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Fourth-order interactions in the canonically transformed d–p model for Cu–O superconductors

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Abstract. The low-energy Hamiltonian for localized Cu spins and mobile O holes is rederived from the minimal version of the Emery model ascribed to a CuO_2 layer in high-T_c superconductors. By means of a computational algorithm the Schrieffer–Wolff transformation is performed, at large but finite Hubbard repulsion U on Cu sites, up to fourth order in the d–p (Cu–O) hopping amplitude t. The resultant interactions in $O(t^4)$ involve spin–spin superexchange, a Kondo-like spin–hole exchange opposite in sign to that in $O(t^2)$, and a Hubbard-type attraction between symmetrized O holes within a CuO_4 group. An effective t_{pp}–J_{dd}–J_{dp}–J_{pp} model is established for the special case $U = 2\epsilon$, where ϵ is the charge transfer energy.

1. Introduction

The electronic properties of a Cu–O plane, as a basic structural element of the high-T_c superconductors $La_{2-x}Sr_xCuO_4$ and $YBa_2Cu_3O_{7-y}$, can be described by the Emery model [1]. Such an approach allows us to distinguish the role of the copper (Cu) d-states and oxygen (O) p-states by assuming that strong electronic correlations exist (at least on Cu sites) and holes added by doping go predominantly to O sites. Treating the Cu–O hybridization perturbatively, a canonical transformation from the original Hamiltonian to an approximate effective one brings out the low-lying exitations in the CuO_2 layers. The Schrieffer–Wolff transformation [2] and other perturbation techniques (as used, e.g., in [3, 4]) have been applied to derive from the Emery model, or from the Anderson lattice model, a lot of spin exchange models [3–19]. The transformed models include local Cu-spins and mobile O-holes in the spin-fluctuation regime [3]; for the charge-fluctuation regime cf. [19]. The fourth-order contribution with respect to the d–p hopping amplitude, t, contains, as a standard result [20], the Cu–Cu superexchange of Heisenberg type. Additionally, there must occur [3] spin–hole, spin–spin–hole, hole–hole–spin, and hole–hole interactions in $O(t^4)$. In particular, a carrier–carrier attraction was obtained in [3]; Cu–O Kondo-like couplings with different signs arise from $O(t^4)$ in [4]. Some ambiguities in $O(t^4)$ concerning the structure of the interactions and the renormalization of the coupling parameters have motivated us to reconsider the problem.

The aim is to give a straightforward microscopic foundation of an effective model Hamiltonian for describing the interplay between magnetism and superconductivity in the Cu-spin and O-hole subsystems. Usually, the single-band strongly correlated

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Hubbard model is canonically transformed into the t–J model for high-T_c superconductivity. However, within the framework of a two-band model one can handle questions related to both Cu and O degrees of freedom. We are especially interested in an explicit expression for the superexchange parameter in dependence on the doping concentration. Further, a crucial point is how the Hubbard repulsion on Cu sites yields (among other interactions) an attraction between doped O holes.

In this paper we present the complete Hamiltonian up to fourth order in t based on the minimal version of Emery's d–p model at large but finite U (with the Hubbard repulsion strength U between d-holes). For this purpose one of us [21] has developed a computational algorithm to carry out the Schrieffer–Wolff transformation. The resulting Hamiltonian is projected onto the subspace of singly occupied Cu sites. The compact effective model found here simplifies considerably in the (not unrealistic [22–25]) case $U = 2\epsilon$, where ϵ is the charge transfer energy.

2. Schrieffer–Wolff transformation up to $O(t^4)$

The Hamiltonian for a CuO_2 layer is based on the Emery model [1] in its simplest form (in hole notation relative to a filled shell ($3d^{10}$, $2p^6$) configuration)

$$H = H_{\epsilon_d} + H_{\epsilon_p} + H_U + H_t = \epsilon_d \sum_{i\sigma} n^d_{i\sigma} + \epsilon_p \sum_{l\sigma} n^p_{l\sigma} + U \sum_i n^d_{i\uparrow} n^d_{i\downarrow} + t \sum_{i\sigma} \sum_{l(\neq i)}{}' (-1)^{\alpha_{il}} (d^+_{i\sigma} p_{l\sigma} + p^+_{l\sigma} d_{i\sigma}) \tag{1}$$

where the operator $d^+_{i\sigma}$ ($d_{i\sigma}$) creates (destroys) a hole with spin σ in the $3d_{x^2-y^2}$ orbital at the Cu site i, and $p^+_{l\sigma}$ ($p_{l\sigma}$) creates (destroys) a hole with spin σ in the $2p_x$ or $2p_y$ orbital at the O site l. The hole number operators read $n^d_{i\sigma} = d^+_{i\sigma} d_{i\sigma}$ and $n^p_{l\sigma} = p^+_{l\sigma} p_{l\sigma}$. $\sum'_{l(\neq i)}$ means summation over the four nearest-neighbour (NN) O sites around the Cu site i in the two-dimensional lattice involving one Cu and two O atoms per unit cell. ϵ_d and ϵ_p denote the atomic energies of d and p holes and U is the Hubbard interaction strength at a Cu site. The NN Cu–O hybridization amplitude t is accompanied by the phase factor [16, 17]

$$(-1)^{\alpha_{il}} = \pm 1 \qquad \text{if } \boldsymbol{R}_l = \boldsymbol{R}_i \mp \tfrac{1}{2}\boldsymbol{e}_x,\ \boldsymbol{R}_l = \boldsymbol{R}_i \pm \tfrac{1}{2}\boldsymbol{e}_y \tag{2}$$

in units of the Cu–Cu distance.

Realistic parameter values [22–25] suggest the strong-coupling regime, i.e., the d–p hopping t is assumed to be weaker than the charge transfer energy ϵ and the Coulomb repulsion U. In view of perturbation theory we consider formally the case [3, 15]

$$t \ll \epsilon,\ U - \epsilon \qquad \epsilon = \epsilon_p - \epsilon_d > 0. \tag{3}$$

Let us decompose $H = H_0 + H_1$ into the unperturbed part H_0 and the perturbation H_1 by setting

$$H_0 = H_{\epsilon_d} + H_{\epsilon_p} + H_U \qquad H_1 = H_t \tag{4}$$

according to (1). The canonical Schrieffer–Wolff transformation [2] is defined by

$$H' = e^{-S} H e^{S} = H_0 + \tfrac{1}{2}[H_1, S] + \tfrac{1}{3}[[H_1, S], S] + \tfrac{1}{8}[[[H_1, S], S], S] + \cdots \tag{5}$$

provided that the generator S satisfies the condition $H_1 + [H_0, S] = 0$. This yields

$$S = t \sum_{i\sigma} {\sum_{l(\neq i)}}' (-1)^{\alpha_{il}} \left[\frac{1}{\epsilon} - \left(\frac{1}{\epsilon} + \frac{1}{U-\epsilon} \right) n^{\mathrm{d}}_{i,-\sigma} \right] (d^{+}_{i\sigma} p_{l\sigma} - p^{+}_{l\sigma} d_{i\sigma}). \tag{6}$$

To the order of t^2 the calculation of H' from (5) by means of (1), (4), and (6) leads to

$$H'_2 = \tfrac{1}{2}[H_t, S] = H^{(2)}_{\mathrm{kin}} + H^{(2)}_{\mathrm{dp}} + H^{(2)}_{\mathrm{double}} \tag{7}$$

where

$$H^{(2)}_{\mathrm{kin}} = \frac{t^2}{\epsilon} \left(-4 \sum_i n^{\mathrm{d}}_i + \sum_{i\sigma} {\sum_{l(\neq i)}}' {\sum_{m(\neq i)}}' (-1)^{\alpha_{il}+\alpha_{im}} p^{+}_{l\sigma} p_{m\sigma} \right) \tag{8a}$$

$$\begin{aligned} H^{(2)}_{\mathrm{dp}} &= t^2 \left(\frac{1}{\epsilon} + \frac{1}{U-\epsilon} \right) \sum_{i\sigma} {\sum_{l(\neq i)}}' {\sum_{m(\neq i)}}' (-1)^{\alpha_{il}+\alpha_{im}} \\ &\quad \times (d^{+}_{i,-\sigma} d_{i\sigma} p^{+}_{l\sigma} p_{m,-\sigma} - d^{+}_{i,-\sigma} d_{i,-\sigma} p^{+}_{l\sigma} p_{m\sigma}) \qquad (8b) \\ &= 2t^2 \left(\frac{1}{\epsilon} + \frac{1}{U-\epsilon} \right) \sum_{i} {\sum_{l(\neq i)}}' {\sum_{m(\neq i)}}' (-1)^{\alpha_{il}+\alpha_{im}} \left(s_{lm} \cdot S_i - \tfrac{1}{4} n^{\mathrm{p}}_{lm} n^{\mathrm{d}}_i \right) \end{aligned}$$

$$\begin{aligned} H^{(2)}_{\mathrm{double}} &= \frac{t^2}{\epsilon} \sum_{\langle i,j \rangle \sigma} d^{+}_{i\sigma} d_{j\sigma} + \frac{t^2}{2} \left(\frac{1}{\epsilon} + \frac{1}{U-\epsilon} \right) \Bigg(8 \sum_{i\sigma} n^{\mathrm{d}}_{i\sigma} n^{\mathrm{d}}_{i,-\sigma} \\ &\quad - \sum_{\langle i,j \rangle \sigma} d^{+}_{i\sigma} d_{j\sigma} (n^{\mathrm{d}}_{i,-\sigma} + n^{\mathrm{d}}_{j,-\sigma}) + \sum_{i\sigma} {\sum_{l(\neq i)}}' {\sum_{m(\neq i)}}' (-1)^{\alpha_{il}+\alpha_{im}} \\ &\quad \times (d^{+}_{i\sigma} d^{+}_{i,-\sigma} p_{m,-\sigma} p_{l\sigma} + p^{+}_{l\sigma} p^{+}_{m,-\sigma} d_{i,-\sigma} d_{i\sigma}) \Bigg). \end{aligned} \tag{8c}$$

Here $n^{\mathrm{d}}_i = \sum_\sigma n^{\mathrm{d}}_{i\sigma}$ and $n^{\mathrm{p}}_{lm} = \sum_\sigma p^{+}_{l\sigma} p_{m\sigma}$, and $\langle i, j \rangle$ refers to the summation over all the NN Cu sites. In (8*b*) the local spin operators for d holes and the non-local spin operators for p holes are defined by

$$S_i = \frac{1}{2} \sum_{\sigma\sigma'} d^{+}_{i\sigma} \sigma_{\sigma\sigma'} d_{i\sigma'} \qquad s_{lm} = \frac{1}{2} \sum_{\sigma\sigma'} p^{+}_{l\sigma} \sigma_{\sigma\sigma'} p_{m\sigma'} \tag{9}$$

respectively, via the vector $\sigma = (\sigma_x, \sigma_y, \sigma_z)$ of the Pauli matrices. In particular, the kinetic term (8*a*) describes an effective p-hole hopping on O sites, the Kondo-like interaction (8*b*) stands for the Cu–O spin exchange, whereas (8*c*) involves doubly occupied Cu sites which will be projected out below. Note that up to $O(t^3)$ all contributions to H' resulting from (5) were given completely in [15]. Therein, however, the fourth order in t was calculated only with respect to the Cu–Cu superexchange and was not influenced by O-hole doping.

Let us outline our calculation scheme in two steps. First, we compute H' according to (5) up to $O(t^4)$. Second, we project the resulting H' onto the subspace of singly occupied Cu sites. Note that this procedure is not invertible. The projection is carried out only at the end of the calculation. This means, in particular, $H^{(2)}_{\text{double}}$ from (8*c*) as well as the $O(t^3)$ terms are projected out after having done their job in producing fourth-order contributions involving only the Cu^{2+} configuration.

We are now interested in the total H' in $O(t^4)$ projected onto the subspace of singly occupied Cu sites. The canonical transformation is performed by using the computational program COMMUT which was developed [21] in the symbolic mode of REDUCE. Additionally, the projection operator $P = \prod_i (n^{\text{d}}_{i\uparrow} - n^{\text{d}}_{i\downarrow})^2$ is applied to establish precisely the single occupation of the d-hole states. This means that Cu^{2+} should be stable under doping. Only such fourth-order terms H'_4 are retained which survive under the operation $P H'_4 P$. Furthermore, in order to prove the correctness of our computations we have checked the spin–rotational invariance of H'_4. Thus we arrive straightforwardly from (5) with (1), (4), and (6) at the following result

$$H'_4 = \tfrac{1}{8}[[[H_t, S], S], S] = H^{(4)}_{\text{kin}} + H^{(4)}_{\text{dp}} + H^{(4)}_{\text{dd}} + H^{(4)}_{\text{pp}} + H^{(4)}_{\text{ddp}} \tag{10}$$

where

$$H^{(4)}_{\text{kin}} = \frac{t^4}{\epsilon^3}\Bigg(20\sum_i n^{\text{d}}_i - 4\sum_{i\sigma}\sum_{l(\neq i)}{}'\sum_{m(\neq i)}{}'(-1)^{\alpha_{il}+\alpha_{im}} p^+_{l\sigma}p_{m\sigma} + \sum_{\langle i,j\rangle\sigma}\sum_{m(\neq i)}{}'\sum_{r(\neq j)}{}'(-1)^{\alpha_{im}+\alpha_{jr}} p^+_{r\sigma}p_{m\sigma}\Bigg) \tag{11a}$$

$$\begin{aligned} H^{(4)}_{\text{dp}} = {} & -J_{\text{dp}}\sum_{i\sigma}\sum_{l(\neq i)}{}'\sum_{m(\neq i)}{}'(-1)^{\alpha_{il}+\alpha_{im}}(d^+_{i\sigma}d_{i,-\sigma}p^+_{l,-\sigma}p_{m\sigma} - d^+_{i,-\sigma}d_{i,-\sigma}p^+_{l\sigma}p_{m\sigma}) \\ & + \tilde{J}_{\text{dp}}\sum_{\langle i,j\rangle\sigma}\sum_{l(\neq i)}{}'\sum_{r(\neq j)}{}'(-1)^{\alpha_{il}+\alpha_{jr}}(d^+_{i\sigma}d_{i,-\sigma}p^+_{l,-\sigma}p_{r\sigma} \\ & - d^+_{i,-\sigma}d_{i,-\sigma}p^+_{l\sigma}p_{r\sigma} + d^+_{j\sigma}d_{j,-\sigma}p^+_{l,-\sigma}p_{r\sigma} - d^+_{j,-\sigma}d_{j,-\sigma}p^+_{l\sigma}p_{r\sigma}) \qquad (11b) \\ = {} & -2J_{\text{dp}}\sum_i\sum_{l(\neq i)}{}'\sum_{m(\neq i)}{}'(-1)^{\alpha_{il}+\alpha_{im}}(s_{lm}\cdot S_i - \tfrac{1}{4}n^{\text{p}}_{lm}n^{\text{d}}_i) \\ & + 2\tilde{J}_{\text{dp}}\sum_{\langle i,j\rangle}\sum_{l(\neq i)}{}'\sum_{r(\neq j)}{}'(-1)^{\alpha_{il}+\alpha_{jr}}[s_{lr}\cdot(S_i+S_j) - \tfrac{1}{4}n^{\text{p}}_{lr}(n^{\text{d}}_i + n^{\text{d}}_j)] \end{aligned}$$

$$\begin{aligned} H^{(4)}_{\text{dd}} = {} & J_{\text{dd}}\sum_{\langle i,j\rangle\sigma}(d^+_{i\sigma}d_{i,-\sigma}d^+_{j,-\sigma}d_{j\sigma} - d^+_{i\sigma}d_{i\sigma}d^+_{j,-\sigma}d_{j,-\sigma}) \\ = {} & 2J_{\text{dd}}\sum_{\langle i,j\rangle}(S_i\cdot S_j - \frac{1}{4}n^{\text{d}}_i n^{\text{d}}_j) \end{aligned} \tag{11c}$$

$$\begin{aligned} H^{(4)}_{\text{pp}} = {} & -\sum_{i\sigma}\sum_{lmnr(\neq i)}{}'(-1)^{\alpha_{il}+\alpha_{im}+\alpha_{in}+\alpha_{ir}}(J_{\text{pp}} - \tfrac{1}{2}J_{\text{ddp}}n^{\text{d}}_i)p^+_{l\sigma}p^+_{m,-\sigma}p_{n,-\sigma}p_{r\sigma} \\ = {} & -\frac{1}{2}\sum_{i\sigma}\sum_{lm(\neq i)}{}'(-1)^{\alpha_{il}+\alpha_{im}}(J_{\text{pp}} - \tfrac{1}{2}J_{\text{ddp}}n^{\text{d}}_i)p^+_{l\sigma}p_{m\sigma} \end{aligned}$$

$$+\sum_{i}\sum_{lmnr(\neq i)}{}'(-1)^{\alpha_{il}+\alpha_{im}+\alpha_{in}+\alpha_{ir}}$$
$$\times (J_{pp}-\tfrac{1}{2}J_{ddp}n_i^d)(s_{lm}\cdot s_{nr}-\tfrac{1}{4}n_{lm}^p n_{nr}^p) \tag{11d}$$

$$H_{ddp}^{(4)}=J_{ddp}\sum_{(i,j)\sigma}\sum_{l(\neq i)}{}'\sum_{r(\neq j)}{}'(-1)^{\alpha_{il}+\alpha_{jr}}(d_{i,-\sigma}^{+}d_{i,-\sigma}d_{j,-\sigma}^{+}d_{j,-\sigma}p_{l\sigma}^{+}p_{r\sigma}$$
$$-d_{i\sigma}^{+}d_{i,-\sigma}d_{j,-\sigma}^{+}d_{j,-\sigma}p_{l,-\sigma}^{+}p_{r\sigma}-d_{i,-\sigma}^{+}d_{i,-\sigma}d_{j,-\sigma}^{+}d_{j\sigma}p_{l\sigma}^{+}p_{r,-\sigma}$$
$$+d_{i\sigma}^{+}d_{i,-\sigma}d_{j,-\sigma}^{+}d_{j\sigma}p_{l,-\sigma}^{+}p_{r,-\sigma}) \tag{11e}$$
$$=J_{ddp}\sum_{(i,j)}\sum_{l(\neq i)}{}'\sum_{r(\neq j)}{}'(-1)^{\alpha_{il}+\alpha_{jr}}[\tfrac{1}{4}n_i^d n_j^d n_{lr}^p+n_{lr}^p(S_i\cdot S_j)$$
$$-s_{lr}\cdot(n_i^d S_j+n_j^d S_i)+2is_{lr}\cdot(S_i\times S_j)].$$

The coupling coefficients in (11) are found to be

$$J_{dp}=8t^4\left(\frac{1}{\epsilon^3}+\frac{1}{\epsilon^2(U-\epsilon)}+\frac{1}{\epsilon(U-\epsilon)^2}+\frac{1}{(U-\epsilon)^3}\right) \tag{12a}$$

$$\tilde{J}_{dp}=\frac{t^4}{2}\left(\frac{2}{\epsilon^3}+\frac{1}{\epsilon^2(U-\epsilon)}-\frac{1}{\epsilon(U-\epsilon)^2}\right) \tag{12b}$$

$$J_{dd}=\frac{t^4}{2}\left(\frac{2}{\epsilon^3}+\frac{3}{2\epsilon^2(U-\epsilon)}-\frac{1}{2\epsilon(U-\epsilon)^2}\right) \tag{12c}$$

$$J_{pp}=\frac{t^4}{2}\left(\frac{2}{\epsilon^3}+\frac{3}{\epsilon^2(U-\epsilon)}+\frac{1}{\epsilon(U-\epsilon)^2}\right) \tag{12d}$$

$$J_{ddp}=t^4\left(\frac{1}{\epsilon^3}+\frac{1}{\epsilon^2(U-\epsilon)}-\frac{1}{\epsilon(U-\epsilon)^2}-\frac{1}{(U-\epsilon)^3}\right). \tag{12e}$$

3. Discussion of the effective Hamiltonian

Let us now turn from H' given in (5) to an effective Hamiltonian H_{eff} according to the prescription $P\,H'\,P$. Thus, the d-charge degrees of freedom are frozen-in. As a consequence, H_U and $H_{double}^{(2)}$ from (8*c*) are projected out. Moreover, it can be shown that the $O(t^3)$ terms have cancelled, since $P\,H_3'\,P=0$ with $H_3'=\frac{1}{3}[[H_t,S],S]$. In summarizing we recall (5) on the the basis of (1), (4), (7), (8*a*), (8*b*), (10), and (11*a*) to (11*e*) to get the effective Hamiltonian up to $O(t^4)$ as

$$H_{eff}=H_{\epsilon_d}+H_{\epsilon_p}+H_{kin}^{(2)}+H_{dp}^{(2)}+H_{kin}^{(4)}+H_{dp}^{(4)}+H_{dd}^{(4)}+H_{pp}^{(4)}+H_{ddp}^{(4)} \tag{13}$$

which must be supplemented by the constraint that there is exactly one hole per Cu site. Within this subspace $n_i^d=1$ holds because $P\,n_i^d\,P=P^2=P$. The model (13) includes mobile O holes and localized Cu spins. Note that all the contributions to H_{eff} survive, in view of (12), in the strong-correlation limit $U\to\infty$. The fourth-order interactions inherent in (13) are the Cu–O exchange $H_{dp}^{(4)}$ of Kondo type, the Cu–Cu superexchange $H_{dd}^{(4)}$ of Heisenberg type, the carrier–carrier correlation in $H_{pp}^{(4)}$

between the O holes, and the four-centre processes $H^{(4)}_{\mathrm{ddp}}$ between localized Cu and itinerant O spins.

The result (13) can be compared with the Hamiltonians derived from the Anderson lattice Hamiltonian by means of the canonical perturbation theory in [3] and of the canonical perturbation expansion in [4]. In particular, the coupling parameter $2J_{\mathrm{dd}}$ occuring in (11*c*) coincides, in view of (12*c*), with J_{ss} (CPT) in formula (5.3) of [3]. The factor $J_{\mathrm{pp}} - \frac{1}{2}J_{\mathrm{ddp}}$ entering (11*d*) at $n_i^{\mathrm{d}} = 1$ agrees (apart from a factor of two) with $\tilde{J}_{\mathrm{cc}}$ given in formula (4.2) of [3]. The present fourth-order interactions have a similar spin structure as those in [4] (cf. formulae (35) and (A.25) therein) but differ in the coefficients. Moreover, the O-spin operators s_{lm} defined in (9) lead to four-site contributions in contrast to the three-site restriction in [4] with local s_m.

A doping-influenced Heisenberg coupling can be deduced from the hole–spin–spin operator form $n^{\mathrm{p}}_{lr}\boldsymbol{S}_i \cdot \boldsymbol{S}_j$ in (11*e*) by averaging ($\langle\langle \ldots \rangle\rangle$) in a mean-field approximation over the p part. Introducing the mean hole number per O site as $n^{\mathrm{p}} = \langle n^{\mathrm{p}}_{ll}\rangle = \sum_\sigma \langle p^+_{l\sigma} p_{l\sigma}\rangle$ one finds from (11*e*), by restricting O-site indices to $l = r$ between i and j, together with (11*c*) the total superexchange parameter

$$\tilde{J}_{\mathrm{dd}} = 2J_{\mathrm{dd}} - n^{\mathrm{p}} J_{\mathrm{ddp}}. \tag{14a}$$

Let $\delta = 2n^{\mathrm{p}}$ be the doping concentration per unit cell (i.e., $\delta_{\max} = 4$). Then one gets from (14*a*) via (12*c*) and (12*e*) in the limit $U \to \infty$ [17]:

$$\tilde{J}_{\mathrm{dd}}\big|_{U\to\infty} = \frac{2t^4}{\epsilon^3}\left(1 - \frac{\delta}{\delta_{\max}}\right). \tag{14b}$$

Note that (14*b*) would also be valid for other definitions of δ, e.g., related to n^{p} or $4n^{\mathrm{p}}$. The NN coupling $\tilde{J}_{\mathrm{dd}}|_{U\to\infty}$ (> 0) remains antiferromagnetic in the presence of doping, also. There is no magnetic frustration with increasing O-hole concentration δ in agreement with the conclusions of [17] and [19], provided that a direct O–O overlap is absent in the original d–p model.

Representative values (in eV) for the parameters concerning the minimal version of the Emery model are, e.g., $t = 1.3$–1.5, $\epsilon = 1$, $U = 5$–6 [1]; 1.38, 4, 10 [22]; 1.3, 3.6, 10.5 [23]; 1.13, 3.3, 8.5 [24]; and 1.6, 3.4–5.9, 8.5 [25]. This means in our case that, for instance, at $\epsilon = 4$ and $U = 8$ the coupling parameter $2J_{\mathrm{dd}}$ takes acceptable values (cf. [11, 23]) for $t = 1.2$ (1.3), namely $2J_{\mathrm{dd}} = 0.1$ (0.13) (all in eV).

The range of physically realistic parameters allows us to consider the special case $U = 2\epsilon$. Then, according to (12*e*), J_{ddp} is equal to zero, so that H_{ddp} in (11*e*) exactly vanishes. To illustrate the remaining three kinds of interaction we introduce the symmetric (s) linear combination of O states around the Cu site i as [20]

$$p^{\mathrm{s}}_{i\sigma} = \frac{1}{2}\sum_{l(\neq i)}{}'(-1)^{\alpha_{il}} p_{l\sigma}. \tag{15}$$

By means of the bilinear operators

$$\begin{aligned} b^{\mathrm{pd}}_{ij} &= \frac{1}{\sqrt{2}}\left(d_{j\downarrow}p^{\mathrm{s}}_{i\uparrow} - d_{j\uparrow}p^{\mathrm{s}}_{i\downarrow}\right) \\ b^{\mathrm{dd}}_{ij} &= \frac{1}{\sqrt{2}}\left(d_{j\downarrow}d_{i\uparrow} - d_{j\uparrow}d_{i\downarrow}\right) \\ b^{\mathrm{pp}}_{ij} &= \frac{1}{\sqrt{2}}\left(p^{\mathrm{s}}_{j\downarrow}p^{\mathrm{s}}_{i\uparrow} - p^{\mathrm{s}}_{j\uparrow}p^{\mathrm{s}}_{i\downarrow}\right) \end{aligned} \tag{16}$$

we can form the d–p^s, d–d, and p^s–p^s singlet-pairings. Taking into account (15) and (16) one gets from (13) (with (1), (8*a*), (8*b*), (11), and (12)) the compact effective model at $U = 2\epsilon$:

$$H_{\text{eff}}\Big|_{U=2\epsilon} = \left(\epsilon_{\text{d}} - 4\frac{t^2}{\epsilon} + 20\frac{t^4}{\epsilon^3}\right)\sum_i n_i^{\text{d}} + \epsilon_{\text{p}}\sum_{l\sigma} p_{l\sigma}^{+} p_{l\sigma}$$
$$+ \left(4\frac{t^2}{\epsilon} - 22\frac{t^4}{\epsilon^3}\right)\sum_{i\sigma} p_{i\sigma}^{\text{s}+} p_{i\sigma}^{\text{s}} + 4\frac{t^4}{\epsilon^3}\sum_{(i,j)\sigma} p_{i\sigma}^{\text{s}+} p_{j\sigma}^{\text{s}} \qquad (17)$$
$$\left(-16\frac{t^2}{\epsilon} + 256\frac{t^4}{\epsilon^3}\right)\sum_i b_{ii}^{\text{pd}+} b_{ii}^{\text{pd}} - 8\frac{t^4}{\epsilon^3}\sum_{(i,j)}(b_{ii}^{\text{pd}+} b_{ji}^{\text{pd}} + b_{ij}^{\text{pd}+} b_{jj}^{\text{pd}})$$
$$- 3\frac{t^4}{\epsilon^3}\sum_{(i,j)} b_{ij}^{\text{dd}+} b_{ij}^{\text{dd}} - 48\frac{t^4}{\epsilon^3}\sum_i b_{ii}^{\text{pp}+} b_{ii}^{\text{pp}}.$$

Note, there appears to be a competition effect in the local p^s–d Kondo coupling. The antiferromagnetic behaviour in $O(t^2)$ acts against the ferromagnetic one in $O(t^4)$, as can be seen already from (8*b*) and from the first term of (11*b*), respectively. The last term of (17) offers an attractive p^s–p^s interaction. This local attraction between symmetrized O-hole states is of Hubbard type, cf. the first expression in (11*d*). Such an attraction can be predicted more generally since $J_{\text{pp}} - \frac{1}{2}J_{\text{ddp}} > 0$ holds for all $U > 1.44\epsilon$.

In summary, the Schrieffer–Wolff transformation was carried out to deduce, from the minimal version of the Emery model parametrized by t, ϵ, and U, an effective model in the spin-fluctuation regime for large but finite U. The limit $U \to \infty$ is involved; the special case $U = 2\epsilon$ is discussed. As a consequence of the computational program COMMUT [21] the resultant Hamiltonian H_{eff} can be established completely up to $O(t^4)$ under the constraint that the Cu sites are singly occupied. H_{eff} can be used to describe the low-energy properties of the planar Cu–O network in high-T_c superconductors. The following interactions are incorporated:

(i) different expressions of a Kondo-like Cu–O exchange with competing couplings in $O(t^2)$ and $O(t^4)$;
(ii) a spin-$\frac{1}{2}$ Heisenberg Cu–Cu superexchange, which does not change its antiferromagnetic sign under doping (no frustration);
(iii) many-site processes between localized Cu spins and itinerant O spins, which vanish only at $U = 2\epsilon$;
(iv) an attractive Hubbard-type interaction between O holes in symmetrized p states (within a CuO_4 cluster), which indicates a possible Cooper instability.

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