Comparison of effective models for CuO_2 layers in oxide superconductors

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Several effective models, as derived from a general two-band Hubbard model for CuO_2 layers in oxide superconductors, are studied. In particular, we compare the Hubbard model with the hole-spin models (unsymmetrized and symmetrized) and a generalized effective single-band (t-J) model. The exact calculation of energy spectra on a chain of four cells shows that states for a single additional hole are quite well reproduced by reduced models, taking into account the renormalization of constants. Less satisfactory is the agreement for the undoped system, especially for small charge-transfer energies. The same analytical procedure is applied to the square lattice system, where the parameters are estimated also from the levels of a single CuO_4 group. The results for quasiparticle spectra indicate that corrections to the t-J model are even smaller than in the case of the single-band Hubbard model.

I. INTRODUCTION

Due to their relevance for oxide superconductors (SC), models for strongly correlated electronic systems are at present at the center of theoretical investigations in condensed matter physics.[1] For the description of electrons in CuO_2 layers, which are the essential ingredient of SC having highest T_c, several microscopic models have been proposed and studied so far. The most realistic seems to be the Hubbard model, incorporating several bands,[2] in particular the hybridized Cu $d_{x^2-y^2}$ and O p_σ orbitals. In the following we shall restrict ourselves to the consideration of the latter model, although the physics would be quite different, if, e.g., the nonhybridizing orbitals would become essential.[3] The general Hubbard model is appropriate for the interpretation of electron spectroscopy results[4] etc., it is, however, too complicated for the model studies of quasiparticle properties and even more for the study of SC properties. A large number of orbitals per unit cell thus prevents the exact diagonalization of systems with reasonable sizes, it makes the analytical analysis less transparent, etc. Assuming that by doping the reference substance, i.e., La_2CuO_4 or $Y_2BaCu_3O_6$, the holes enter predominantly on O orbitals,[5] a coupled hole-spin model has been derived[6,7] and studied by several authors.[8–10] The advantage of this model is that it incorporates in a natural way the relevant degrees of freedom: the localized spins at Cu sites, relevant for the reference substance, and the mobile charge carrier holes. Also, it allows in principle a perturbational treatment of single- and two-hole properties, although the coupling of both degrees is not weak. Even more extensively studied is the single-band effective model, the so-called t-J model, derived originally as the representation of strongly correlated electrons in the single-band Hubbard model,[11,12] but expected to account well also for the properties of CuO_2 layers.[13] The t-J model, describing the hopping of fermions with the exclusion of doubly occupied sites, has the smallest basis of states per cell and is therefore suitable also for numerical calculations.[14] On the other hand, the model is nonperturbative in character although an expression in the transverse exchange coupling has been employed by several authors.[15–17]

Our aim is to perform a quantitative comparison of these models. We restrict ourselves to the regime of low doping, so that we in fact analyze only the models for the undoped system and the states of a single additional hole. Analytically the reduction of the initial Hubbard model to the hole-spin models can be performed within the perturbation theory[6,7] using the hybridization energy as a small parameter. Although the latter requirement is not always fulfilled, we nevertheless retain in the reduced model only the simplest invariants. The underlying idea is that higher-order perturbation corrections mainly renormalize the model parameters. We test this assumption by comparing low-lying states, as obtained for all discussed models, by the exact diagonalization of a small one-dimensional system. We show that the effective models, i.e., the hole-spin model and the t-J model, quantitatively account very well for single-hole states. In particular, the agreement remains satisfactory even for smaller charge-transfer energies, i.e., in the mixed valence regime. On the other hand, for the reference (undoped) system the mapping on the Heisenberg spin model becomes more questionable in the same regime, since results can differ even qualitatively. In this way, the value of the charge-transfer energy will be crucially needed for the proper determination of the physical regime, as also recognized by other authors.[4,7,13]

For the square-lattice case the analogous exact diagonalizations were not performed due to the exceeding numerical effort.[18,19] We, however, rely on the one-dimensional results and on the results for a single CuO_4 group,[4,13] and use them as the basis for the analytical symmetrization of the hole-spin model and the reduction to a generalized t-J model.

In Sec. II we present the models and show the relations between parameters as obtained within the perturbation analysis. Section III is devoted to the quantitative com-

parison of results for all models on a one-dimensional chain. Since the dependence on the charge-transfer energy is most pronounced, we study both the mixed valence and the charge-transfer regime. In Sec. IV models are compared for a single CuO_4 group, while the analytical procedure is repeated for a real square-lattice system. Discussion and conclusions are given in Sec. V.

II. MODELS

Assuming that in CuO_2 layers Cu $d_{x^2-y^2}$ orbitals and O p_σ orbitals are essential for the electronic properties, we adopt the *two-band Hubbard model* for such a system, as first introduced by Emery,[2]

$$H_{\rm Hubb}=-t_{pd}\sum_{(i,j)s}c_{is}^{\dagger}c_{js}+\Delta\sum_{(i\in p)}n_i+\sum_i U_i n_{i\uparrow}n_{i\downarrow}+V_0\sum_{\langle i,j\rangle}n_i n_j\ . \tag{2.1}$$

Here, operators $c_{is}^{\dagger}(c_{js})$ represent a creation (annihilation) of holes on Cu sites, i.e., on d sublattice ($i\in d$), or on the O sites ($i\in p$), respectively. The corresponding vacuum are filled electronic shells Cu d^{10} and O p^6. Terms in Eq. (2.1) can be interpreted as follows: the hybridization (t_{pd}) contribution from the hopping between neighboring sites (ij), the charge-transfer (Δ) term, the Hubbard on-site repulsion with $U_{i\in p}=U_{pp}$, $U_{i\in d}=U_{dd}$, and the intersite repulsion (V_0) term. Symbol $\langle ij\rangle$ denotes the summation over the pairs of neighboring sites. In the hybridization term we do not introduce the explicit relative phases of p-d orbitals, since they can be transformed out[9] by redefining the p sublattice operators $c_i(i\in p)$ with phase factors $\exp(i\mathbf{Q}\cdot\mathbf{R}_i)$, $\mathbf{Q}=(\pi,\pi)$.

For the undoped system (i.e., for $\bar{n}=1$/cell) with $\Delta>0$ and $U_{dd}\gg t_{pd}$ it is expected that the model (2.1) can be described by the Heisenberg model for spin degrees on Cu sites. Additional holes introduced by doping (mainly) on O sites can be however mobile, hopping between neighboring O sites since $\Delta<U_{dd}$. For this case, the mobile holes and localized spins on Cu sites are the relevant degrees of freedom and the *coupled hole-spin model*[6,7] has been derived, treating t_{pd} as the smallest quantity

$$H_{hs}=J\sum_{\langle i,j\rangle}\mathbf{S}_i\cdot\mathbf{S}_j-\tilde{t}\sum_{\substack{l,m\in i\\ i,s}}c_{ls}^{\dagger}c_{ms}+V_1\sum_{\substack{l,m\in i\\ i,s,s'}}\tfrac{1}{2}\boldsymbol{\sigma}_{ss'}\cdot\mathbf{S}_i c_{ls}^{\dagger}c_{ms'}+V_2\sum_{(l\in i)i}\mathbf{s}_l\cdot\mathbf{S}_i\ , \tag{2.2}$$

and

$$\mathbf{s}_l=\tfrac{1}{2}\sum_{s,s'}\boldsymbol{\sigma}_{ss'}c_{ls}^{\dagger}c_{ls'}\ .$$

Sites i,j now refer to the d sublattice, while $l,m\in i$ are O sites being neighbors to the ith Cu site. It should be noted that in the V_1 term we have included also the diagonal $l=m$ contribution, so that V_2 is expected to remain smaller. In Eq. (2.2) we have omitted several terms which lead only to energy shifts. Within the lowest order in t_{pd}, parameters in H_{hs} can be expressed in terms of the original ones in $H_{\rm Hubb}$,

$$J=\frac{4t_{pd}^4}{(\Delta+V_0)^2}\left[\frac{1}{U_{dd}}+\frac{2}{U_{pp}+2\Delta}\right],\qquad \tilde{t}=\frac{t_{pd}^2}{2}\left[\frac{1}{U_{dd}-\Delta-2V_0}-\frac{1}{\Delta}\right], \tag{2.3}$$

$$V_1=2t_{pd}^2\left[\frac{1}{U_{dd}-\Delta-2V_0}+\frac{1}{\Delta}\right],\qquad V_2=2t_{pd}^2\left[\frac{1}{U_{pp}+\Delta}-\frac{1}{\Delta}\right]. \tag{2.4}$$

In the realistic situation the perturbation analysis can serve only as a guide, especially in the mixed valence regime where $t_{pd}/\Delta\gtrsim 1$. The question of how well H_{hs} represents the initial $H_{\rm Hubb}$ will be discussed in Secs. III and IV.

The disadvantage of H_{hs} is that it contains two sublattices (p and d) and that the strongest hole-spin coupling is via the hole hopping (V_1) term. These problems can be eliminated by introducing ordinary Wannier functions centered on d sites corresponding to the free hole hopping ($\tilde{t}$) term. In the CuO_2 layer problem there are two such functions per cell, so that the unitary transformation to new orthogonal operators $\tilde{c}_{is}^{\gamma}$ can be generally written as

$$\tilde{c}_{is}^{\gamma}=\sum_l w_{i,l}^{\gamma}c_{ls}\ , \tag{2.5}$$

where i now refer to Cu sites. The explicit forms for $w_{i,l}^{s(a)}$ will be specified in Secs. III and IV.

The transformation of H_{hs} to new symmetrized $H_{\rm sym}$ is now straightforward. We however retain in $H_{\rm sym}$ only a few lowest terms which we will quantify later. Also we are neglecting terms involving antisymmetric $w_{i,l}^{a}$ orbitals that will be justified in Sec. IV. So we denote $\tilde{c}_{is}^{s}\equiv\tilde{c}_{is}$ and get the *symmetrized hole-spin model*

$$H_{\rm sym}=J\sum_{\langle i,j\rangle}\mathbf{S}_i\cdot\mathbf{S}_j-t_0\sum_{(i,j)s}\tilde{c}_{is}^{\dagger}\tilde{c}_{js}+V\sum_i\tilde{\mathbf{s}}_i\cdot\mathbf{S}_i+V'\sum_{(i,j)}\tilde{\mathbf{s}}_j\cdot\mathbf{S}_i+t_1\sum_{(i,j)s,s'}\tfrac{1}{2}\boldsymbol{\sigma}_{ss'}\cdot\mathbf{S}_i(\tilde{c}_{is}^{\dagger}\tilde{c}_{js'}+\tilde{c}_{js}^{\dagger}\tilde{c}_{is'})+t_2\sum_{\substack{(i,j\neq k)\\ s,s'}}\tfrac{1}{2}\boldsymbol{\sigma}_{ss'}\cdot\mathbf{S}_i\tilde{c}_{js}^{\dagger}\tilde{c}_{ks'}\ , \tag{2.6}$$

where the last term represents the hopping between next-nearest-neighbor (NNN) cells jk through the intermediate cell i. All summations are now only over cell indices i,j,k. The largest term is expected to be the Kondo coupling (V) term,

whereas the holes move via the free hopping (t_0) term and the spin-dependent (t_1) term.

When V is large a reduction to the subspace of mobile singlets is natural.[13] The local singlet state, formed out of the local d hole and the symmetrized p hole, can be used as a new vacuum

$$|\tilde{0}_i\rangle = \frac{1}{\sqrt{2}}(\tilde{c}^\dagger_{i\uparrow}c^\dagger_{i\downarrow} - \tilde{c}^\dagger_{i\downarrow}c^\dagger_{i\uparrow})|0\rangle \ . \tag{2.7}$$

Neglecting the participation of the higher-energy triplet state, the $H_{\rm sym}$ can be now rewritten solely in terms of d (Cu site) fermions hopping from the site j onto empty sites $|\tilde{0}_i\rangle$, the process being a representation of the exchange of the singlet between cells i,j. We thus obtain the *generalized t-J model*

$$H_{tJ} = J\sum_{\langle i,j\rangle}\mathbf{S}_i\cdot\mathbf{S}_j - t\sum_{(i,j)s} d^\dagger_{is}d_{js} - t'\sum_{(j,k)s} d^\dagger_{js}d_{ks} + \zeta\sum_{(i,j\neq k)ss'} \tfrac{1}{2}\boldsymbol{\sigma}_{ss'}\cdot\mathbf{S}_i d^\dagger_{js}d_{ks'} \tag{2.8}$$

with $d^\dagger_{is} = c_{is}(1-n_{i-s})$ operators satisfying the requirement of, at most, singly occupied sites. In Eq. (2.8) we included the NNN hopping terms, i.e., the (t') spin-independent hopping between NNN sites (j,k) and the (ζ) hopping dependent on the intermediate spin $\mathbf{S}_i$. Within the lowest-order parameters in the H_{tJ} model can be related to those in Eq. (2.6) by calculating new matrix elements taking into account the redefined local vacuum, Eq. (2.7). However, we can evaluate also the contributions of the second-order processes, where the intermediate state is the local triplet state, formed by the d hole and the p hole, an energy V above the local singlet state. The procedure of the calculation is in principle identical to that used in deriving the hole-spin model. The result is

$$t = -\tfrac{1}{2}t_0 - \tfrac{3}{4}t_1, \quad t' = -\frac{3}{4}\frac{\bar{t}^2}{V}, \quad \zeta = \tfrac{1}{2}t_2 - \frac{\bar{t}^2}{V} \ , \tag{2.9}$$

where $\bar{t} = 1/\sqrt{2}(t_0 + \frac{1}{2}t_1)$. It should be noted that the sign is reversed in hopping terms due to the exchanged role of mobile fermions in the models (2.6) and (2.8).

III. ONE-DIMENSIONAL SYSTEMS

In order to perform the quantitative comparison of different models, introduced in Sec. II, we first study the $d=1$ system on a chain. We expect that relations between parameters of discussed models would not be crucially dependent on the dimensionality of the lattice, although the final physical behavior of $d=1$ and $d=2$ systems would be essentially different. We adopt the view that effective models should reproduce as well as possible the low-energy properties of the original Hubbard model. Hence we compare directly the low-energy spectra and the character of states, as obtained by the exact diagonalization of small systems. In particular, we choose the chain of $N_0=4$ cells, where the number of low-lying energy levels is still reasonable. It should be noted that in $d=1$ the models correspond to a system of the CuO chain with a single O p orbital per cell.

The first question is how well is the Hubbard model, Eq. (2.1), represented by the Heisenberg spin Hamiltonian for the undoped system, i.e., for $N_h=4$ holes (fermions) in our case. In the following we fix some parameters in the model (2.1) to realistic values;[2,4] in particular, we take $t_{pd}=1.4$ (eV), $U_{dd}=7$, and $U_{pp}=1$. Here and further on we express all quantities in units of eV. Since Δ is not known reliably enough[4] and moreover it influences substantially the results, we treat several values $0<\Delta<4$ corresponding to regimes of mixed valence $\Delta \gtrsim 0$ as well as to the charge-transfer regime $t_{pd} \ll \Delta \lesssim U_{dd}$. We considered as well the dependence on the repulsion $0<V_0<1$ and $0<U_{pp}<4$; however, no significant effects were found for the undoped system nor for the spectra of a single added hole, so we discuss in the following mainly the $V_0=0$ and $U_{pp}=1$ results.

The lowest-lying energy levels of the Hubbard model of $N_h=4$ on a chain of $N_0=4$ cells are represented in Fig. 1, shown relative to the spin singlet $S=0$, $q=0$ ground state. At larger $\Delta \approx 4$ the levels map very well on those of the Heisenberg model, which would be for $N_0=4$ just equidistant with an energy difference $\Delta E = J$, while $S=1$, $q=\pm\pi/2$ and $S=0$, $q=\pi$ levels would be degenerate. The best-fitted value $J=0.2$ is however smaller than the perturbative result (2.3) with $J=0.35$. The mapping on the Heisenberg model becomes substantially worse on decreasing Δ. The level scheme is very perturbed in the mixed valence regime $\Delta<2$, also the values obtained for the exchange coupling $J>0.35$ are quite unphysical. Finally at $\Delta \to 0$ even the character of the ground state changes since the $S=1$, $q=\pi$ state appears to have the lowest energy and an explanation for this effect is still lacking. It should be noted that at smaller $\Delta<2$ a substantial improvement cannot be achieved even by including the next-neighbor interactions $\mathbf{S}_i\cdot\mathbf{S}_{i+2}$ in the Heisenberg model. Hence corrections beyond the two-spin interaction are needed, which makes the mapping on a spin model less useful. It should, however, be stressed that the disagreement between the levels of the general Hubbard model and those of effective models appear to be the largest for the undoped system. Since the experiments yield for the CuO_2 layers $J \approx 0.1$ eV,[20] this would be an indication that the system is in the charge-transfer regime $\Delta \gg t_{pd}$ (due possibly to smaller effective t_{pd}) or that the coupling J as determined from the low-energy spectra differs from J as would be obtained from high-energy spin excitations. Hence a proper understanding of the undoped system is still needed.

Let us proceed to the comparison of low-energy spectra for a doped system with one *single additional hole*, $n_h=1$. In Figs. 2 and 3 we present the results for different models corresponding to two charge-transfer energies $\Delta=4$ and 2, respectively, for a system of $N_0=4$

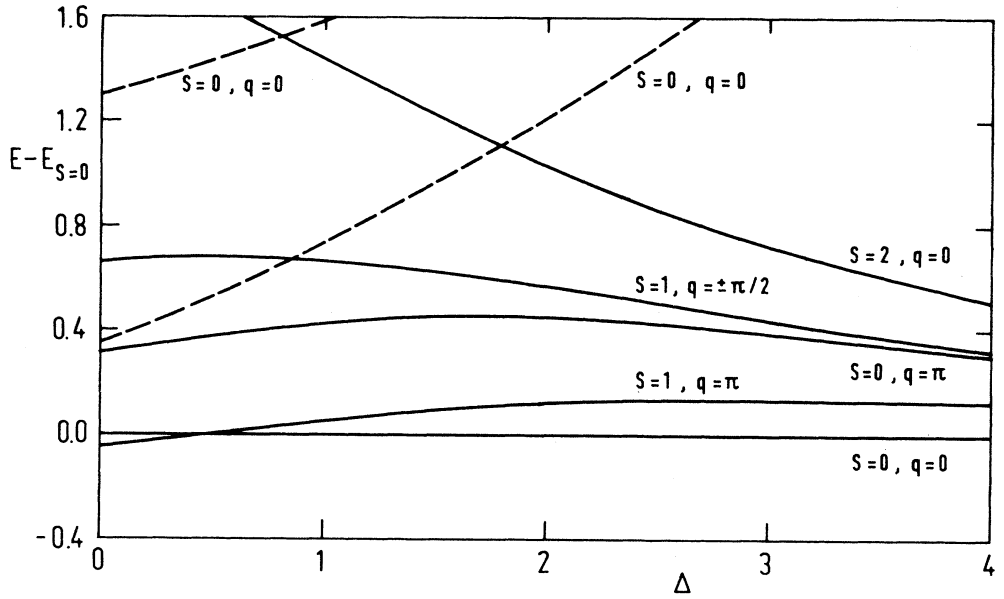

FIG. 1. The lowest-lying energy levels of H_{Hubb} for $N_h=4$ holes on a chain of $N_0=4$ cells, shown relative to the $S=0$, $q=0$ state.

cells. The energies are given relative to the lowest energy state for such a system. In the Hubbard model (2.1) the diagonalization is thus performed for $N_h=5$ holes and only the lowest-lying branches with total spins $S=\frac{1}{2},\frac{3}{2},\frac{5}{2}$ are shown. Comparing Figs. 2(a) and 3(a) we notice that differences between $\Delta=4$ and 2 cases are merely quantitative. Thus the energy scale is somewhat expanded for $\Delta=2$, whereas the pairs of excited states with $S=\frac{1}{2}$ and $\frac{3}{2}$ tend to merge as $\Delta\to 0$. In both cases the ground state appears to be $S=\frac{1}{2}$, $q=\pi/2$.

In Figs. 2(b) and 3(b) the spectra for a single hole $n_h=1$ in the hole-spin model (2.2) are presented. Here, J has been fixed from the analysis of the undoped system, i.e., $J=0.2$ ($\Delta=4$) and $J=0.35$ ($\Delta=2$), while other parameters have been chosen so that the spectra would fit best to those of the Hubbard model. From the figures we

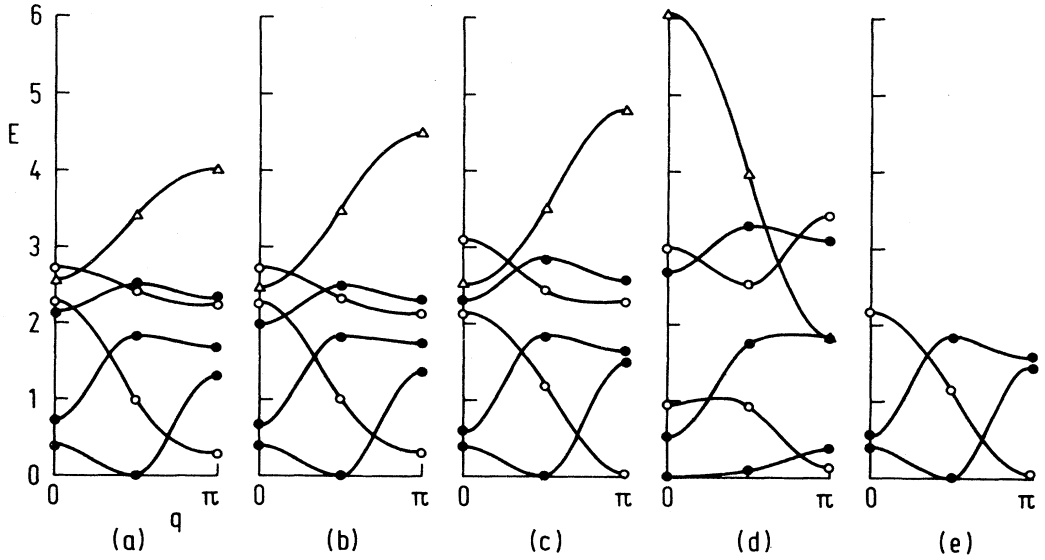

FIG. 2. The lowest-lying branches for a system of $N_h=5$ holes on a chain of $N_0=4$ cells for different models corresponding to charge-transfer energy $\Delta=4$. ● represent the $S=\frac{1}{2}$ energy levels; ○ correspond to the $S=\frac{3}{2}$, and △ to the $S=\frac{5}{2}$ levels, respectively. The solid lines between the points are only a guide to the eye. (a) Hubbard model; (b) hole-spin model; (c) symmetrized hole-spin model; (d) Kondo-lattice model; (e) generalized t-J model.

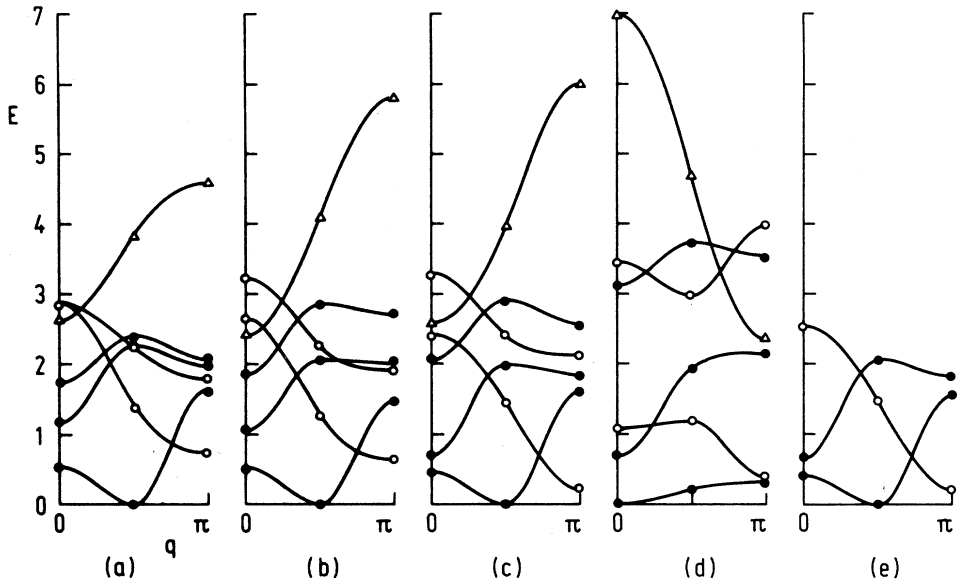

FIG. 3. The same as in Fig. 2 but for the mixed valence regime $\Delta=2$.

see that indeed a satisfactory qualitative and quantitative agreement can be reached, especially for larger $\Delta=4$. The parameters which were used are presented in Table I, where in the parentheses we give the perturbation analysis results, Eqs. (2.3) and (2.4). The perturbation results for parameters remain qualitatively correct in spite of t_{pd}/Δ and $t_{pd}/(U_{dd}-\Delta)$ not being small;[19,21] however, the values are substantially renormalized due to higher-order effects. This is evident for the largest and the most important V_1 coupling, which is reduced by $\approx 40\%$.

Wannier functions (2.5) for the symmetrized model can be given explicitly for the chain (of infinite length)

$$w_{i,l}=\frac{1}{N}\sum_k e^{ik(R_l-R_i)}=\frac{\sin\pi(R_l-R_i)}{\pi(R_l-R_i)}\ , \tag{3.1}$$

where l and i refer to the p and d sites, respectively. Hence parameters in the symmetrized hole-spin model (2.6) can be expressed as

$$t_0=\tilde{t},\quad t_1=\frac{8}{3\pi^2}(2V_1+V_2),\quad t_2=\frac{8}{9\pi^2}(2V_1-3V_2)\ , \tag{3.2}$$

$$V=\frac{8}{\pi^2}(2V_1+V_2),\quad V'=\frac{8}{9\pi^2}(2V_1+5V_2)\ . \tag{3.3}$$

The parameter set used in Figs. 2(c) and 3(c), which is giving the best agreement with original spectra, is presented in Table II. In parentheses we present the values (if they are not the same) obtained from Eqs. (3.2) and (3.3). The difference between calculated and fitted t_1, t_2 can be to a large extent attributed to finite-size effects, since Wannier functions (3.1) are defined for $N_0\to\infty$ system. As seen from Figs. 2(b) and 2(c) and Figs. 3(b) and 3(c), the terms left out in Eq. (2.6) clearly do not disturb the agreement between unsymmetrized and the symmetrized model. It should be also noted that the hopping is still dominated by the spin-dependent t_1 term. Spin-flip hopping is also the reason why spectra are less satisfactorily reproduced by the *Kondo lattice model*,[6,8,10] where one takes into account only the local interaction V and an effective free-hole hopping $t_0^{\rm eff}$, but $V'=t_1=t_2=0$. Here we fix the parameter $t_0^{\rm eff}=t_0+\frac{3}{2}t_1\approx 1.1$ so that from Eq. (2.9), both the symmetrized hole-spin model (2.6) and the Kondo lattice model, give the same value of t in the t-J model. Within the Kondo lattice model the differences between branches remain qualitatively correct, see Figs. 2(d) and 3(d), still the $\mathbf{q}$ dependences are quite perturbed. In particular, a $\mathbf{q}=0$ state appears to be of the lowest energy in the relevant parameter regime.

The t-J model can reproduce only a few lowest branches due to the very restricted basis set. It misses, especially for $\Delta\le 2$, nearly degenerate partner branches with $S=\frac{1}{2}$ and $S=\frac{3}{2}$. Still it reproduces very well the lowest quasiparticle branch, see Figs. 2(e) and 3(e), with

TABLE I. The parameters of H_{hs} which were used in Figs. 2(b) and 3(b). (In the parentheses are given the perturbation analysis values.)

Δ	$\tilde{t}$	V_1	V_2
4	−0.15 (0.08)	1.4 (2.29)	−0.2 (−0.20)
2	−0.35 (−0.29)	2.0 (2.74)	−0.9 (−0.65)

TABLE II. The parameters of $H_{\rm sym}$ used in Figs. 2(c) and 3(c). [In the parentheses are presented the values obtained from Eqs. (3.2)and (3.3).]

Δ	t_0	t_1	t_2	V	V'
4	−0.15	0.85 (0.70)	0.2 (0.31)	2.2	0.16
2	−0.35	1.0 (0.84)	0.3 (0.63)	2.5	−0.05

the values consistent with Eq. (2.9), i.e., $t=-0.56$, $\zeta=0.08$ for $\Delta=4$, and $t=-0.58$, $\zeta=0.14$ for $\Delta=2$, while in both cases $t'\approx 0$.

It should be noted that second-order corrections in Eq. (2.9) are very small. This is not so much the effect of substantial V, but rather of a very small NN hopping matrix element $\bar{t}$ between the spin singlet and the spin triplet state. So we get from Table II, but also from perturbation results Eqs. (2.3), (2.4), and Eq. (3.2) that $|\bar{t}| \ll |t|$ which can be attributed to quite different role of the spin-flip hopping in $\bar{t}$ and t processes and the destructive interference between both types of hopping contributions to $\bar{t}$. Second-order contributions should be compared to those obtained from the reduction of the corresponding single-band Hubbard model, where $\zeta \approx J \gg \bar{t}^2/V$.[11,15] Our $d=1$ results thus seem to indicate that the two-band Hubbard model is nearer to the t-J model (comparing the single quasiparticle properties) than the single-band Hubbard model, which is consistent with some limiting cases.[22]

IV. PLANAR SYSTEM

In a planar system corresponding to the CuO_2 network the possibilities for the exact diagonalization studies are very restricted. A corresponding Hubbard model on a $N_0=4$ cell would be already on the computation limit.[18,19] We, however, expect that the relation between the Hubbard model (2.1) and the hole-spin model (2.2) remains similar as in the one-dimensional case.

In order to show this quantitatively we perform the calculation for a single CuO_4 cluster with a free boundary condition. Although this system is rather trivial and cannot be used to determine J, still we gain some information on the single hole states for both models.[4] For such a system the hole-spin model can be written in the following form:

$$H_{CuO_4} = -4\tilde{t} n_{(s)} + (4V_1 + V_2)\mathbf{s}_{(s)}\cdot\mathbf{S} + V_2(\mathbf{s}_{(d)} + \mathbf{s}_{(p_x)} + \mathbf{s}_{(p_y)})\cdot\mathbf{S} , \quad (4.1)$$

where (s,d,p_x,p_y) stand for symmetrized orbitals formed out of four O p orbitals in the CuO_4 group. Comparing energy levels, obtained by the exact diagonalization of the Hubbard model for the cluster with those obtained from Eq. (4.1), one can uniquely determine the parameters needed for the hole-spin model, Eq. (2.2). The results are presented in Table III. In order to construct the symmetrized model, Eq. (2.6),we define usual Wannier functions, as determined by the free-hole hopping ($\tilde{t}$) term in Eq. (2.2). The corresponding band energies are

TABLE III. The parameters of the hole-spin model H_{CuO_4} as obtained from the results of exact diagonalization of Hubbard model for the CuO_4 cluster.

Δ	$\tilde{t}$	V_1	V_2
4	−0.10	1.05	−0.09
2	−0.23	1.08	−0.14

$$\varepsilon_{ks} = -2\tilde{t}(\cos k_x + \cos k_y + 1) , \quad (4.2)$$

for the symmetric band and $\varepsilon_{ka}=2\tilde{t}$ for the asymmetric band. The wave functions $w_{i,l}^{s(a)}$, Eq. (2.5) are given by

$$w_{i,t}^{\gamma} = \frac{1}{N}\sum_{\mathbf{k}} a_{l\gamma}(\mathbf{k}) e^{i\mathbf{k}\cdot(\mathbf{R}_l - \mathbf{R}_i)} , \quad (4.3)$$

where $\mathbf{R}_i$ refer to symmetrized (Cu) sites, while $a_{l\gamma}$ still depend on the index of the O atom in the cell, i.e.,

$$a_{1s}(\mathbf{k}) = \xi(\mathbf{k})\cos\left[\frac{k_x}{2}\right], \quad a_{2s}(\mathbf{k}) = \xi(\mathbf{k})\cos\left[\frac{k_y}{2}\right], \quad (4.4)$$

$$a_{1a}(\mathbf{k}) = -a_{2s}(\mathbf{k}), \quad a_{2a}(\mathbf{k}) = a_{1s}(\mathbf{k}) , \quad (4.5)$$

and

$$\xi(\mathbf{k}) = \left[\cos^2\left[\frac{k_x}{2}\right] + \cos^2\left[\frac{k_y}{2}\right]\right]^{-1/2} .$$

s Wannier functions defined in this way are in fact identical to those used by Zhang and Rice.[13] They are presented in Fig. 4. It is seen that they are well localized, i.e., much stronger than in a $d=1$ chain, Eq. (3.1).

The transformation to a symmetrized model is now straightforward. A general conclusion is that there is only a weak coupling between s and a hole orbitals; e.g., the largest term comes from the V_2 term in Eq. (2.2) and the coupling strength can be estimated to remain below the value ≈ 0.2. Hence, these terms do not seem to be essential and we neglect them further on. For the s orbital we get by using Eqs. (4.4) and (4.5)

$$t_0 = \tilde{t}, \quad t_1 = 0.54V_1 + 0.13V_2, \quad t_2 = 0.078V_1 , \quad (4.6)$$

$$V = 3.67V_1 + 0.92V_2, \quad V' = 0.078V_1 + 0.24V_2 . \quad (4.7)$$

For our particular values obtained from the levels of the CuO_4 cluster are parameters given in the Table IV, while in the parentheses results from the $d=1$ fit are presented. Although the Kondo coupling V is quite strong, it is still essentially smaller than U_{dd} and moreover smaller than the free-hopping effective bandwidth $W \approx 8t_0^{\text{eff}}$ in the corresponding Kondo model. The definition of the appropriate bandwidth W in the general hole-spin model, Eq. (2.6), is however more involved. Still W is expected to be substantially smaller, i.e., $W < 8t_0^{\text{eff}}$.

The reduction to the t-J model now follows Eq. (2.8). The parameters as given by $t=-0.48$, $\zeta=0.05$ for $\Delta=4$ and $t=-0.55$, $\zeta=0.08$ for $\Delta=2$ while $t'\approx 0$. Again, corrections to the prototype t-J model are very small. In a planar lattice a possibility of a direct p-p hopping should be also considered. The corresponding matrix element has been estimated to $t_{pp} \lesssim 0.5$ eV.[4] This process affects the NN hopping, i.e., it increases t, but the main qualitative difference is in a much stronger NNN hopping t'. In fact, we get $\Delta t = -0.28t_{pp}$ and $\Delta t' = +0.06t_{pp}$ for NNN neighbors along the diagonal, i.e., at distance $R=\sqrt{2}a_0$ (a_0 being the unit cell length) while $\Delta t' = -0.065t_{pp}$ for the NNN hopping along the direction with the distance $R=2a_0$.

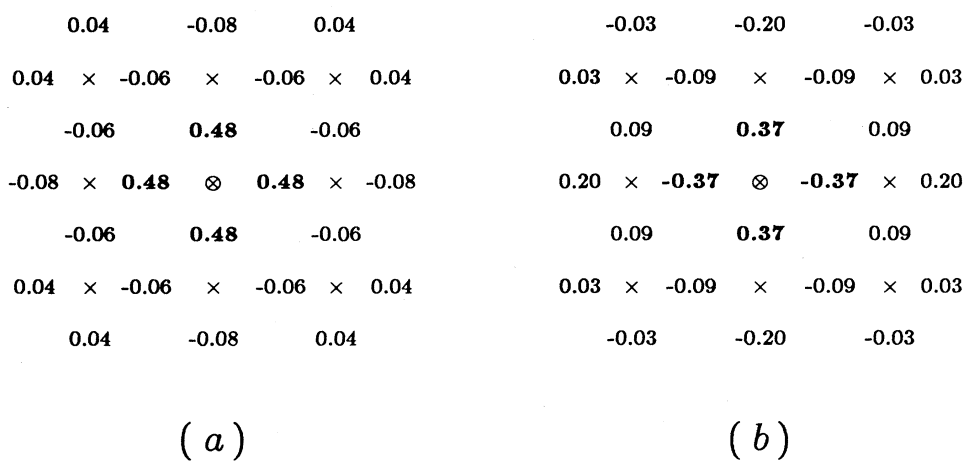

FIG. 4. The values of $w^s_{i,l}$ and $w^a_{i,l}$ on the O sites represent (a) symmetric and (b) antisymmetric Wannier functions centered around Cu site ⊗.

V. CONCLUSIONS

In this paper we have studied the relations between different models, which have been introduced to describe the electronic properties of CuO_2 layers in oxide SC. The comparison is based on the calculations performed mainly for a single mobile quasiparticle (hole) introduced into the reference system. In this way we have not touched the question of the quasiparticle interactions relevant for the SC properties. However, the underlying motivation is that the presumable attraction is not a local hole-hole interaction but is rather mediated through the low-energy excitations of the reference system. Then the effective models as described in Sec. II can be used as a good starting point for the study of the hole binding[8–10,14,16,18] and of possible SC pairing[11,12] under the condition that models adequately describe quasiparticle properties.

Our exact diagonalization results for a finite CuO_2 chain show that spectral properties of a single mobile quasiparticle in a general Hubbard model can be well reproduced by reduced effective models, i.e., by the hole-spin model (unsymmetrized and symmetrized) and by the generalized t-J model. This remains valid even in the mixed valence regime (with $\Delta \approx t_{pd}$),[21] where the straightforward derivation of the hole-spin model is not possible due to the breakdown of the perturbation expression using t_{pd} as a small parameter.

Numerical results for a chain and for a single CuO_4 cluster in a planar lattice show that parameters for a hole-spin model should be substantially renormalized relative to their value obtained via the perturbation analysis. This is especially evident for the most important (symmetrized) Kondo coupling, which is reduced by $\lesssim 50\%$. The hopping in the symmetrized hole-spin model is predominantly a spin-dependent one. This is also the reason why the simple Kondo-lattice model, assuming only a free-hole hopping, misses some quasiparticle properties. Other terms in $H_{\rm sym}$ seem to be less important. In particular, very weak is the (V') term which has been claimed to induce a strong FM coupling[9] between the Cu spins $\mathbf{S}_i$ around a static hole. An apparent reduction of this term relative to the unsymmetrized model is, even in $d=1$, due to the enhancement of the local Kondo coupling, which agrees with the arguments by Zhang and Rice.[13] Although we have shown that the prototype t-J model can describe well the same quasiparticle properties, there are still some conceptual and possibly technical advantages of the hole-spin models, especially in the regime of not too small J. Thus one can get a qualitatively adequate description of the lowest quasiparticle bands (with a nontrivial $\mathbf{q}\neq 0$ ground state) by using a simple picture of a free-hole hopping in a Néel spin background.

Our results confirm that the t-J model represents very well the low-energy properties of the original model. Our focus was on the possible influence of invariants added to the simple t-J model.[19] We could introduce additional terms representing perturbed (Cu) spin correlations around the singlet. Again due to small $V' \ll V$ these corrections appear negligible. We found as relevant only the NNN hopping contributions, spin-dependent and spin-independent ones. It is, however, to some extent surprising that these contributions are even smaller as they would arise from straightforward reduction of a singe-band Hubbard model. This agrees with a recent finding, that in a certain regime the model can be exactly mapped on the t-J model.[22] The origin of this phenomenon in our derivation is less clear. It can be attributed to the fact that due to a particular coherence the

TABLE IV. The parameters of $H_{\rm sym}$ obtained from the levels of the CuO_4 cluster. (In the parentheses are presented results from the $d=1$ fit.)

Δ	t_1	t_2	V	V'
4	0.56 (0.73)	0.08 (0.11)	3.77 (4.95)	0.06 (0.06)
2	0.57 (0.96)	0.09 (0.16)	3.83 (6.51)	0.05 (−0.06)

local singlet has a substantially reduced NN hopping matrix element into the local triplet state. The NNN hopping contributions are, however, enhanced if one takes into account also the direct p-p hopping. These terms are weak, e.g., $|t'|<0.1|t|$, still their influence on the quasiparticle coherent mass as well as on the hole binding can be quite strong at smaller J, as found in a recent numerical study.[23] Whether these terms can yield an essential difference between the quasiparticle pairing in the two-band Hubbard model and in the single-band Hubbard model, is not yet clear. It should be however noted that our analysis of quasiparticle spectra is strictly unique only within the second-order perturbation analysis in t_{pd}, so that the determination of higher-order terms like t' and ζ remains less reliable.

The essential discrepancy between the original Hubbard model and reduced models appears in the properties of the reference (undoped) system. On reducing Δ to the mixed valence regime Heisenberg model even qualitatively fails to reproduce the excitation spectra. In view of the experimentally determined rather small value $J=0.1$ eV,[20] our results could again be an indication that the real system is in the charge-transfer regime $\Delta \gg t_{pd}$ or that models still miss some degrees of freedom which would lead to reduction of the exchange coupling.

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