_1 and t_2. Both the hopping term and the doping effect on the background spin-spin interaction will be investigated. In the limit of small doping we show that the condition for the equivalence between these two models becomes optimum when $t_1\neq 0$ and $t_2=0$. In terms of nonorthogonal operators for a single O^- hole, we show that the exact mapping of the two-band model to a single-band model can also be achieved at $t_1\neq 0$ and $t_2=0$.

Let us start from the two-band Hubbard model with both the on site (oxygen) and intersite (oxygen-copper) Coulomb interactions being set to zero; we study the effective Hamiltonian derived from the small t_0 limit. Up to the second-order the perturbation one obtains[2-5]

$$H_{\rm eff}^{(2)}=\varepsilon_d\sum_{i,\sigma}n_{d,i\sigma}+\varepsilon_p\sum_{l,\sigma}n_{p,l\sigma}-\sum_{(il)\sigma}\frac{v_{il}^2}{\Delta}n_{d,i\sigma}+\sum_{(il)\sigma}\left[\frac{1}{\Delta}+\frac{1}{U_d-\Delta}\right]v_{il}^2(d_{i\sigma}^\dagger d_{i-\sigma}p_{l-\sigma}^\dagger p_{l\sigma}-d_{i\sigma}^\dagger d_{i\sigma}p_{l-\sigma}^\dagger p_{l-\sigma})$$
$$+\sum_{(il)(il'),l\neq l'}\left[\left[\frac{1}{\Delta}+\frac{1}{U_d-\Delta}\right]v_{il}v_{il'}d_{i\sigma}^\dagger d_{i-\sigma}p_{l-\sigma}^\dagger p_{l'\sigma}+\left[\frac{1}{\Delta}n_{d,i\sigma}-\frac{1}{U_d-\Delta}n_{d,i-\sigma}\right]v_{il}v_{il'}p_{l\sigma}^\dagger p_{l'\sigma}\right]. \quad (1)$$

Here $n_{d,i\sigma}=d_{i\sigma}^\dagger d_{i\sigma}$ and $n_{p,l\sigma}=p_{l\sigma}^\dagger p_{l\sigma}$. $d_{i\sigma}^\dagger$ ($p_{l\sigma}^\dagger$) is the operator creating a hole with spin σ on the ith Cu site (lth O site). ε_d and ε_p denote the energy levels occupied by a hole, respectively, on the Cu site and on the O site. From Ref. 3 the phases of the $2p$ and $3d$ wave functions are taken into account according to

$$v_{il}=(-1)^{M_{i,l}}t_0 . \quad (2)$$

Here i represents the site of a Cu atom and l is the site of its nearest-neighboring O atoms. $M_{il}=2$ if $l=i-\hat{\mathbf{x}}/2$ or $i-\hat{\mathbf{y}}/2$ and $M_{il}=1$ if $l=i+\hat{\mathbf{x}}/2$ or $i+\hat{\mathbf{y}}/2$. $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ denote, respectively, the unit vectors along the x and y directions. In terms of the operator, which combines the four oxygen-hole states around a Cu ion,

$$P_{i\sigma}=\tfrac{1}{2}\sum_{l\in i}(-1)^{M_{il}}p_{l\sigma} . \quad (3)$$

The Hamiltonian in Eq. (1) becomes

$$H_{\rm eff}^{(2)}=\left[\varepsilon_d-\frac{4t_0^2}{\Delta}\right]\sum_{i\sigma}n_{d,i\sigma}+\left[\varepsilon_p-\frac{4t_0^2}{\Delta}\right]\sum_{l\sigma}n_{p,l\sigma}$$
$$+4\left[\frac{t_0^2}{\Delta}+\frac{t_0^2}{U_d-\Delta}\right]\sum_{i\sigma}(d_{i\sigma}^{\dagger}d_{i-\sigma}P_{i-\sigma}^{\dagger}P_{i\sigma}-d_{i\sigma}^{\dagger}d_{i\sigma}P_{i-\sigma}^{\dagger}P_{i-\sigma})+4\frac{t_0^2}{\Delta}\sum_{i\sigma}P_{i\sigma}^{\dagger}P_{i\sigma}\ . \tag{4}$$

From Eq. (4) it is interesting to note that these $P_{i\sigma}$ are normalized but not orthogonalized and they obey the following anticommutation relations:[3]

$$\{P_{i\sigma},P_{j\sigma}^{\dagger}\}=\delta_{\sigma\sigma'}(\delta_{ij}-\delta_{\langle ij\rangle}/4)\ , \tag{5}$$

$$\{P_{i\sigma},P_{j\sigma'}\}=\{P_{i\sigma}^{\dagger},P_{j\sigma'}^{\dagger}\}=0\ , \tag{6}$$

where $\delta_{\langle ij\rangle}=1$ if i and j are nearest neighbors and vanishes otherwise. Before we go any further, let us use the following Wannier functions for the Cu site at $\mathbf{R}_i$ with N_s as the number of Cu sites:

$$\phi_{i\sigma}=N_s^{-1/2}\sum_{\mathbf{k}}P_{\mathbf{k}\sigma}e^{i\mathbf{k}\cdot\mathbf{R}_i}\ , \tag{7}$$

$$P_{\mathbf{k}\sigma}=N_s^{-1/2}\beta_k\sum_{i}P_{i\sigma}e^{-i\mathbf{k}\cdot\mathbf{R}_i}\ , \tag{8}$$

where $\beta_k=[1-(\cos k_x+\cos k_y)/2]^{-1/2}$ is a normalization factor. The operator $\phi_{i\sigma}$ is complete and orthogonalized in the oxygen-hole space. Using Eqs. (7) and (8), we have

$$P_{i\sigma}=N_s^{-1}\sum_{j,k}\beta_k^{-1}\phi_{j\sigma}e^{-i\mathbf{k}\cdot(\mathbf{R}_j-\mathbf{R}_i)}\ . \tag{9}$$

For convenience we shall choose the $3d$ level $\varepsilon_d=4t_0^2/\Delta$ and the nearest-neighboring Cu-Cu distance equal to 1. Substituting $P_{i\sigma}$ defined in Eq. (9) into the Hamiltonian in Eq. (4) and considering only terms up to the nearest-neighboring hopping process in the Wannier representation, $H_{\rm eff}^{(2)}$ can be shown to take the following form:

$$H_{\rm eff}^{(2)}=(\varepsilon_p-4t_1)\sum_{l\sigma}p_{l\sigma}^{\dagger}p_{l\sigma}+4t_1\sum_{i,\sigma}\phi_{i\sigma}^{\dagger}\phi_{i\sigma}+4(t_1+t_2)\lambda^2\sum_{i\sigma}(d_{i\sigma}^{\dagger}d_{i-\sigma}\phi_{i-\sigma}^{\dagger}\phi_{i\sigma}-d_{i\sigma}^{\dagger}d_{i\sigma}\phi_{i-\sigma}^{\dagger}\phi_{i-\sigma})$$
$$+4(t_1+t_2)\lambda_1^2\sum_{i,j,\sigma}(d_{i\sigma}^{\dagger}d_{i-\sigma}\phi_{j-\sigma}^{\dagger}\phi_{j\sigma}-d_{i\sigma}^{\dagger}d_{i\sigma}\phi_{j-\sigma}^{\dagger}\phi_{j-\sigma})-t_1\sum_{i,j,\sigma}\phi_{j\sigma}^{\dagger}\phi_{i\sigma}$$
$$+4(t_1+t_2)\lambda\lambda_1\sum_{i,j,\sigma}(d_{i\sigma}^{\dagger}d_{i-\sigma}\phi_{j-\sigma}^{\dagger}\phi_{i\sigma}-d_{i\sigma}^{\dagger}d_{i\sigma}\phi_{j-\sigma}^{\dagger}\phi_{i-\sigma})$$
$$+4(t_1+t_2)\lambda\lambda_1\sum_{i,j,\sigma}(d_{i\sigma}^{\dagger}d_{i-\sigma}\phi_{i-\sigma}^{\dagger}\phi_{j\sigma}-d_{i\sigma}^{\dagger}d_{i\sigma}\phi_{i-\sigma}^{\dagger}\phi_{j-\sigma})\ . \tag{10}$$

Here t_1 and t_2 have been defined at the beginning of this paper. The first four terms in Eq. (10) are the self-energy terms which we call $H_0^{(2)}$ and the remaining terms are the hopping terms which will be denoted by $H_1^{(2)}$. The parameters λ and λ_1 are defined as

$$\lambda=N_s^{-1}\sum_k\beta_k^{-1}=\frac{1}{(2\pi)^2}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi}\beta_k^{-1}dk_xdk_y\simeq 0.96\ ,$$
$$\lambda_1=\tfrac{1}{4}N_s^{-1}\sum_k\beta_k^{-1}e^{i\mathbf{k}\cdot(\mathbf{R}_i-\mathbf{R}_j)}=\frac{1}{(2\pi)^2}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi}dk_xdk_y\beta_k^{-1}(\cos k_x+\cos k_y)\simeq -0.14\ , \tag{11}$$

with $\mathbf{R}_i$ and $\mathbf{R}_j$ as the nearest neighbors. The spin of doped hole on the oxygen sites around a Cu ion at site i may form a local singlet or triplet state with the spin ($3d^9$) on this Cu ion. The singlet state ϕ_{i-} and the triplet states ϕ_{i+} and $\phi_{i\sigma\sigma}$ are constructed as follows:

$$\psi_{i\pm}=\frac{d_{i\uparrow}\phi_{i\downarrow}\pm d_{i\downarrow}\phi_{i\uparrow}}{\sqrt{2}}\ ,$$
$$\psi_{i\sigma\sigma}=d_{i\sigma}\phi_{i\sigma}\ . \tag{12}$$

In terms of these local singlet and triplet states and using the identity $d_{i\uparrow}^{\dagger}d_{i\uparrow}+d_{i\downarrow}^{\dagger}d_{i\downarrow}=1$, which ensures the Cu ion always being singly occupied, $H_{\rm eff}^{(2)}=H_0^{(2)}+H_1^{(2)}$ in Eq. (10) can be separated into the self-energy part,

$$H_0^{(2)}=(\varepsilon_p-4t_1)\sum_{l\sigma}p_{l\sigma}^{\dagger}p_{l\sigma}-[8(t_1+t_2)\lambda^2-4t_1]\sum_i\psi_{i-}^{\dagger}\psi_{i-}+4t_1\sum_i\psi_{i+}^{\dagger}\psi_{i+}+4t_1\sum_{i\sigma}\psi_{i\sigma\sigma}^{\dagger}\psi_{i\sigma\sigma}\ , \tag{13}$$

and the part for hopping processes,

$$H_1^{(2)}=t_1\sum_{(ij)\sigma}(\psi_{j\sigma\sigma}^{\dagger}d_{i\sigma}^{\dagger}d_{j\sigma}\psi_{i\sigma\sigma}+\frac{1}{\sqrt{2}}\psi_{j\sigma\sigma}^{\dagger}d_{i-\sigma}^{\dagger}d_{j\sigma}\psi_{i+}+$$
$$+\frac{1}{\sqrt{2}}\psi_{i\sigma\sigma}^{\dagger}d_{j-\sigma}^{\dagger}d_{i\sigma}\psi_{j+}+\tfrac{1}{2}\psi_{j+}^{\dagger}d_{i\sigma}^{\dagger}d_{j\sigma}\psi_{i+})-(\tfrac{1}{2}t_1+t_2)\sum_{(ij)\sigma}\psi_{j-}^{\dagger}d_{i\sigma}^{\dagger}d_{j\sigma}\psi_{i-}$$
$$+\frac{1}{\sqrt{2}}t_2\sum_{(ij)\sigma}(\sigma\psi_{j-}^{\dagger}d_{i\sigma}^{\dagger}d_{j-\sigma}\psi_{i\sigma\sigma}+\sigma\psi_{j\sigma\sigma}^{\dagger}d_{i-\sigma}^{\dagger}d_{j\sigma}\psi_{i-})+\frac{t_2}{2}\sum_{(ij)\sigma}(\sigma\psi_{j+}^{\dagger}d_{i\sigma}^{\dagger}d_{j\sigma}\psi_{i-}+\sigma\psi_{j-}^{\dagger}d_{i\sigma}^{\dagger}d_{j\sigma}\psi_{i+})+\text{H.c.} \quad (14)$$

In deriving $H_0^{(2)}$ and $H_1^{(2)}$ we have neglected the contribution from $\lambda_1^2(\simeq 0.02)$ and set $8\lambda_1\lambda\simeq -1$. From $H_0^{(2)}$ it is straightforward to show that the energy separation between the triplet and singlet states is

$$\Delta E=E_+-E_-=8(t_1+t_2)\lambda^2\simeq 8(t_1+t_2)\ .$$

This result is very close to that obtained in Ref. 3. In Eq. (14), the first and second terms, respectively, correspond to hoppings from triplet to triplet states and from singlet to singlet states. The last two terms represent the hybridization between the singlet and triplet states. In order to ensure the equivalence between the t-J model and the two-band model in the antiferromagnetic background, the contribution of the hybridization terms to the lowest-energy state needs to be small. For the purpose of estimating the effect of the hybridization terms, we consider the problem of two nearest-neighboring sites (1 and 2) according to the Hamiltonian H_{12} derived from Eqs. (13) and (14) by neglecting the first term in Eq. (13) and the contribution of the hopping terms from one triplet to other triplet states in Eq. (14). This approximation simplifies the mathematics but may underestimate the contribution of the triplet states to the lowest-energy state. The Hamiltonian H_{12} can be diagonalized by the basis operators of two independent subspaces. One of them contains six operators: $d_{1\uparrow}^{\dagger}\psi_{1-}$, $d_{2\uparrow}^{\dagger}\psi_{2-}$, $d_{1\uparrow}^{\dagger}\psi_{1+}$, $d_{2\uparrow}^{\dagger}\psi_{2+}$, $d_{1\downarrow}^{\dagger}\psi_{1\downarrow\downarrow}$, and $d_{2\downarrow}^{\dagger}\psi_{2\downarrow\downarrow}$. The basis operators for the other subspace are simply obtained by reversing all spins. The diagonalized H_{12} takes the following form:

$$H_{12}=\sum_{i=1}^{6}E_i(\phi_i^{\dagger}\phi_i+\phi_i'^{\dagger}\phi_i')\ , \quad (15)$$

where E_i is the eigenenergy, ϕ_i is the annihilation operator for a quasiparticle in state i, and $\phi_i'=\phi_i$ (with all spins reversed). The lowest-energy state is represented by the eigenenergy E_1 and the operator ϕ_1:

$$E_1=-\tfrac{1}{2}\{(9t_2+t_1/2)-[(9t_2+t_1)^2+4(18t_1^2+36t_1t_2+3t_2^2/4)]^{1/2}\}\ , \quad (16)$$
$$\phi_1=c[d_{1\uparrow}^{\dagger}\psi_{1-}+d_{2\uparrow}^{\dagger}\psi_{2-}+c_1(d_{1\uparrow}^{\dagger}\psi_{1+}+d_{2\uparrow}^{\dagger}\psi_{2+})-c_2(d_{1\downarrow}^{\dagger}\psi_{1\downarrow\downarrow}+d_{1\downarrow}^{\dagger}\psi_{1\downarrow\downarrow})]\ .$$

In Eq. (16), c is a normalized constant, $c_1=t_2/2(4t_1-E_1)$, and $c_2=t_2/\sqrt{2}(4t_1-E_1)$. The first two terms represent the contribution from the singlet states and the remaining terms come from the triplet states. For $t_1=0$ and $t_2\neq 0$, the coefficients in front of the triplet states, $c_1=0.055$ and $c_2=0.078$. In $\phi_1^{\dagger}\phi_1$, while two terms correspond to the transition process between singlet 1 and singlet 2 states, there are eight terms representing various hopping processes from 1 singlet to triplet 2 and vice versa. Therefore, the weight due to the contribution of the triplet states in $\phi_1^{\dagger}\phi_1$ should be more than the coefficients c_1 and c_2 indicated. For example, in a antiferromagnetic background, it is straightforward to show that the weight of the triplet states in $\phi_1^{\dagger}\phi_1$ is $2c_1\simeq 11\%$. For $t_1=t_2$, which is the limit studied in Ref. 3, $c_1\simeq 0.025$ and $c_2\simeq 0.039$. If these coefficients can be regarded as small and are neglected,[3] then the one band t-J model and the two-band model are approximately equivalent to each other as long as the background spin-spin interaction does not include the quantum operators for oxygen coordinates. Although the method of deriving Eq. (14) involves approximations, we expect that the terms being neglected in Eq. (14) should be very small. Therefore, according to Eq. (14), the equivalence between these two models reaches optimum in the limit $t_1\neq 0$ and $t_2=0$. Under this condition the coupling between the singlet and triplet states vanishes or becomes very small, the doped hole always stays in the lower-energy singlet state, and the operators associated with the oxygen coordinates can be eliminated from Eq. (14).

We have also employed the fourth-order perturbation to derive correction to the background spin-spin interaction from the two-band Hubbard model. The procedure is tedious but the result is simple:

$$H_{\text{eff}}^{(4)}=\sum_{\langle ilj\rangle}\left[\frac{4t_0^4}{\Delta^2U_d}+\frac{4t_0^4}{2\Delta^3}\right](1-n_{p,l\uparrow}-n_{p,l\downarrow})\mathbf{s}_i\cdot\mathbf{s}_j$$
$$-\sum_{\langle ilj\rangle}\frac{4t_0^4}{U_d\Delta(U_d-\Delta)}(n_{p,l\uparrow}+n_{p,l\downarrow})\mathbf{s}_i\cdot\mathbf{s}_j\ . \quad (17)$$

The first term on the right-hand side of the preceding equation describes the neighboring copper sites (i,j) antiferromagnetic superexchange interaction via the middle (O^{2-}) state l. The second term represents the nearest-neighboring copper site (i,j) ferromagnetic superexchange interaction if an O^- hole exists at the middle site l. To our knowledge this is the first time that the expression for the ferromagnetic superexchange interaction between two copper spins with O^- site in the middle has been explicitly derived.

In the small doping limit, if the number operator in Eq. (17) is treated as a doping parameter $n_{p,l\uparrow}+n_{p,l\downarrow}\simeq\delta\ll 1$, and in view of small values for c_1 and c_2 in Eq. (16), it may be a good approximation to replace the two-band model by the t-J model. The problem of whether the operator $n_{p,l\uparrow}+n_{p,l\downarrow}$ can indeed be treated as a C number and whether the singlet-to-triplet hybridization term can really be neglected without losing additional physics requires further investigation. Our result for the hopping Hamiltonian $H_1^{(2)}$ in Eq. (14) shows that the transition between the triplet and singlet states vanishes or becomes very small for $t_1\neq 0$ and $t_2=0$. Under this limit $H_1^{(2)}$ describes only the hopping process from lower-energy singlet-i-to-singlet-j states; the equivalence between the t-J model and the two-band model becomes almost exact when the O-hole occupation number in Eq. (17) is treated as a parameter. For other values of t_1 and t_2, the singlet-to-triplet hybridization terms always exist in $H_1^{(2)}$. For $t_1=0$ and $t_2\neq 0$, these hybridization terms contribute the most to $H_1^{(2)}$. In the following we shall examine this conclusion from a different point of view by using nonorthogonal operators for the O^- hole. According to Ref. 6, the second-order effective Hamiltonian derived from a two-band Hubbard model in the representation of a set of nonorthogonal operators is easily obtained as

$$H_{\rm eff}^{(2)}=-4(2t_2+t_1)\sum_i f_{i-}^\dagger f_{i-}+4t_1\sum_i f_{i+}^\dagger f_{i+}+4t_1\sum_{i\sigma} f_{i\sigma\sigma}^\dagger f_{i\sigma\sigma} \tag{18}$$

with a spin singlet and triplet states defined by

$$f_{i\pm}=\frac{d_{i\uparrow}P_{i\downarrow}\pm d_{i\downarrow}P_{i\uparrow}}{\sqrt{2}},\quad f_{i\sigma\sigma}=d_{i\sigma}P_{i\sigma}\ .$$

Using Eqs. (5) and (6), the following commutation relations are obtained:

$$\begin{aligned}[f_{i\pm},f_{j\pm}^\dagger]&=\delta_{ij}\left[1-\tfrac{1}{2}\sum_\sigma(d_{i\sigma}^\dagger d_{i\sigma}+P_{i\sigma}^\dagger P_{i\sigma})\right]+\tfrac{1}{8}\delta_{\langle ij\rangle}\sum_\sigma d_{j\sigma}^\dagger d_{i\sigma}\ ,\\ [f_{i-},f_{j+}^\dagger]&=\tfrac{1}{2}\delta_{ij}\sum_\sigma\sigma(d_{i\sigma}^\dagger d_{i\sigma}-P_{i\sigma}^\dagger P_{i\sigma})-\tfrac{1}{8}\delta_{\langle ij\rangle}\sum_\sigma\sigma d_{j\sigma}^\dagger d_{i\sigma}\ ,\\ [f_{i-},f_{j-}]&=[f_{i-},f_{j+}]=0\ .\end{aligned} \tag{19}$$

When a hole is added to a ferromagnetic background formed by the copper spins, the basis states can be described by[6]

$$|A_{i\mp}\rangle=f_{i\mp}^\dagger d_{i\downarrow}\prod_{j=1}^N d_{j\downarrow}^\dagger|0\rangle\ . \tag{20}$$

It is straightforward to show that the transfer integral between neighboring triplet and singlet states for $t_1=0$ and $t_2\neq 0$ does not vanish:

$$t_{+-}=\langle A_{i+}|H_{\rm eff}^{(2)}|A_{j-}\rangle=\langle A_{i-}|H_{\rm eff}^{(2)}|A_{j+}\rangle=t_2\ . \tag{21}$$

In this limit the result in Eq. (21) implies that $H_{\rm eff}^{(2)}$ contains both singlet-to-triplet and triplet-to-singlet hopping terms and thus cannot be mapped exactly to a single-band model. However, when $t_1\neq 0$ and $t_2=0$, it is readily seen that $t_{+-}=0$, and $H_{\rm eff}^{(2)}$ does not consists of any hopping term between the singlet and triplet states. Therefore, only in the limit of $t_1\neq 0$ and $t_2=0$ (or $U_d\to\infty$) the mapping between these two models can be exact. This result corresponds to the same fixed point for both models mentioned previously by Anderson.[7] Although the preceding conclusion is consistent with our result shown in Eq. (14), it is contrary to the result of Zhang[6] in which the exact mapping occurs at $t_1=0$ and $t_2\neq 0$. The cause for this discrepancy is due to the commutation relation $[f_{i-},f_{j+}^\dagger]$ listed in Eq. (19) being missing in Ref. 6. Finally, we wish to point out that the exact mapping of the two-band to single-band model should also hold at $t_1\neq 0$ and $t_2=0$ even in an antiferromagnetic background. This is because t_{+-} is expected to vanish according to Eq. (18) in this limit.

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*Permanent address: Institute of Physics, Chinese Academy of Sciences, Beijing, China.

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