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Low-energy limit of the three-band model for electrons in a CuO_2 plane

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The three-band model with the O–O direct hopping near to unit filling is considered. We present the general procedure of reduction of this model to the low-energy limit. At unit filling the three-band model in the charge-transfer limit is reduced to the Heisenberg model and we calculate the superexchange constant. For the case of small electron doping the three-band model is reduced to the t–J model and we calculate electron hopping parameters at the nearest and next neighbors. We derive the structure of corrections to the t–J model and calculate their magnitudes. The values of the hopping parameters for electron- and hole-doping differ by approximately 40%.

1. Introduction

Since the discovery of electron-doped superconductors [1] there has been growing interest in the structure and properties of these systems [2–4]. The electron- and hole-doped high-temperature superconductors (such as $Nd_{2-x}Ce_xCuO_4$ and $La_{2-x}Sr_xCuO_4$) both have CuO_2 planes with the same structure constant. In spite of the similar structure, the experiments show strong asymmetry in the properties of these compounds. Thus, the critical temperature for $Nd_{2-x}Ce_xCuO_4$ is only 22 K, in contrast with $T_c = 40$ K for $La_{2-x}Sr_xCuO_4$ [5]. Also, the doping concentrations which destroy the AF order for electron- and hole-doped systems are $\sim 15\%$ and 2–3%, respectively [2,3]. To study such asymmetrical phenomena might help to illuminate the nature of superconductivity in these compounds.

Since the structure of the CuO_2 plane is the same for these compounds, one can expect that the well-known three-band hamiltonian [6] should be suitable for both of them.

In this paper we investigate one electron over unit filling in a CuO_2 plane. We start from the Emery hamiltonian [6] with the O–O direct hopping. On the basis of our general approach to the low-energy reduction [7], we obtain the effective single-band hamiltonian. The equivalence of this single-band hamiltonian and the t–J model is discussed and the second-order corrections to the t–t'–J model are derived. The effective parameters of the t–t'–J model for the electron are calculated in the realistic region of Emery model parameters. Effective hopping is less than in the case of hole-doping. A similar conclusion was obtained in the work by Zhang and Benneman [8], but they used the perturbation theory over the parameters t_{pd}/U_d, $t_{pd}/(\epsilon_p - \epsilon_d)$ which does not work, as was argued in our previous works [7,9].

In section 2 we represent the three-band model in more suitable terms for reduction to the single-band model. We use a three-step procedure. At the first step we introduce the symmetrical and antisymmetrical oxygen operators. At the second step we separate out the one-site hamiltonian and get its solution. At the third step we represent the primary hamiltonian in terms of the Hubbard operators which reflect the structure of the solution of the one-site problem. In section 3 we briefly consider the three-band model at unit filling. Then, we apply the Schieffer–Wolff transformation [10] for getting the J-term of the low-energy hamiltonian. In section 4 we get the effective electron hopping parameters and the correction to them. Also, we discuss the accuracy of the t–t'–J models for the electron-doped system. Section 5 presents our conclusions. In the Appendix

some details of our considerations are given.

2. Three-band hamiltonian

The three-band model with the direct O–O hopping is given by the following hamiltonian [6]:

$$H=\epsilon_d \sum_{l,\alpha} d^+_{l\alpha} d_{l\alpha} + \epsilon_p \sum_{m,\alpha} p^+_{m\alpha} p_{m\alpha} + U_d \sum_l d^+_{l\uparrow} d_{l\uparrow} d^+_{l\downarrow} d_{l\downarrow} + H' , \quad (1)$$

where $d^+_{l\alpha}$ ($d_{l\alpha}$) creates (annihilates) the hole in a Cu $d_{x^2-y^2}$ state at site l, $p^+_{m\beta}$ ($p_{m\beta}$) creates (annihilates) the hole in an O $p_{x(y)}$ state at site m, ϵ_d and ϵ_p are the energies of Cu and O levels, respectively, U_d is an intrasite Coulomb repulsion at the copper site.

The hybridization term H' is given by

$$H' = t \sum_{\langle lm\rangle\alpha} (d^+_{l\alpha} p_{m\alpha} + \text{h.c}) - t_p \sum_{\langle mm'\rangle\alpha} (p^+_{m\alpha} p_{m'\alpha} + \text{h.c.}) , \quad (2)$$

where $\langle lm\rangle$ denotes the nearest-neighbor Cu and O sites, $\langle mm'\rangle$ denotes the nearest-neighbor O sites. In eq. (2) we follow the sign convention of refs. [11,12].

As was first noted by Zhang and Rice [13], it is conveniently to use the orthonormalized oxygen states on the four oxygens around a Cu site. In our previous work [7] we have represented the hamiltonian (1), (2) in terms of orthogonal symmetrical and antisymmetrical oxygen cluster states,

$$q_l = \sum_{\boldsymbol{k}} (1+\gamma_{\boldsymbol{k}})^{-1/2} (\cos(k_x/2) p_{\boldsymbol{k}x} + \cos(k_y/2) p_{\boldsymbol{k}y}) \exp(-i\boldsymbol{k}\boldsymbol{r}_l) ,$$

$$\tilde{q}_l = \sum_{\boldsymbol{k}} (1+\gamma_{\boldsymbol{k}})^{-1/2} (-\cos(k_y/2) p_{\boldsymbol{k}x} + \cos(k_x/2) p_{\boldsymbol{k}y}) \exp(-i\boldsymbol{k}\boldsymbol{r}_l) , \quad (3)$$

where summation in eq. (3) is produced over the Brillouin zone with $\gamma_{\boldsymbol{k}} = \frac{1}{2}(\cos(k_x a) + \cos(k_y a))$ and $p_{\boldsymbol{k}x,y}$ are the Fourier images of $p_{mx,y}$,

$$p_{\boldsymbol{k}x,y} = \sum_{m\in x,y} p_m \exp(-i\boldsymbol{k}\boldsymbol{r}_m) . \quad (4)$$

The physical reason for the introduction of q_l and $\tilde{q}_l$ states [13] is as follows. The hole at the copper can hop only at the symmetrical combinations of the oxygen states. If we separate out the oxygen states which interact strongly with the copper states, we can solve the problem of determination of the low-energy two-hole states or vacuum states at the background of the one-hole states (spins). The states q_l, $\tilde{q}_l$ (3) are independent at different sites and are orthonormalized. They are very convenient for solving this problem.

The original hamiltonian (1), (2) in terms of q_l, $\tilde{q}_l$ takes the form

$$H_0 = \epsilon_d \sum_{l,\alpha} d^+_{l\alpha} d_{l\alpha} + \epsilon_p \sum_{l,\alpha} (q^+_{l\alpha} q_{l\alpha} + \tilde{q}^+_{l\alpha} \tilde{q}_{l\alpha}) + U_d \sum_l d^+_{l\uparrow} d_{l\uparrow} d^+_{l\downarrow} d_{l\downarrow} ,$$

$$H' = 2t \sum_{\langle ll'\rangle\alpha} \lambda_{ll'} (d^+_{l\alpha} q_{l'\alpha} + \text{h.c.}) - t_p \sum_{\langle ll'\rangle\alpha} \{\mu_{ll'} (q^+_{l\alpha} q_{l'\alpha} - \tilde{q}^+_{l\alpha} \tilde{q}_{l'\alpha}) + \nu_{ll'} (q^+_{l\alpha} \tilde{q}_{l'\alpha} + \text{h.c.})\} , \quad (5)$$

where the explicit form of the coefficients $\lambda_{ll'}$, $\mu_{ll'}$, $\nu_{ll'}$ can be obtained from eqs. (1), (2) and (3),

$$\{\lambda,\mu,\nu\}_{ll'} \equiv \{\lambda,\mu,\nu\}(\boldsymbol{l}-\boldsymbol{l}') = \sum_{\boldsymbol{k}} \{\lambda,\mu,\nu\}_{\boldsymbol{k}} \exp(-i\boldsymbol{k}(\boldsymbol{l}-\boldsymbol{l}')) , \quad (6)$$

with

$$\lambda_{\boldsymbol{k}} = (1+\gamma_{\boldsymbol{k}})^{1/2} ,$$

$$\mu_{\boldsymbol{k}} = 8\cos^2(k_x/2)\cos^2(k_y/2)(1+\gamma_{\boldsymbol{k}})^{-1/2} , = 4\cos(k_x/2)\cos(k_y/2)(\cos^2(k_x/2) - \cos^2(k_y/2))(1+\gamma_{\boldsymbol{k}})^{-1/2} .$$

These coefficients decrease rapidly with increasing $|\boldsymbol{l}-\boldsymbol{l}'|$. The values of λ, μ and ν for small $|\boldsymbol{l}-\boldsymbol{l}'|$ are given in table 1. One can easily get that $\nu_{00} \equiv 0$ and, therefore, the mixing of q and $\tilde{q}$ at the same sites is absent. The transformed hamiltonian (5) is equivalent to the three-band hamiltonian (1), (2).

We divide the hamiltonian (5) into local and hopping parts:

$$H_{\text{loc}} = \epsilon_d \sum_{l,\alpha} d^+_{l\alpha} d_{l\alpha} + (\epsilon_p - \mu_0 t_p) \sum_{l,\alpha} q^+_{l\alpha} q_{l\alpha}$$

Table 1
The values of the coefficients $\lambda(l-l')$, $\mu(l-l')$, $\nu(l-l')$ as functions of $(l-l')=nx+my$

n, m	$\lambda_{n,m}=\lambda_{m,n}$	$\mu_{n,m}=\mu_{m,n}$	$\nu_{n,m}=-\nu_{m,n}$
0, 0	0.9581	1.4567	0.0
1, 0	0.1401	0.5497	0.2678
1, 1	−0.0235	0.2483	0.0
2, 0	−0.0137	−0.1245	0.0812
2, 1	0.0069	−0.0322	0.0609
2, 2	0.0035	0.0231	0.0

$$+(\epsilon_p+\mu_0 t_p)\sum_{l,\alpha}\tilde{q}^+_{l\alpha}\tilde{q}_{l\alpha}+U_d\sum_l d^+_{l\uparrow}d_{l\uparrow}d^+_{l\downarrow}d_{l\downarrow}$$

$$+2t\lambda_0\sum_{ll'\alpha}(d^+_{l\alpha}q_{l\alpha}+\text{h.c.}),$$

$$H_{hop}=2t\sum_{ll'\alpha}\lambda_{ll'}(d^+_{l\alpha}q_{l'\alpha}+\text{h.c.})$$

$$-t_p\sum_{ll'\alpha}\{\mu_{ll'}(q^+_{l\alpha}q_{l'\alpha}-\tilde{q}^+_{l\alpha}\tilde{q}_{l'\alpha})$$

$$+\nu_{ll'}(q^+_{l\alpha}\tilde{q}_{l'\alpha}+\text{h.c.})\}. \qquad (7)$$

Hereafter, a sum over l, l' denotes $l\neq l'$. One can see that the hybridization term in H_{loc} (7) includes only the symmetric oxygen state in agreement with Zhang and Rice [13]. The direct O–O hopping, once taken into account, does not mix local states with the opposite symmetry.

For the case of unit filling there is one hole per unit cell. Therefore, one can introduce the set of one-hole cluster states

$$|d_\alpha\rangle\equiv d^+_\alpha|0\rangle,\quad |q_\alpha\rangle\equiv q^+_\alpha|0\rangle,$$
$$|\tilde{q}_\alpha\rangle\equiv\tilde{q}^+_\alpha|0\rangle, \qquad (8)$$

and rewrite H_{loc} in these terms:

$$H^1_{loc}=\sum_{l,\alpha}\{\epsilon_d X^{dd}_{l\alpha}+(\epsilon_p-\mu_0 t_p)X^{qq}_{l\alpha}$$

$$+(\epsilon_p+\mu_0 t_p)X^{\tilde{q}\tilde{q}}_{l\alpha}+2t\lambda_0(X^{dq}_{l\alpha}+\text{h.c.})\}, \qquad (9)$$

where

$$X^{ab}_{l\alpha}\equiv|a_{l\alpha}\rangle\langle b_{l\alpha}| \qquad (10)$$

is the Hubbard operator at the site l, and $\alpha=\pm\frac{1}{2}$ is the spin projection. It is convenient to introduce the Hubbard operators because they form the natural basis for description of one-site states. If we also introduce the non-diagonal Hubbard operators we can simply express all operators in our hamiltonian (7) in their terms. Diagonalization of H^1_{loc} (9) is performed for each site independently. After diagonalization, H^1_{loc} is given by

$$H^1_{loc}=\sum_{l,\alpha}\{\epsilon_f X^{ff}_{l\alpha}+\epsilon_g X^{gg}_{l\alpha}+(\epsilon_p+\mu_0 t_p)X^{\tilde{q}\tilde{q}}_{l\alpha}\}, \qquad (11)$$

with

$$|f_\alpha\rangle=U|d_\alpha\rangle-V|q_\alpha\rangle,$$
$$|g_\alpha\rangle=V|d_\alpha\rangle+U|q_\alpha\rangle,$$
$$U=((R_1+\tilde{\Delta})/2R_1)^{1/2}, \qquad (12)$$
$$V=((R_1-\tilde{\Delta})/2R_1)^{1/2},$$

where $R_1=(\tilde{\Delta}^2+4t^2\lambda_0^2)^{1/2}$, $\tilde{\Delta}=(\Delta-\mu_0 t_p)/2$, and $\epsilon_{f,g}=-\Delta_1\mp R_1$, $\Delta_1=(\Delta+\mu_0 t_p)/2$, $\Delta=\epsilon_p-\epsilon_d$. As discussed in ref. [7], we assume that at unit filling the groundstate of the CuO_2 plane is the low $|f\alpha\rangle$ - states on each cluster (the hole on the copper with admixture of symmetrical combination of the hole on the nearest four oxygens) with a virtual transition at neighbors. Such transitions give the superexchange interaction in the section order of perturbation theory.

The hopping part of the hamiltonian (7) contains transitions between vacuum, one- and two-hole states at the different sites. For a detailed consideration of this subject see ref. [7].

3. Superexchange interaction

Here we consider only the terms of H_{hop} that are relevant to intersite interaction:

$$H_{hop}=\sum_{ll'\alpha\beta,y}F^{y,\alpha}_{ll',\beta}\{X^{y,f\alpha}_l X^{0,f\beta}_{l'}+X^{f\beta,0}_l X^{f\alpha,y}_{l'}\}, \qquad (13)$$

where y is the set of two-hole states, which are five singlets and three triplets [7], $F^{y,\alpha}_{ll',\beta}$ are matrix elements of the hamiltonian for transition from $\{f_l, f_{l'}\}$ to $\{y_l, 0_{l'}\}$ states.

By applying the Schrieffer–Wolff transformation to eq. (13) (see Appendix and refs. [7,10]) one can get

$$H_J=\sum_{ll'}(J_{ll'}\boldsymbol{S}_l\boldsymbol{S}_{l'}+Y_{ll'}\hat{N}_l\hat{N}_{l'}), \qquad (14)$$

$$\boldsymbol{S}_l=\tfrac{1}{2}\sigma_{\alpha\beta}X^{\alpha\beta}_l,\quad \hat{N}_l\equiv X^{\uparrow\uparrow}_l+X^{\downarrow\downarrow}_l.$$

The expressions for the $J_{ll'}$ and $Y_{ll'}$ constant are given in the Appendix.

Thus, we have established that at unit filling the groundstate of the CuO_2 plane is the system of local spins which interact antiferromagnetically. Since $J_{ll'}$ decreases rapidly with increasing $|l-l'|$, we hold only the nearest-neighbor term in eq. (14) and receive the Heisenberg hamiltonian. One can check that $Y_{\langle ll'\rangle} \simeq -\frac{1}{4} J_{\langle ll'\rangle}$ and so

$$H_J = J \sum_{\langle ll'\rangle} (\boldsymbol{S}_l \boldsymbol{S}_{l'} - \tfrac{1}{4} \hat{N}_l \hat{N}_{l'}) ,$$

$$J \equiv J_{\langle ll'\rangle} . \qquad (15)$$

The second term in the hamiltonian (15) can be essential when the system goes away from unit filling.

4. Electron-doped system

The doping of the CuO_2 plane by the electron is equivalent to removal of a hole from one of the clusters. Hence, in the hole picture the electron is "zero" or vacuum state. If the hole (spin) is taken away from cluster, the neighboring holes (spins) can hop to the empty site. Thus, the mechanism of the movement of the electron is different from the movement of the added hole. The electron moves as a "hole-in-hole", whereas the hole moves as a local singlet.

4.1. Hopping hamiltonian

From the expression for H_{hop} (7) with the definitions (12) and (10) one can easily get the zero-order electron hopping hamiltonian,

$$H_t = \sum_{ll'\alpha} T^{\mathrm{e}}_{ll'} X^{0,f\alpha}_l X^{f\alpha,0}_{l'} , \qquad (16)$$

with

$$T^{\mathrm{e}}_{ll'} = -4t\lambda_{ll'} UV - t_{\mathrm{p}} \mu_{ll'} V^2 . \qquad (17)$$

The electron hopping hamiltonian (16) coincides with the hole hopping hamiltonian derived in refs. [7,9]. They correspond to the t–t'–... terms of the t–t'–J hamiltonian. But the expression for the hole-singlet hopping is more complicated [7]:

$$T^{\mathrm{h}}_{ll'} = 2t\lambda_{ll'} (\sqrt{2}\, U_1 U - W_1 V) \times (\sqrt{2}\, V_1 V - W_1 U) - t_{\mathrm{p}} \mu_{ll'} (\sqrt{2}\, V_1 V - W_1 U)^2/2 , \qquad (18)$$

where U and V were determined in eq. (12), and U_1, V_1, W_1 are the components of the eigenfunction of the local singlet.

Thus, we have mapped the three-band model for one electron over unit filling to the t–t'–J model. The hamiltonian (15), (16) in terms of the Hubbard operators can be rewritten in a more usual form:

$$H_{t-J} = t \sum_{\langle ll'\rangle,\alpha} \tilde{c}^{+}_{l\alpha} \tilde{c}_{l'\alpha} + J \sum_{\langle ll'\rangle} (\boldsymbol{S}_l \boldsymbol{S}_{l'} - \tfrac{1}{4} \hat{n}_l \hat{n}_{l'}) , \qquad (19)$$

$$\tilde{c}_{l\alpha} = c_{l\alpha}(1 - \hat{n}_{l,-\alpha}) , \quad \tilde{c}^{+}_{l\alpha} = (\tilde{c}_{l\alpha})^{+} ,$$

$$\boldsymbol{S}_l = \tfrac{1}{2} c^{+}_l \sigma c_l , \quad \hat{n}_l = (c^{+}_l \cdot c_l) .$$

Here $c^{+}_{l\alpha}$, $c_{l\alpha}$ are the electron creation and annihilation operators.

4.2. Second-order corrections

With the help of Schrieffer–Wolff transformation we shall obtain the second-order corrections to the t–t'–J hamiltonian. The corrections to the first hopping parameter will be small and the t–J model may be valid. The corrections to the other hopping parameters are not relatively small and, therefore, models with the hopping at neighbors farther than the nearest must be more complicated than the simple t–t'–... type.

First of all we shall obtain the correction to the energy of the electron. Such a correction arises due to the virtual process of hopping of the electron at the neighbors with transition to the excited state and back. The corresponding hamiltonian is given in the Appendix. The resulting second-order correction is

$$\delta H_{\mathrm{E}} = -\sum_{ll'} M_{ll'} X^{00}_l \hat{N}_{l'} \qquad (20)$$

with

$$M_{ll'} = \frac{|T^{g}_{l'f}|^2}{\epsilon_g - \epsilon_f} ,$$

$$T^{g}_{l'f} = 2t\lambda_{ll'} (U^2 - V^2) + t_{\mathrm{p}} \mu_{ll'} UV . \qquad (21)$$

The hamiltonian δH_{E} (20) coincides completely with δH_{E} in ref. [7], but the expression (21) for the $M_{ll'}$ is sufficiently more simple than for the hole one.

Corrections to the direct hopping parameters can

be obtained by transformation of the hamiltonian (13). The result is

$$\delta H_t = \Sigma_{lnl'\alpha\beta,y} T^{y}_{lnl'} \{x_y X_l^{0,f\alpha} X_{l'}^{f\alpha,0} \hat{N}_n + z_y X_l^{0,f\beta} X_{l'}^{f\alpha,0} (\sigma_{\alpha\beta} \boldsymbol{S}_n)\}, \quad (22)$$

where y is the set of two-hole states, $x_y = \frac{1}{2}$ for singlets and $x_y = \frac{3}{4}$ for triplets, $z_y = 1$ for singlets and $z_y = -\frac{1}{2}$ for triplets. The expressions for $T^{y}_{lnl'}$ are given in the Appendix. As was shown, the corrections to the t–t'–J hamiltonian have a complicated nature and depend on the filling ($\hat{N}$-term) and spin state of the neighbors ($\boldsymbol{S}$-term). The corrections for the hole single-band model [7] and the electron one are quite different.

4.3. Quantitative results

We have argued [7] that our general approach to the low-energy reduction of a three-band model is essentially more correct than the other one, because we construct the perturbation theory over the ratio of the effective hopping parameters between the different local states to the energy gap between them. This ratio for the case of a CuO_2 plane is of the order of 0.1. All values of the effective sing-band hamiltonian have been derived for arbitrary parameters of the three-band model, without any assumption about a relationship among t, Δ and U_d. In our calculation we take $U_d = 8.2$ eV, $t = 1.4$ eV, $t_p = 0.7$ eV, $U_p = V_{pd} = 0$ according to the different papers [14–16]. Also, we have taken the experimental value of $J = 126$ meV [17] and have selfconsistently determined the charge-transfer gap to be $\Delta = 5.07$ eV. In table 2 we present the following effective parameters of the one-band model: the hopping parameters to the first, second and third neighbors; the contribution of the direct O–O hopping; corrections to hopping and energy; value of the ratio t_1/J.

We obtain for the electron hopping $t^e \equiv t_1 \approx 0.39$ eV, that is 1.36 times less than the hole hopping [7] $t^h \approx 0.53$ eV. The role of the direct O–O hopping for the electron-doped system is lower than for the hole one. Actually, the admixture of the O-state for one hole on a cluster is small, unlike for the hole singlet, where the added hole is mainly on the oxygen. Thus, the O–O hopping contribution to the hopping at the nearest-neighbors for the electron $(t_{p1}/t_1)^e \approx 20\%$ and for the hole $(t_{p1}/t_1)^h \approx 36\%$.

As for the validity of t–J, t–t'–J and other models to the electron-doped system, our conclusions are similar to the case of the hole-doped system. Thus, if we hold only the hopping at the nearest-neighbors, the corrections to the t–J model on a ferromagnetic background are near to 0.13% for electrons and 2.5% for holes, and the t–J model is valid. If we are interested in the next-neighbors hopping, it is necessary to include the correction (22) to the effective hamiltonian. This correction has a complicated structure and does not reduce to the simple direct hopping.

5. Conclusion

We have studied electron doping of the CuO_2 plane in the framework of the three-band model. By applying our general procedure of the low-energy reduction to the electron-doped system, we conclude that the t–J model is valid as well as to the hole-doped

Table 2
The first three hopping parameters, the contributions of the direct O–O hopping to them, second-order corrections to them on a ferromagnetic background, second-order corrections to the energy, and the ratio t_1/J

Neighbor number, n	Direct hopping t_n^{eff}, (eV)	Direct O–O hopping t_{pn}^{eff}, (eV)	Corrections δt_n^{eff}, (%)
1	−0.3896	−0.0765	0.125
2	0.0180	−0.0345	122.5
3	0.0480	0.0173	24.2
Correction to the energy (eV)	−0.0931	Ratio $\lvert t_1/J \rvert$	3.081

system. We established some asymmetrical properties. The effective hopping parameter for the electron is 1.36 times less than the hole one. Corrections to the single-band electron and hole t–J models have different magnitudes. Such corrections are important for transitions at the next-nearest neighbors.

It is doubtful that the difference in the parameters of the one-band model may lead to the drastic difference in behavior of hole-doped and electron-doped systems with doping. The strong asymmetrical dependence of the critical concentration for the disappearance of antiferromagnetism is probably connected with the nature of antiferromagnetic ordering in this system [18]. In the hole-doped systems antiferromagnetism has a quasi-two-dimensional character and is associated with Cu spins. In the electron-doped systems the contribution of Nd or Pr spins in the antiferromagnetic ordering is essential and three-dimensional effects are more important.

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Appendix. The second-order corrections to the hopping process

For obtaining such corrections we use the Schrieffer–Wolff transformation

$$H \Rightarrow \tilde{H} = \exp(-S) H \exp(S) ,$$
$$S^{+} = -S . \qquad (A.1)$$

The first-order generator of transformation and the second-order correction are

$$[H_0, S] = -H' , \quad \delta H^2 = \tfrac{1}{2}[H', S] , \qquad (A.2)$$

for this model $H_0 \equiv H_{\mathrm{loc}}$ (eq. (7)). For the derivation of the J-term $H' \equiv H_{\mathrm{hop}}$ (eq. (13)). Expressions for the $J_{ll'}$ and $Y_{ll'}$ integrals are given by

$$J_{ll'} = \sum_{y} x_y \frac{|F^{y}_{ll'}|^2}{\epsilon_y + \epsilon_0 - 2\epsilon_f} ,$$

$$Y_{ll'} = -\sum_{y} z_y \frac{|F^{y}_{ll'}|^2}{\epsilon_y + \epsilon_0 - 2\epsilon_f} , \qquad (A.3)$$

where y is the set of two-hole states at a cluster, ϵ_y are the eigenenergies, $\epsilon_0 \equiv 0$ is the energy of the vacuum state. Values $x_y = 2$, $z_y = \frac{1}{2}$ for singlets and $x_y = -2$, $z_y = \frac{3}{4}$ for triplets. Matrix elements $F^{y}_{ll'}$ are obtained in ref. [7]. One can check that the major contribution to J and Y originates from the matrix element of the transition to the lowest singlet and so $Y_{\langle ll' \rangle} \simeq \frac{1}{4} J_{\langle ll' \rangle}$.

The terms of H_{hop} (7), which lead to the energy correction, are given by

$$H'_{\mathrm{E}} = \sum_{ll'\alpha} F^{g}_{ll',f} \{ X^{0,f\alpha}_{l} X^{g\alpha,0}_{l'} + X^{0,g\alpha}_{l'} X^{f\alpha,0}_{l} \} . \qquad (A.4)$$

The corresponding generator of the transformation is

$$S_{\mathrm{E}} = -\sum_{ll'\alpha} \frac{F^{g}_{ll',f}}{\epsilon_g - \epsilon_f} \{ X^{0,f\alpha}_{l} X^{g\alpha,0}_{l'} - X^{0,g\alpha}_{l'} X^{f\alpha,0}_{l} \} , \qquad (A.5)$$

where $|f_\alpha\rangle$ and $|g_\alpha\rangle$ are the one-hole states (12) with their energies ϵ_f and ϵ_g. Thus, the second-order correction to the energy has the form (20).

Corrections to the direct hopping (22) can be obtained from the transformation of the hamiltonian (13). Magnitudes $T^{y}_{lnl'}$ are given by

$$T^{y}_{lnl'} = \frac{F^{y}_{ln} F^{y}_{nl'}}{\epsilon_y + \epsilon_0 - 2\epsilon_f} . \qquad (A.6)$$

The expressions of F^{y}_{ln} were obtained analytically and computed for definite values of parameters of the three-band model in ref. [7].

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