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Magnetic interactions and dynamics of holes in CuO_2 planes of high-T_c superconducting materials

V. Hizhnyakov,* E. Sigmund, and M. Schneider
Institut für Theoretische Physik, Teil III, Universität Stuttgart, Pfaffenwaldring 57,
7000 Stuttgart 80, Federal Republic of Germany

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Starting from the two-band Hubbard Hamiltonian a systematic derivation of the spin-dependent interactions within the CuO_2 planes of the perovskite high-T_c superconductors is presented, taking the remarkably strong Cu-O hybridization of these materials into account. We show that in the case of hole doping the kinetic energy of the holes plays a dominant role leading to a ferromagnetic ordering in the surrounding of an additional hole (ferron state). In addition we show that any reduction of the two-band model to a one-band model clearly underestimates the influence of the kinetic energy of the holes.

I. INTRODUCTION

It is generally accepted that models with strong on-site Coulomb interactions in a partially filled $3d_{x^2-y^2}$ Cu band can be used for the description of the electronic states of CuO_2 planes in the high-T_c superconducting copper oxides.[1] In one such model, the so-called two-band Hubbard model,[2] both the $d_{x^2-y^2}$ band of the Cu ions and the $p\sigma$ bands of the oxygen ions are incorporated. The corresponding electronic on-site energies of the localized orbitals are given by ε_d and ε_p, respectively. In the case of a half-filled Cu band, each of the $d_{x^2-y^2}$ Cu orbitals is occupied by one electron, only the spin of which is responsible for the magnetic behavior of the Cu ion. The overlap of the orbitals between nearest-neighboring Cu and O ions is described by the exchange integral T. The Coulomb repulsion probed by a second electron added to the Cu orbital is included via the Cu on-site (Hubbard) repulsion potential U. The parameters of the model are taken within the range (see, e.g., Ref. 3) $U \sim 8-10$ eV, $T \sim 1.3$ eV, and $\varepsilon = |\varepsilon_p - \varepsilon_d| \sim 1.5-5.3$ eV, where the Coulomb repulsion on oxygen is incorporated by Hartree-Fock approximation. In Ref. 3, the best fit to experiments was given by $\varepsilon \sim 1.5$ eV. In most of the papers the hole representation is used instead of the electron one. The two representations can easily be connected: the Hubbard parameter U remains unchanged, the hopping integral T changes sign, while the difference of the one-electron energies ε should be replaced by $\varepsilon_h = U - \varepsilon$.

The two-band Hubbard Hamiltonian can be written in the form

$$H = H_0 + H_U + H_T , \tag{1}$$

where

$$H_0 = \varepsilon_d \sum_{m,\sigma} n^d_{m\sigma} + \varepsilon_p \sum_{m,\sigma} n^p_{m'\sigma} , \tag{2a}$$

$$H_U = (U/2) \sum_{m,\sigma} n^d_{m\sigma} n^d_{m-\sigma} , \tag{2b}$$

$$H_T = T \sum_{(m,m'),\sigma} (d^\dagger_{m\sigma} p_{m'\sigma} + \text{H.c.}) . \tag{2c}$$

$n^d_{m\sigma}$ and $n^p_{m'\sigma}$ are the electronic occupation numbers of the $d_{x^2-y^2}$ and $p\sigma$ orbitals, respectively, $d^\dagger$ (d) and $p^\dagger$ (p) are electronic creation (annihilation) operators in the corresponding Cu and O orbitals obeying Fermi statistics. m,m' denote the lattice sites occupied by Cu and O ions, (m,m') represents the summation over nearest neighbors only. The spin index σ indicates the spin directions ($\sigma = \uparrow, \downarrow$). H_0 is the sum over all single-particle states, H_U describes the Coulomb repulsion for two electrons on the same Cu site with opposite spins and H_T is the transfer term (hybridization) between Cu ions and the four nearest O ions responsible for the mobility of the particles. We do not consider the O-O transfer proportional to the exchange integral t, because t is remarkably smaller than T; the effect of the O-O transfer has been studied intensively in Ref. 4.

The large value of the Hubbard energy U leads to strong electron-electron correlation effects in these systems. For totally filled $p\sigma$ bands and a half-filled $d_{x^2-y^2}$ band (corresponding to La_2CuO_4 or $YBa_2Cu_3O_6$), these effects result in the appearance of the energy gap above the highest occupied state and in a strong spin-spin interaction causing antiferromagnetic ordering of the Cu^{2+} ions.

To estimate this Cu^{2+} spin-spin interaction in the materials under consideration, the theory of superexchange[5] is used commonly. According to this theory, the coupling constant J of the spin-spin interaction equals (see, e.g., Ref. 6)

$$J = 2T^4 \left[\frac{1}{(U-\varepsilon)^3} + \frac{2}{U(U-\varepsilon)^2} \right] . \tag{3}$$

Expression (3) is usually derived via the Schrieffer-Wolff transformation,[7] which leads to an expansion in orders of $T/(U-\varepsilon)$ and T/ε. For the half-filled case (undoped situation), the terms proportional T/ε cancel, as can be seen from Eq. (3). For arbitrary band fillings, however, the convergence of this expansion is only guaranteed if the conditions $U-\varepsilon \gg T$ and $|\varepsilon| \gg T$ are satisfied. This corresponds to materials with strong Cu on-site Hubbard interaction and weak hybridization of nearest Cu and O ions. In the superconducting oxides, however, the Cu and O orbitals strongly hybridize and, therefore, the last condition is not satisfied.

Indeed, taking into account that each Cu ion is surrounded by four nearest O ions one finds[8] that the strength of the hybridization is determined by the parameter $4T/|\varepsilon|$. For $4T \ll |\varepsilon|$, the hybridization has to be considered as weak, whereas in the case of $4T \gtrsim |\varepsilon|$, one is in the strong hybridization region. For the high-T_c materials the latter relation holds true, corresponding to a strong Cu-O hybridization. Therefore, in order to describe the transport behavior and the interactions in these materials, we have to use a treatment adequate for the parameter range $U \gg \varepsilon, T$ and $4T \gtrsim \varepsilon = |\varepsilon_p - \varepsilon_d|$. (In the case $U, \varepsilon \gg T$ and $4T \gtrsim |U-\varepsilon|$, and analogous treatment can be used by simply replacing ε by $U-\varepsilon$, leading to similar results.)

We will see that, only for the undoped systems, the spin-spin interaction resulting from our calculation and the one described by formula (3) coincide (up to terms $\sim T^2/[U(U-\varepsilon)] \ll 1$). For the doped situation, more general expressions have to be used.

It was suggested by Anderson[9] that the properties of the low-energetic excitations of the two-band Hubbard model are close to those of the one-band Hubbard model or even to those of the simpler *t-J* model. In the case of $|\varepsilon| \gg T$, this statement was proved by Zhang and Rice[6] and its validity was discussed by many other authors.[10,11] Although we will show that the considerations of Ref. 6 do not hold for the actual case $|\varepsilon| \sim T$, the idea[9] itself is interesting and we will discuss it in the last section. The calculations in Ref. 6 are based on including the lowest-lying energy states in every $\mathrm{CuO_4}$ plaquette only and neglecting the four other states totally. In the given parameter range $|\varepsilon| \sim T \ll U$, the validity of this approximation has to be studied carefully when one wants to map the two-band Hubbard model onto the *t-J* model. In this communication we propose an approach which allows us to find answers to these questions.

II. FIRST UNITARY TRANSFORMATION

In contrast to the calculations usually performed when deriving the spin-spin interaction[7] (3), we make use of the smallness of the parameters T/U and ε/U only, but not of the parameter T/ε. To do so we separate the Hamiltonian H_T into two terms

$$H_T = H_{T1} + H_{T2} , \tag{4}$$

where the first term

$$H_{T1} = T \sum_{(m,m'),\sigma} (1 - n^d_{m-\sigma})(d^\dagger_{m\sigma} p_{m'\sigma} + \mathrm{H.c.}) \tag{5a}$$

does not change the number of the double-occupied Cu sites, while the second one

$$H_{T2} = T \sum_{(m,m'),\sigma} n^d_{m-\sigma}(d^\dagger_{m\sigma} p_{m'\sigma} + \mathrm{H.c.}) \tag{5b}$$

changes this number, creating or annihilating double-occupied Cu sites (an analogous separation was used for transforming the one-band Hubbard model to the *t-J* model[12]). In the case of totally filled $p\sigma$ bands and a half-filled $d_{x^2-y^2}$ band, the first term, H_{T1}, vanishes since there are no doubly or zero-occupied Cu sites. The second one, H_{T2}, contributes to the energy of the system by mixing Cu states with single and double occupancy. Due to the large energetic difference $\sim U$ between the states involved, one can calculate the contribution of H_{T2} by a perturbational approach with T/U as the expansion parameter. For the general case of arbitrary band fillings, a more convenient realization of the calculations can be found using the method of unitary transformations (see, e.g., Ref. 8).

As a first step we transcribe the system with the unitary exponential transformation

$$H_1 = \exp\{S_1\} H \exp\{-S_1\} . \tag{6}$$

S_1 is chosen to be

$$S_1 = \frac{T}{U_1} \sum_{(m,m'),\sigma} n^d_{m-\sigma}(d^\dagger_{m\sigma} p_{m'\sigma} - \mathrm{H.c.})$$

and $U_1 = U - \varepsilon \sim U$. This transformation eliminates the term H_{T2} and replaces it by a series of new effective interactions depending on the product of T and powers of the small parameter T/U_1 only. We expand the transformed Hamiltonian up to the fourth order and keep all terms up to T^3/U_1^2, but only those terms proportional to T^4/U_1^3 whose mean values differ from zero for the half-filled d band. This leads to

$$H_1 \approx H_0 + H_{T1} + H'_U + H_2 + H_3 + H_4^0 . \tag{7}$$

H'_U coincides with H_U if U is replaced by $U_2 = U + 8T^2/U_1$. H_2, H_3, and H_4^0 describe the second-, third-, and fourth-order effects.

The second-order Hamiltonian reads

$$H_2 = H_2^{(0)} + H_2^{(1)} + H_2^{(2)} + H_2^{(3)} + H_{pd}^{ss} . \tag{8}$$

Here

$$H_2^{(0)} = \frac{2T^2}{U_1} \sum_m n^d_m N^p_m \tag{9}$$

describes the induced correlation interaction between Cu electrons and electrons on nearest oxygen sites. $N^P_m = \sum_\sigma P^\dagger_{m\sigma} P_{m\sigma}$, where

$$P^\dagger_{m\sigma} = \tfrac{1}{2} \sum_{(m')} p^\dagger_{m'\sigma} \tag{10}$$

is the totally symmetric oxygen electron operator of a $\mathrm{CuO_4}$ plaquette. (m') denotes the sum over four oxygen sites which are nearest to the mth Cu site. The Hamiltonian

$$H_2^{(1)} = \frac{T^2}{U_1} \sum_{(m,m_1),\sigma} n^d_{m-\sigma}(1 - n^d_{m_1-\sigma})(d^\dagger_{m\sigma} d_{m_1\sigma} + \mathrm{H.c.}) \tag{11}$$

describes the conditional hopping of electrons between the nearest Cu ions [(mm_1) indicates summation over the nearest Cu sites] while

$$H_2^{(2)}=\frac{T^2}{U_1}\sum_{(m,m_1),\sigma} n^d_{m-\sigma}n^d_{m_1-\sigma}(d^\dagger_{m\sigma}d_{m_1\sigma}+\text{H.c.}) \qquad (12)$$

takes into account the motion of electrons for a more than half-filled d band.

$$H_2^{(3)}=-4\frac{T^2}{U_1}\sum_{m\sigma}(d^\dagger_{m\sigma}d^\dagger_{m-\sigma}P_{m\sigma}P_{m-\sigma}+\text{H.c.}) \qquad (13)$$

is responsible for the two-particle motion and

$$H^{ss}_{pd}=8\frac{T^2}{U_1}\sum_m (s^d_m s^P_m-\tfrac{1}{4}n^d_m N^P_m) \qquad (14)$$

describes the Cu-O spin-spin interaction. We introduced spin operators according to

$$d^\dagger_{m\uparrow}d_{m\downarrow}=s^d_{xm}+is^d_{ym},\quad d^\dagger_{m\uparrow}d^d_{m\uparrow}=\tfrac{1}{2}n^d_m+s^d_{zm}\ ,$$
$$P^\dagger_{m\uparrow}P_{m\downarrow}=s^P_{xm}+is^P_{ym},\quad P^\dagger_{m\uparrow}P_{m\uparrow}=\tfrac{1}{2}N^P_m+s^P_{zm}\ .$$

The third-order term equals

$$H_3=\frac{8T^2}{3U_1}H_2+H_3^{(1)}+H_3^{(2)}+H_3^{(3)}\ , \qquad (15)$$

where

$$H_3^{(1)}=-\frac{8T^3}{U_1^2}\sum_{m,\sigma}(1+\tfrac{1}{3}n^d_{m\sigma})P^\dagger_{m\sigma}P_{m\sigma}(d^\dagger_{m-\sigma}P_{m-\sigma}+\text{H.c.})$$
$$+\frac{T^3}{U_1^2}\sum_{(m,m_1),\sigma}(1+\tfrac{5}{3}n^d_{m_1\sigma})n^d_{m\sigma}$$
$$\times(d^\dagger_{m_1-\sigma}P_{m-\sigma}+\text{H.c.}) \qquad (16)$$

describes the hybridization dependence of Cu and O ions from their valences.

The equation

$$H_3^{(2)}=\frac{T^3}{U_1^2}\sum_{(m,m_1),\sigma}(1+\tfrac{5}{3}n^d_{m_1\sigma})$$
$$\times(d^\dagger_{m_1-\sigma}d^\dagger_{m\sigma}d_{m-\sigma}P_{m\sigma}+\text{H.c.}) \qquad (17)$$

takes into account the hopping processes with flipping of spins, and

$$H_3^{(3)}=3\frac{T^3}{U_1^2}\sum_{(m,m_1),\sigma} n^d_{m_1\sigma}(d^\dagger_{m\sigma}d^\dagger_{m-\sigma}d_{m_1-\sigma}P_{m\sigma}+\text{H.c.}) \qquad (18)$$

contributes to the two-particle transport. The only fourth-order term which has a nonzero mean value for the half-filled d band is of the form

$$H_4^{(0)}=\frac{T^4}{U_1^3}\sum_{(m,m_1)}(s^d_m s^d_{m_1}-\tfrac{1}{4}n^d_m n^d_{m_1})n^p_{m'}\ , \qquad (19)$$

where m' numbers the oxygen site situated between the mth and m_1-th Cu site.

III. SECOND UNITARY TRANSFORMATION

If one projects H_1 onto the electronic subspace of half-filled Cu $d_{x^2-y^2}$ orbitals and totally filled O p orbitals, all terms except H_0, H_2^0, and H_4^0 turn out to be zero. The first two terms do not depend on Cu spins, whereas the term H_4^0 does. Consequently, H_4^0 describes the Cu spin-spin interaction, which is of the order T^4/U_1^3.

There is, however, an additional contribution to the Cu spin-spin interaction resulting from the conditional hopping term $H_2^{(1)}$ in the second order. To prove that we perform a second unitary transformation

$$\bar{H}=\exp\{S_2\}H_1\exp\{-S_2\}\ , \qquad (20)$$

where

$$S_2=\frac{T^2}{U_1U_2}\sum_{(m,m_1),\sigma} n^d_{m-\sigma}(d^\dagger_{m\sigma}d_{m_1\sigma}-\text{H.c.})\ . \qquad (21)$$

By this transformation the term $H_2^{(1)}$ is totally removed. Instead, a number of terms $\sim T^4/U^3$ (and a series of smaller, higher-order terms) are built up. Among them the term

$$H_4^{(1)}=\frac{4T^4}{U_2U_1^2}\sum_{(m,m_1)}(s^d_m s^d_{m_1}+\tfrac{1}{4}n^d_m n^d_{m_1}) \qquad (22)$$

is the only one which has a nonzero mean value for the half-filled d band.

The total Hamiltonian, which is obtained after the second transformation and after excluding terms with double-occupied Cu sites, takes the form

$$H=H_0+H_{T1}+H_3+H^{ss}_{pd}+H_{\text{se}}\ . \qquad (23)$$

The last term, H_{se}, describing the Cu superexchange interaction, is given by

$$H_{\text{se}}=H_4^{(0)}+H_4^{(1)}\ . \qquad (24)$$

For the undoped case, the Cu spin-spin interaction takes the following form (up to an additional constant which is of no relevance):

$$H_{\text{se}}=J\sum_{(m,m_1)} s^d_m s^d_{m_1}\ , \qquad (25)$$

where

$$J=\frac{2T^4}{U_1^3}(1+2U_1/U_2)\approx 6\frac{T^4}{U^3} \qquad (26)$$

is the interaction constant (see also Ref. 8 where this expression was presented without derivation). We want to underline here that the only condition for the validity of the formula (26) is $|\varepsilon|,T\ll U$. In this case, expression (26) is equivalent to (3). This is due to the fact that, in the undoped case, the term linear in T (5a) in the Hamiltonian does not work and, therefore, that the expansion of the Schrieffer-Wolff transformation[7] and our transformations (6) and (20) are identical.

IV. SPIN-SPIN INTERACTION IN THE DOPED CASE

The situation changes drastically when one goes away from half-filling. When adding a hole to the undoped system, it has two important consequences concerning the magnetic interactions and the kinetic energy of the hole.

First, expression (25) describes the spin-spin interaction of two nearest Cu^{2+} ions in that case only when an O^{2-} ion is situated between them. If the charge of this O ion equals -1 (i.e., a hole is localized on it), another much stronger Cu spin interaction starts to work, which is due to the above-mentioned Cu-O spin-spin interaction $H_{pd}^{ss} \sim T^2/U$ (14). This interaction is only zero if $\langle s_{m'}^{P} \rangle = 0$, which corresponds to diamagnetic O^{2-} or to O^0 ions, but not to O^{1-} ions. As a result, the O^{1-} ion causes an effective spin-spin interaction between the two neighboring Cu^{2+} ions, which is ferromagnetic (see also, Ref. 13). In our model this interaction has the form

$$J' \approx \frac{4T^2}{U_1} w \ , \tag{27}$$

where w is the probability of the appearance of the configuration $Cu^{2+}-O^{1-}-Cu^{2+}$. The sign of this interaction depends on the O^{1-} spin.

Second, the presence of a hole in the antiferromagnetic- (AF) ordered CuO_2 plane causes an additional, even more stronger interaction depending on the spin orientation. This is due to the fact that, in contrast to other treatments, the conditioned hopping term H_{T1} in our theory remains unchanged throughout both transformations. Indeed, the corresponding kinetic energy of a hole strongly depends on the spin orientation of the nearest Cu ions. For example, when the surrounding of the hole is ferromagnetically polarized, the hole can delocalize, which leads to a remarkable lowering of the kinetic energy of the system. For one turned Cu spin this gain of delocalization energy already equals 0.45 T (if $|\varepsilon| \leq 4T$).[8] For the assumed parameter range this energy is much larger than the energy $8J$ one needs for turning one spin. Therefore, for $U \gg 4T \geq |\varepsilon|$, a hole in the AF-ordered CuO_2 planes will create a ferromagnetically ordered cluster[8,14–16] (ferron) (see also Refs. 4 and 17 where magnetic and kinetic interactions are studied in detail numerically). Experimental evidences for hole ferrons in these materials have been found by magnetic[18] (and dielectric[19]) susceptibility measurements (see also Ref. 20, and references therein). Evidences for the ferron formation are also indicated in optical measurements (see Refs. 18–22, and references therein).

V. ONE-BAND APPROXIMATION

In this section we discuss the validity of a one-band approximation derived for the parameter range $4T \geq \varepsilon$. First, however, we want to add some remarks concerning the derivation of the t-J model.[6]

As we have pointed out, the treatment of the starting Hamiltonian (1) with the usual Schrieffer-Wolff transformation[7] leads to serious problems in the case of a strong hybridization $\varepsilon \sim T$ since the expansion parameter T/ε of the transformation is not small and the convergence of the expansion is therefore not guaranteed. This convergence, however, is necessary when treating the transport processes within a perturbation theory as it is done in Ref. 6. This shortcoming can be avoided by applying the modified transformation (6) to the Hamiltonian (1).

Another point of criticism is the introduction of local singlet and triplet states. In Refs. 6 and 23 this local consideration is motivated by the small effective transport terms of the t-J model leading to a triplet energy much higher than the singlet energy. On the other hand, Emery *et al.*[24] were able to show, for a special situation of the t-J model, that, in the exact ground-state wave function, there is a remarkable admixture of triplet states. Further on, the derivation[6] of the t-J model does not depend on the type of the magnetic ordering, which is physically not satisfactory since the hole transport depends strongly on the spin orientation (see Nagaoka's theorem[25]).

In the following we demonstrate an alternative way for reducing the two-band model to a one-band model, taking into account from the very beginning the strong Cu-O hybridization ($4T \geq |\varepsilon|$).

As we have shown, the kinetic energy of a hole originates from the interaction H_{T1} (5a) which, in an AF-ordered CuO_2 plane, acts only within CuO_4 units. This is due to Pauli's exclusion principle. Because of the fourfold symmetry axis of the CuO_2 plane, the interaction only involves a totally symmetric linear combination of the oxygen operators in the CuO_4 plaquettes,

$$\begin{aligned} P_{m\sigma} &\equiv P_{m_x,m_y\sigma} \\ &= \tfrac{1}{2}(p_{x,m_x m_y \sigma} + p_{x,m_x m_{y+1}\sigma} \\ &\qquad + p_{y,m_x m_y \sigma} + p_{y,m_{x-1} m_y \sigma}) \ . \end{aligned} \tag{28}$$

Here m_x and m_y are x and y coordinates of the site m, indices x and y describe the two oxygen states in the mth unit cell. The operators $P_{m\sigma}$ are normalized but not orthogonal to each other;[10] their anticommutator equals

$$[P_{m\sigma}, P^{\dagger}_{m'\sigma'}]_+ = \delta_{\sigma\sigma'}(\delta_{mm'} + \delta_{(mm')}/4) \ . \tag{29}$$

Following Zhang and Rice,[6] we get rid of the nonorthogonality by expanding $P_{m\sigma}$ via the Wannier operators $P'_{m\sigma}$,

$$P'_{m\sigma} = (1/N) \sum_k e^{-ikm} P'_{k\sigma} \ , \tag{30}$$

which are both normalized and orthogonal. Here,

$$P'_{k\sigma} = \tfrac{1}{2}\beta_k [p_{x,k\sigma}(1+e^{ik_y}) + p_{y,k\sigma}(1+e^{-ik_x})] \tag{31}$$

are oxygen operators in k representation which are normalized and orthogonal:

$$\beta_k = [1 + \tfrac{1}{2}(\cos k_x + \cos k_y)]^{-0.5}$$

is the normalization factor. The expansion of the original $P_{m\sigma}$ in terms of the $P'_{m\sigma}$ is as follows:

$$P_{m\sigma} = \lambda_0 P'_{m\sigma} + \lambda_1 \sum_{(m')} P'_{m'\sigma} + \cdots \ , \tag{32}$$

where $\lambda \approx 0.96$, $\lambda_1 \approx 0.14$. (m') denotes the sum over the Cu sites nearest to m. Only the two largest terms of this expansion are taken into account, the terms proportional to λ_i ($i=2,3,\ldots$) are neglected (e.g., $\lambda_2 \approx 0.015$). The $P_{m\sigma}$

are identical with the p^s_m of Ref. 6.

The operators $P'_{m\sigma}$, however, do not give the complete set of oxygen operators of the considered oxygen sublattice with two oxygen atoms in the unit cell. Therefore, to be consistent, an additional set of Wannier operators has to be constructed. The corresponding operators are $Q'_{m\sigma}$

$$Q'_{m\sigma}=(1/N)\sum_{k} e^{-ikm}Q'_{k\sigma} \tag{33}$$

with

$$Q'_{k\sigma}=\tfrac{1}{2}\beta_k[p_{x,k\sigma}(1+e^{ik_x})-p_{y,k\sigma}(1+e^{-ik_y})] . \tag{34}$$

Now the $P'_{m\sigma}$ and $Q'_{m\sigma}$ together form a complete set of orthogonal and normalized oxygen operators. The $Q'_{m\sigma}$ introduced here differ from the asymmetric operators $p^a_{m\sigma}$ of Zhang and Rice,[6] since their $p^a_{m\sigma}$ are not orthogonal to the $p^s_{m\sigma}$.

Using the approximate expansion (32), the first two terms of the Hamiltonian (7) take the form

$$H_0+H_{T1}\approx\tilde{H}_0+\tilde{H}_{T1} , \tag{35}$$

where

$$\begin{aligned}\tilde{H}_0=\sum_{m,\sigma}[&\varepsilon_d d^\dagger_{m\sigma}d_{m\sigma}+\varepsilon_p P'^\dagger_{m\sigma}P'_{m\sigma}\\&+2\lambda_0 T(d^\dagger_{m\sigma}P'_{m\sigma}+\text{H.c.})(1-n^d_{m-\sigma})\\&+\varepsilon_p Q'^\dagger_{m\sigma}Q'_{m\sigma}]\end{aligned} \tag{36}$$

describes the on-site energy:

$$\tilde{H}_{T1}=2\lambda_1 T\sum_{(m,m'),\sigma}(d^\dagger_{m\sigma}P'_{m'\sigma}+\text{H.c.})(1-n^d_{m-\sigma}) \tag{37}$$

takes into account the hopping process to neighboring plaquettes. The on-site Hamiltonian $\tilde{H}_0$ can be diagonalized by using the operators

$$c^{(1)}_{m\sigma}=(\sin\alpha)d_{m\sigma}+(\cos\alpha)P'_{m\sigma} , \tag{38a}$$

$$c^{(2)}_{m\sigma}=(\cos\alpha)d_{m\sigma}-(\sin\alpha)P'_{m\sigma} , \tag{38b}$$

where

$$\alpha=\arctan[4\lambda_0 T/(\varepsilon+2\Omega)]$$

and

$$\Omega=\left[4\lambda_0^2T^2+\frac{\varepsilon^2}{4}\right]^{1/2} .$$

In this representation, the on-site energies are equal to $\varepsilon_p\pm\Omega$ and ε_p.

Following the proposal of Anderson,[9] we assume that all the states except the highest one are filled with electrons. An extra hole can be brought into the system by removing an electron from the highest occupied state as long as possible virtual transitions to other states are neglected. We also neglect the double-electron occupancy of the Cu sites. Under these conditions, the effective Hamiltonian in hole representation, which describes the motion of the hole and which is obtained by projecting the total Hamiltonian (7) to the state mentioned, takes the following standard form [the half-filled d band ($\text{Cu}^{2+}\equiv 3d^9$) and the totally empty p bands ($\text{O}^{2-}\equiv 2p^6$) are taken as the vacuum state]:

$$\begin{aligned}H_{\text{eff}}=(\varepsilon_p+\Omega)\sum_{m,\sigma}n_{m\sigma}&+t\sum_{(m,m'),\sigma}(c^\dagger_{m\sigma}c_{m'\sigma}+\text{H.c.})\\&+J'\sum_{(m,m')}s_m s_{m'} ,\end{aligned} \tag{39}$$

where

$$J'=2\frac{T^4}{U^3}(1+2U_1/U_2)$$

and

$$t=\lambda_1 T\sin(2\alpha) .$$

For $|\varepsilon|\le T$, the exchange integral t is $\sim 0.13T$,

$$c_{m\sigma}=c^{(1)}_{m\sigma}(1-n_{m,-\sigma}),$$

s_m is the spin operator of the site m, and $n_{m\sigma}$ is the hole number operator. Here only the strongest terms of the expansion are taken into account.

In order to compare the transformed two-band model (7) and the one-band model (39) derived from it, we calculate the energy of a hole in the rigid AF-ordered spin lattice with one turned Cu spin. As it was mentioned above, in the two-band model the delocalization energy equals $0.45T$.[8] For the same parameters, the delocalization energy in the one-band model (39) equals 0.27 (for $\varepsilon\sim 4T$ one gets an energy of $\sim 0.19T$). From that we conclude that, qualitatively, the main effect of the kinetic and magnetic interactions, namely, the formation of the ferron-type hole state, is analogous in both models, although within a one-band model (39) the influence of the kinetic energy is strongly underestimated. This also explains that, in a t-J model, the ferrons (ferromagnetic hole clusters), as proposed in Ref. 8, only appear for a very large ratio $t/J\ge 19$,[26] which corresponds to $U/T\ge 6$. In contrast, in a two-band model, the ferron states already appear for $U/T\sim 3$.[4,8]

VI. CONCLUSION

In this communication we studied the interplay between magnetic interactions and the kinetic energy of holes in the CuO_2 planes of superconducting cuprates. We started from a two-band Hubbard Hamiltonian and transcribed it by two unitary transformations. The transformations are chosen in such a form that, for the assumed parameter range ($U\gg T,\varepsilon$; $4T\ge|\varepsilon|$), the series expansion of the transformed Hamiltonian converges. It turned out that, in the undoped situation, our results coincide with the commonly used results for the spin-spin interactions. In the hole-doped case, however, we could show that, taking into account the dynamical behavior of additional holes consistently, the formation of small ferromagnetic hole clusters is favored energetically.[4,8] In addition, we proved that any reduction of the two-band model to a one-band model strongly underestimates the influence of the kinetic hole energy.

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[*] Also at Institute of Physics, Estonian Academy of Sciences, Riia 142, Tartu, Estonia, 202400 U.S.S.R.

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