Exact-diagonalization study of electron-lattice coupling in the effective two-band t-J model

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The effective two-band t-J Hamiltonian for holes in Cu-O planes of cuprates is obtained from the three-band Hubbard Hamiltonian. In this model a doped oxygen hole together with two neighboring copper holes is treated as a composite spin-$\frac{1}{2}$ three-sites particle. The model is studied by exact diagonalization in a $Cu_{16}O_{32}$ square cluster. Both binding energy and hole-hole correlation function indicate that two holes bind together for $J/t>0.11$ and are predominantly located on the next-nearest oxygen sites in the same Cu-O chain. Electron-phonon interaction is studied in the adiabatic phonons approximation. Copper $(\pi,0)$ ''half-breathing'' mode is shown to couple strongly to doped holes and increase the hole-hole correlation as well as the binding energy. These results are compared with experimental data. [S0163-1829(98)01538-0]

I. INTRODUCTION

A large number of experimental observations on the superconducting cuprates indicate that the lattice effects in the systems with strong electron correlation are unusual, and may even be playing a role in the high-temperature superconductivity.[1–10] In particular, the strong softening of longitudinal-optical (LO) phonon modes with hole doping[2,3] is a matter of great interest, since the inelastic neutron-scattering data[4] show that the dispersion of this mode changes significantly at low temperatures leading to local unit-cell doubling in the CuO_2 planes, suggesting dynamic short-range charge ordering. The numerical studies[11,12] of the Holstein-Hubbard and Holstein t-J models indicate the existence of a subtle interplay between electron-electron and electron-phonon (el-ph) interactions. In particular, it was shown that the critical el-ph coupling for the small polaron formation is substantially reduced due to the charge carriers ''prelocalization'' in the antiferromagnetic spin background.

Systems with strong electron-electron correlation are most commonly described by the Hubbard Hamiltonian that can be reduced in certain limits to the t-J Hamiltonian. The latter is simple enough for numerical diagonalization to be carried out on sufficiently large clusters, up to 20 cites for two-doped holes.[13–15] In the t-J Hamiltonian a hole in the Cu d orbital and a hole in the symmetrized O p orbital are treated as a composite spin zero particle, the Zhang-Rice singlet.[16] By construction, such a state is symmetric and centered on Cu. However, this may be an oversimplification, since a doped hole primarily resides on oxygen sites in the CuO_2 unit cell and there is no *a priori* reason to view its ground state (GS) centered around a copper ion. This is especially true if there is more then one doped hole in the system and/or there exists a charge ordering on the rows of *oxygen ions* as suggested in the recent result.[4] In order to make the t-J model more realistic in this paper we propose its two-band version, which at the same time is compact enough to carry out numerical studies on large clusters. Another advantage of this model is that the effect of different lattice distortion patterns in cuprates can be incorporated explicitly by changing the corresponding t and J values in the Hamiltonian.

II. HAMILTONIAN

To obtain a simple two-band model we first follow the work by Ogata and Shiba[17] (OS) and start from the three-band Hubbard Hamiltonian:

$$H_{\mathrm{Hubb}}=H_0+H_{\mathrm{hop}},$$

$$H_0=\varepsilon_d\sum_{i,\sigma} n_{d\sigma i}+\varepsilon_p\sum_{j,\sigma} n_{p\sigma j}+U_d\sum_i n_{di\uparrow}n_{di\downarrow}$$

$$+U_p\sum_j n_{pi\uparrow}n_{pi\downarrow}, \tag{1}$$

$$H_{\mathrm{hop}}=-t_{pd}\sum_{\langle i,j\rangle,\sigma} d^{+}_{\sigma i}p_{\sigma j}+\mathrm{H.c.},$$

where $d_{\sigma i}$ and $p_{\sigma j}$ are hole annihilation operators for Cu ith and O jth sites correspondingly. The summation is taken over the first-neighbor Cu-O bonds and σ denotes two possible spin orientations. On each Cu and O site there can be two (opposite spins), one (spin up or down) or zero holes, which together with the cluster size and the number of spin-up and spin-down holes define the Hilbert space of the model. Next we truncate that Hilbert space to a subspace in which copper sites are always occupied by a single hole and all additional holes are doped on oxygen sites. In the zeroth-order approximation ($H_{\mathrm{hop}}=0$) this space forms the basis of a degenerate GS, while the rest of the configurations of the original Hilbert space are treated as excited states. The hopping term in the three-band Hubbard Hamiltonian (t term) is considered as a small perturbation, so that the perturbation theory can be applied to obtain a simplified effective model:

$$H_{\mathrm{eff}}=\varepsilon_d N_{\mathrm{Cu}}+\varepsilon_p n_h+H^{(2)}_{\mathrm{Cu-chtr}}+H^{(2)}_{\mathrm{Cu\text{-}O}}+H^{(2)}_{\mathrm{O\text{-}hop}}+H^{(4)}_{\mathrm{Cu\text{-}Cu}}, \tag{2}$$

where N_{Cu} is the number of Cu sites and n_h is the number of doped O holes. To the second order in t_{pd} one obtains the Cu charge-transfer term (Cu hole hopping to the nearest O site and back):

$$H^{(2)}_{\text{Cu-chtr}} = -(4N_{\mathrm{Cu}} - n_h)\,\frac{t_{pd}^2}{\Delta}, \tag{3}$$

the Cu-O exchange term:

$$H^{(2)}_{\text{Cu-O}} = \sum_{\langle i,j\rangle} 2\left(\frac{t_{pd}^2}{U_p+\Delta} + \frac{t_{pd}^2}{U_d-\Delta}\right)\left(\mathbf{S}_i\cdot\mathbf{S}_j - \frac{1}{4}\,n_{pj}\right) \tag{4}$$

and the O-hole first-nearest neighbor ($j \to k$) hopping terms:

$$H^{(2)}_{\text{O-hop}} = \sum_{\langle i,j,k\rangle,\sigma} (t_1+t_2)\,d^{+}_{\sigma i}d_{-\sigma i}p^{+}_{-\sigma k}p_{\sigma j} - (t_2 n_{d-\sigma i} - t_1 n_{d\sigma i})\,p^{+}_{\sigma k}p_{\sigma j} + \text{H.c.}, \tag{5}$$

where $t_1 = t_{pd}^2/\Delta$ and $t_2 = t_{pd}^2/(U_d-\Delta)$. Out of many fourth-order terms only the Cu-Cu superexchange:

$$H^{(4)}_{\text{Cu-Cu}} = \sum_{\langle i,i'\rangle} 4\left(\frac{t_{pd}^4}{\Delta^2 U_d} + \frac{2t_{pd}^4}{\Delta^2(2\Delta+U_p)}\right)\left(\mathbf{S}_i\cdot\mathbf{S}_{i'} - \frac{1}{4}\right) \tag{6}$$

plays an important role, since all the rest engage O holes and therefore give a small input if the concentration of doped holes is low. Here $\Delta = \varepsilon_p - \varepsilon_d > 0$ is the charge-transfer energy and one of the varied parameters.

After the effective Hamiltonian is obtained, OS apply it to Cu_4O_8, Cu_8O_{16}, and $Cu_{10}O_{20}$ clusters doped with 0, 1, and 2 holes, assuming $U_p = 0$. The first important conclusion follows from the comparison of their results for H_{eff} with those given by the original Hubbard model in a Cu_4O_8 cluster. It follows that the effective Hamiltonian reproduces the results of the Hubbard model quite closely for $\Delta > 3.5$ eV. For lower values of Δ H_{eff} becomes increasingly divergent, which is natural, since H_{eff} was obtained in the assumption of $t/\Delta \ll 1$. Since the experimental value of Δ is in the range of 2–4 eV for cuprates this divergence is of concern, while it does not stop us from proceeding carefully. The second important result concerns the state of doped holes in the antiferromagnetic Heisenberg background. OS notice that the spin configuration of the three-hole Cu-O-Cu triad in the GS of Cu_4O_8 is almost the same as that in the ground state of an isolated three-site Cu-O-Cu cluster with Cu-O exchange interaction:

$$|\varphi\uparrow\rangle = 2|\uparrow\Downarrow\uparrow\rangle - |\downarrow\Uparrow\uparrow\rangle - |\uparrow\Uparrow\downarrow\rangle, \tag{7}$$

(or spin-reverse), since the corresponding GS coefficients for Cu_4O_8 are: 0.1099, −0.0533, −0.0533. Here ↑ and ⇑ denote Cu- and O-site spin correspondingly. The reason for this is quite clear: the Cu-O exchange term determining the *internal* triad spin configuration is of the order t^2, while the Cu-Cu superexchange term governing the triad interaction with the background is of the order t^4 in H_{eff}. Therefore, the intra-triad dynamics happen on a much shorter time scale than its communication with the surrounding spin system, so that these two processes are practically *decoupled*.

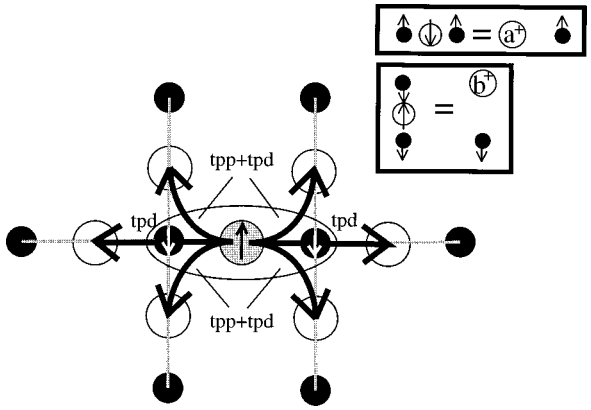

FIG. 1. The Cu-O-Cu triad interacting with the surrounding Cu sites are shown by filled circles, O sites by open circles. Gray lines represent Cu-Cu superexchange terms (J), black lines indicate triad hopping terms (t). The same picture rotated by 90° illustrates the part of Hamiltonian for a triad in vertical position.

Considering these results by OS it seems reasonable to simplify H_{eff} further by introducing a composite three-spin system constructed of one hole on an O site and two holes on the neighboring Cu sites with their spin configuration as given by Eq. (7). One can consider such a Cu-O-Cu system as an effective composite particle with spin-$\frac{1}{2}$, interacting with the surrounding copper spins via the superexchange between the spins of two Cu in the triad and the six neighboring spins, the J term in Fig. 1. In fact, such a construction has been proposed by Emery and Reiter[18] (ER) earlier, but to the best of our knowledge no exact numerical studies have been carried out.

Such a quasiparticle will have a self-energy due to the Cu-O exchange inside the triad. Clearly, it plays no role in the dynamics of a hole unless triads are made nonequivalent, for example by distortion of the lattice. The motion of the quasiparticle occurs through the O-hole hopping to the next available neighboring site (the t term). In the discussion below we follow the arguments by ER. At first let us rewrite Eq. (7) as a linear superposition of the ''left'' and ''right'' singlets:

$$|\varphi\uparrow\rangle = (\uparrow\Downarrow - \downarrow\Uparrow)\uparrow - \uparrow(\Uparrow\downarrow - \Downarrow\uparrow) = S_L\uparrow + \uparrow S_R. \tag{8}$$

By applying Eq. (5) to this expression one can easily verify that S_L hops coherently to the *left*, while S_R hops coherently to the *right*, i.e.,

$$\begin{aligned}
|\uparrow\varnothing S_L\uparrow\rangle &\xrightarrow{(5)} -(t_1+2t_2)|\uparrow S_R\varnothing\uparrow\rangle,\\
|\downarrow\varnothing S_L\uparrow\rangle &\xrightarrow{(5)} -(t_1+2t_2)|\downarrow S_R\varnothing\uparrow\rangle,\\
|\uparrow S_R\varnothing\uparrow\rangle &\xrightarrow{(5)} -(t_1+2t_2)|\uparrow\varnothing S_L\uparrow\rangle,\\
|\uparrow S_R\varnothing\downarrow\rangle &\xrightarrow{(5)} -(t_1+2t_2)|\uparrow\varnothing S_L\downarrow\rangle,
\end{aligned} \tag{9}$$

where $\varnothing$ denotes an empty oxygen site. Therefore, taking into account a factor of 1/2 due to the $|\varphi\uparrow\rangle$-singlet overlap, the quasiparticle hopping amplitude is given by

$$t=-\frac{t_1+2t_2}{2}. \tag{10}$$

Notice that the hopping amplitude becomes negative in analogy with the t-J model.[16] ER suggest to use

$$t=-\frac{t_1+2t_2}{3}, \tag{11}$$

rather than Eq. (10), arguing that an additional factor of $\approx 2/3$ arises due the zero-point spin fluctuations in the GS of the Heisenberg model. Finally, from Eq. (9) one can see that the quasiparticle is free to move to any vacant neighboring O site and the direction of its spin after the hopping is always the same as the spin of the Cu site newly absorbed in the triad.

Two neighboring triads interact with each other via the superexchange between their Cu spins. In the case of two triads sharing the same Cu site the whole system of three Cu and two O spins is assumed to be in the spin-$\frac{1}{2}$ state[18] interacting with the background via the Cu-Cu superexchange. The spin background is described by the Heisenberg superexchange Hamiltonian $H^{(4)}_{\text{Cu-Cu}}$. Since the on-site ε_d and ε_p terms as well as the Cu charge-transfer term (3) produce a constant input to the GS energy, they are omitted in our model. Therefore, it becomes similar to the t-J model, except that the Zhang-Rice singlets are substituted by the Cu-O-Cu spin-$\frac{1}{2}$ composite particles which can occupy the x-O and y-O sites separately.

The Hamiltonian thus obtained can be written in terms of only the Cu site operators, if one introduces two spinless creation operators, a_i^+ and b_i^+, for triads at x- and y-oxygen sites correspondingly of the ith unit cell (see inset in Fig. 1). This cell is associated with the ith copper site. The spin of the corresponding a and b triads is stored as the spin at the next Cu site to the right and down correspondingly, and is created by the same d_i^+ operator as the rest of the background spins. Therefore, a triad particle is represented by the two neighboring Cu sites of which the first marks its orientation and the second its spin. Then one obtains the two-band t-J Hamiltonian:

$$H_{2tJ}=-t\left(\sum_{\langle i,i'\rangle} d^+_{\sigma i}d_{\sigma i'}a^+_{i'}a_i+\sum_{\langle i,i''\rangle} d^+_{\sigma i}d_{\sigma i''}b^+_{i''}b_i\right)$$

$$-t'\sum_{\langle i,i'\rangle} d^+_{\sigma i}d_{\sigma i'}(a^+_{i'}b_i+b^+_i a_{i'}) \tag{12}$$

$$+J\sum_{\langle i,i'\rangle}\left(\mathbf{S}_i\mathbf{S}_{i'}+n_{ni'}\mathbf{S}_i\mathbf{S}_{i''}+n_{bi'}\mathbf{S}_i\mathbf{S}_{i'''}-\frac{1}{4}\right)+\text{H.c.}$$

Here the t term describes the a-triad (horizontal) hopping right or left and the b-triad (vertical) hopping up or down, while the t' term stands for the a triad moving up or down and vice versa (Fig. 1). The first term in the J sum accounts for the background superexchange and the first part of the background-triad superexchange, since a triad occupies two Cu sites and only one of them keeps the triad spin. The next two terms describe the second part of the background-triad superexchange with the second triad Cu spin by ''substituting'' the spinless a or b hole with the second triad Cu site (i'' and i''' correspondingly). The parameters J, t and t' are given by Eqs. (6) and (11):

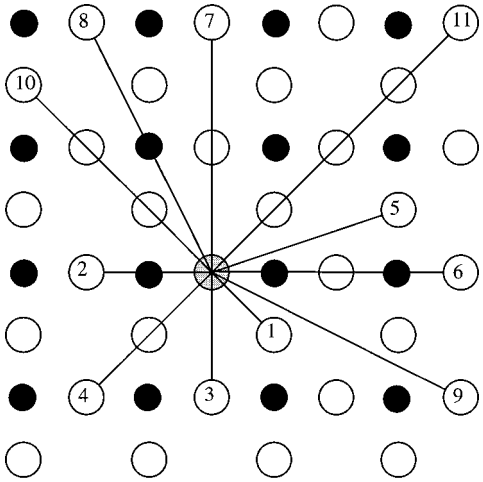

FIG. 2. $Cu_{16}O_{32}$ cluster with possible hole-hole correlation positions.

$$t=\frac{1}{3}\left(\frac{t_{pd}^2}{\Delta}+2\frac{t_{pd}^2}{U_d-\Delta}\right), \tag{13}$$

$$t'=t+t_{pp},$$

$$J=4\left(\frac{t_{pd}^4}{\Delta^2 U_d}+\frac{2t_{pd}^4}{\Delta^2(2\Delta+U_p)}\right). \tag{14}$$

Since the 4×4 cluster that we considered is known to have an unwanted hypercube symmetry, the t' term has been modified by adding a small constant O-O hopping ($t_{pp}=0.1$ for the first-nearest neighbor and $t_{pp}=0$ for all other neighbors—see Fig. 1) to remove this symmetry. The Hamiltonian (12) is exact for a single hole. For the case of two and more holes the terms for triad-triad superexchange must be added and also triads motion close to each other must be considered more carefully. These terms are easy to account for in numerical calculations, while as written analytically they appear rather complicated in the proposed representation. So for the sake of clarity they are omitted from Eq. (12). Since there are only four possible states on each Cu site $\{d^+_\uparrow, d^+_\downarrow, a^+, b^+\}$, the system configurations can be compactly stored in the binary representation. One can see that the dimension of the new Hilbert space is approximately 2^n times that of the t-J model, where n is the number of oxygen holes.

The model was studied by exact diagonalization[19,20] on a square $Cu_{16}O_{32}$ cluster with the periodic boundary conditions (Fig. 2). Values of $U_d=12$, $U_p=4$, and $t_{pd}=1$ were fixed, whereas Δ has been varied to modify the ratio of the magnetic and kinetic terms in the Hamiltonian. The variation of Δ may be considered as a chemical shift of O atomic levels which comes from the influence of the surrounding out-of-plane ions in the cuprates.

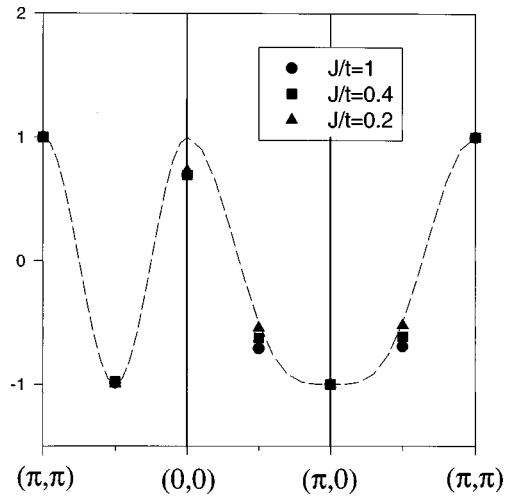

FIG. 3. One-hole dispersion curve $\varepsilon_{1h}(\mathbf{k})$ for various values of t/J. Here $\varepsilon_{1h}(\mathbf{k})=E_{1h}(\mathbf{k})-E_{0h}(\mathbf{k})$, where $E_{nh}(\mathbf{k})$ is the lowest energy of the cluster at a given $\mathbf{k}$. For $\mathbf{k}=(0,0)$ and $\mathbf{k}=(\pi,\pi)$ these values are different from the position of the quasiparticle poles in the Green function (Ref. 23). For each value of t/J the energy range was normalized to the $[-1,1]$ interval.

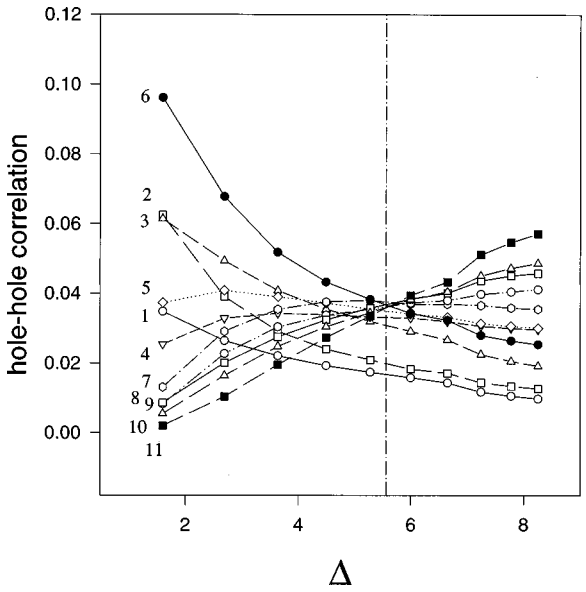

FIG. 4. The GS hole-hole density correlation function (15) for various values of Δ. Numbers on the plot mark different possible hole-hole positions shown in Fig. 2.

III. RESULTS AND DISCUSSION

A. Undistorted cluster

We first will discuss the results for the undistorted cluster and then will see what differences appear when various patterns of lattice distortion are added. In the absence of doped holes our model is purely magnetic and equivalent to the regular t-J model of which GS characteristics are well established. For one doped hole the symmetry properties of the GS obtained in both models are also very similar. In the strong correlation regime $\Delta<\Delta_2=6.9$ ($J/t>0.07$) we obtained two close lowest-energy states: a doublet with $\mathbf{k}=(\pi,0)$ and a quadruplet with $\mathbf{k}=(\pi/2,\pi/2)$. For $\Delta<\Delta_1=4.6$ ($J/t=0.18$) the $\mathbf{k}=(\pi,0)$ state has a lower energy, and then they switch. Both states have the total spin $\mathbf{S}=1/2$. Above Δ_2 there are several almost degenerate states, $\mathbf{k}=(\pi,\pi)$, $\mathbf{S}=5/2$ state being the lowest, then a transition to the completely symmetric $\mathbf{k}=(0,0)$ ferromagnetic ($\mathbf{S}=\mathbf{S}_{\max}$) state takes place at $\Delta_3=7.4$ ($J/t=0.06$). The change of total spin $\mathbf{S}$: $1/2\rightarrow 5/2$ at $\Delta=6.9$ and $5/2\rightarrow\mathbf{S}_{\max}$ at $\Delta=7.4$ is very close to what was obtained by OS for the $Cu_{10}O_{20}$ square cluster. Our results are also in good agreement with those given by the t-J model for which one obtains $(J/t)_1=0.2$ and $(J/t)_2=(J/t)_3=0.075$.[14] Also, in both models the GS is completely symmetric under the cluster point-group operations (x-, y- reflections and a $x\leftrightarrow y$ reflection) in the whole range of Δ. Such a close similarity to the t-J model follows from the dynamics of a single Cu-O-Cu triad in the strong antiferromagnetic background. Since bonds around one of the triad's Cu spins become frustrated, the best kinetic path for the O hole on the triad will be around that Cu site, thus keeping the number of frustrated bonds to a minimum. In this way a symmetric Zhang-Rice-type state can be formed in the strong-correlation regime.

A single hole dispersion spectrum is shown in Fig. 3. In a whole it is very similar to the one obtained for the t-J model,[21] though the (0,0) point is slightly higher in our case. The curve shown in Fig. 3 by a dashed line has a functional form $\varepsilon_{1h}(\mathbf{k})=\text{const}(J)\cdot(\cos k_x+\cos k_y)^2+\text{const}$, that can be obtained from an effective tight-binding Hamiltonian.[22] The bandwidth W/t calculated as the difference of energy between the maximum and minimum values of $\varepsilon_{1h}(\mathbf{k})/t$ was 0.78, 1.7, and 4.0 for J/t equal to 0.2, 0.4, and 1 correspondingly. These values are considerably larger then those obtained for the t-J Hamiltonian, which may be due to the fact that in our model an oxygen hole has six nearest neighbors, while in the one-band t-J model it has only four.

For a system with two doped holes we found the GS with the momentum $\mathbf{k}=(\pi,0)$, symmetric under y reflection, and antisymmetric under x reflection (or vice versa) for $\Delta<5.75$ ($J/t>0.11$). The momentum changes to $\mathbf{k}=(0,0)$ for larger values of Δ, and the GS space symmetry crosses over from d- to s-type around $\Delta=7.7$ ($J/t=0.05$). The GS total spin $\mathbf{S}$ is zero in the whole range of Δ. The t-J model calculations on a 4×4 cluster give the same d- to s-type crossover at $J/t<0.1$, with the degenerate $\mathbf{k}=(\pi,0)$ and (0,0) states as the GS below that value, and the $\mathbf{k}=(0,0)$ GS above.[14] This degeneracy is due to an additional hypercube symmetry of the 4×4 cluster mentioned above. It can be removed by using a cluster of different geometry or by adding extra hopping terms. Then the GS of the regular t-J model is found to be the same in the whole range of the J/t ratio.[15] This is different from the present result. While in our case the energies of the $(\pi,0)$ and (0,0) states are close to each other in the whole Δ range, there is a significant difference in their physical properties. In particular, this can be seen by comparing their hole-hole correlation functions, defined by

$$C(\mathbf{R})=\left\langle \frac{1}{2}\sum_i n_h(\mathbf{r}_i)n_k(\mathbf{r}_i+\mathbf{R})\right\rangle, \tag{15}$$

which gives the probability that there is a hole at $\mathbf{R}$ given there is one at the origin. In Fig. 4 one can see that up to $\Delta=5$ the maximum of the hole-hole correlation density is in

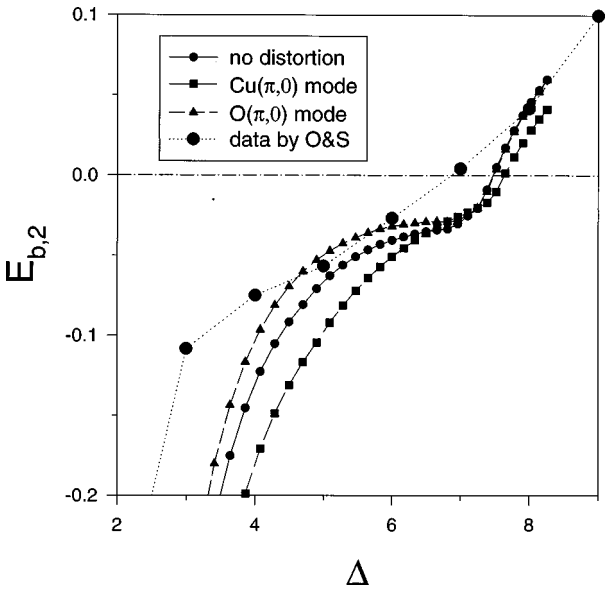

FIG. 5. Two-hole binding energy $E_{b,2}$ as a function of Δ for undistorted and distorted clusters, compared to the result by OS. The distortion assumed for the O and Cu modes is 2%.

the configuration where two holes are located at the second-nearest oxygen sites in the same Cu-O chain (See No. 6 in Fig. 2), therefore we assume that in this region ($\Delta<5$) two holes are bound in a pair. Analysis of spin-spin correlation functions shows that the paired holes in this configuration have opposite spins. The next favored configurations are those with holes facing each other in the neighboring chains (No. 3) and also Nos. 2 and 5. It is interesting to note that the loss of pairing correlation coincides with the crossover of the true GS from the $(\pi,0)$ to (0,0) symmetry (at $\Delta=5.75$, $J/t=0.11$). Therefore, we may conclude that the $(\pi,0)$ GS momentum obtained in this work is of physical importance. These results agree with OS, who also obtained the maximum of the hole-hole correlation in the Nos. 6, 3, and 5 configurations, which are degenerate for the $Cu_{10}O_{20}$ square cluster geometry, and a bound state for $J/t>0.08$.

The two-hole binding energy $E_{b,2}$ defined as

$$E_{b,2}=(E_{2h}-E_{0h})-2(E_{1h}-E_{0h}), \tag{16}$$

where E_{nh} is the GS energy for the system with n doped holes is shown in Fig. 5. The binding energy obtained for $H_{\rm eff}$ model by OS for an undistorted $Cu_{10}O_{20}$ cluster and $U_d=20$ is shown for comparison. Our result and the result by OS tend to diverge at small Δ, which may be a size effect, since we used different clusters. If we consider this point the agreement between the two models is reasonably good, which proves that the Cu-O-Cu particle approximation is indeed valid in a broad range of parameters. From Fig. 5 one can see that in the strong-correlation regime $E_{b,2}$ has very large absolute values, as in the t-J model, and becomes positive (no binding) only around $\Delta=7.2$. On the other hand, the correlation function (Fig. 4) shows that the bound state disappears at a smaller Δ value (somewhere between 5 and 6). Clearly, Eq. (16) overestimates the true binding energy presumably due to the size effect. Indeed, in the 4×4 cluster two doped holes have a large probability of crossing each other's path even without binding, reducing in this way the overall background frustration. In order to obtain the correct pair-binding energy, Eq. (16) must be applied to a cluster of a much larger size.

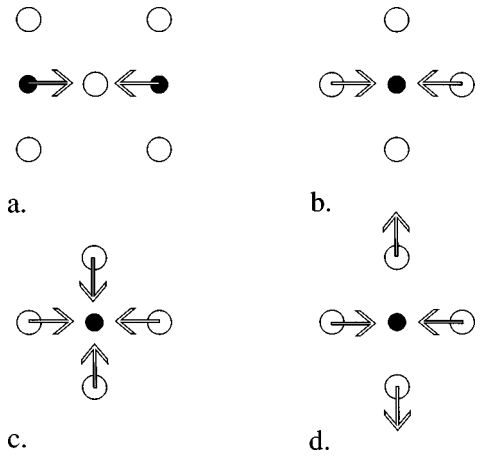

FIG. 6. Patterns of phonon distortion studied. (a) Cu$(\pi,0)$ half-breathing mode, (b) O$(\pi,0)$ half-breathing mode, (c) O(π,π) breathing mode, (d) O(π,π) ''quadrupole'' mode.

B. Effect of lattice distortion

We now discuss the effect of various phonon modes shown in Fig. 6 as different patterns of static lattice distortion, studied in the adiabatic approximation. The parameters t_{pd} and t_{pp} in Eq. (13) are replaced by

$$t_{pd}^{ij}=t_{pd}\left(1-\frac{7}{2}D_{pd}^{ij}\right),$$
$$t_{pp}^{jj'}=t_{pp}(1-2D_{pp}^{jj'}), \tag{17}$$

where D_{pd}^{ij} and $D_{pp}^{jj'}$ are the relative changes in each p-d and p-p bondlengths. Coefficients 7/2 and 2 in Eq. (17) imply corresponding power laws for p-d and p-p transfer integrals.[24] This modulation of the t set by a phonon represents the adiabatic limit of a nonlocal el-ph interaction described by the Su-Shrieffer-Heeger (SSH) model.[25] Also the self-energy of a Cu-O-Cu composite particle must be changed if it occupies a site with distorted Cu-O bonds. The corresponding formulas were obtained by solving the Hubbard Hamiltonian for the Cu-O-Cu spin triad distorted in accordance with the patterns in Fig. 6. Since the change of the triad self-energy is local and proportional to the O-site hole density, it is appropriate to associate it with the Holstein model.[26] We found that the energy input of this term is a slow-varying function of Δ that decreases the total energy approximately by the same amount for all phonon modes. However, for the Cu$(\pi,0)$ and O$(\pi,0)$ modes that were found to produce the strongest energy decrease, the major part of it was found to be due to the change of the kinetic energy of a hole, i.e., due to the nonlocal SSH part of the el-ph interaction.

Out of four phonon modes shown in Fig. 6 those with $\mathbf{q}=(\pi,\pi)$ (c) and (d) were found to produce no significant effect on the system with one- and two-doped holes as compared with the undoped cluster. In other words, they couple mostly to the spin background. On the other hand, the $\mathbf{q}$

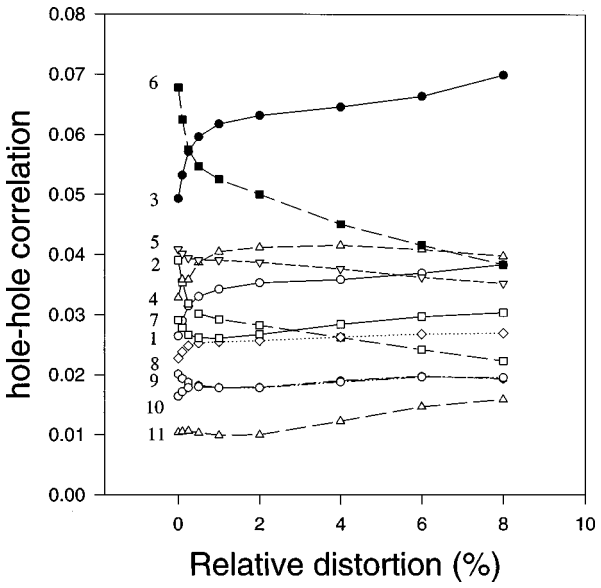

FIG. 7. $C(\mathbf{R})$ for the cluster with Cu$(\pi,0)$ distortion and $\Delta = 2.7$ eV.

$=(\pi,0)$ modes (a) and (b) show a strong influence on doped holes. Specifically, O ''half-breathing'' mode (b) lowers the GS energy of one-hole system quite strongly in agreement with the study of one-dimensional Hubbard Hamiltonian.[27] This strong coupling may be due to the fact that for this distortion pattern the GS $\mathbf{k}$ vector is $(\pi,\pi/2)$, and is located on the boundary of the new Brillouin zone, and therefore the quasiparticle wave function actively interferes with the lattice. This is in agreement with the experimental results for $YBa_2Cu_3O_{7-\delta}$, $La_{2-x}Sr_xCuO_4$,[2] and $Ba_{1-x}K_xBiO_3$,[3] which show strong softening for the branch with O half-breathing distortion at the $\mathbf{q}=(\pi,0)$ point. At the same time, the mode produces no significant energy decrease as the second hole is added. As a result, $E_{b,2}$ was found to decrease with increasing distortion (Fig. 5).

On the other hand, the effect of the Cu half-breathing mode turned out to be the most prominent in the system when two doped holes are present. Figure 7 shows $C(\mathbf{R})$ calculated for this mode. One can see that now the maximum of the hole-hole correlation density shifts into position 3, so that the pair becomes more localized. It is remarkable that this shift happens when distortion is still very small (0.25%), even though the GS symmetry remains unchanged by distortion.[28] In addition, a robust decrease in the two-hole GS energy takes place, which strongly increases the pair binding energy, up to 50% for $\Delta=4.5$, as can be seen in Fig. 5. This unusual feature may be viewed as a sign of a resonance of different hole pair configurations instigated by the discussed lattice distortion. These results show that the Cu half-breathing mode produces a major effect on *paired* holes in the antiferromagnetic background. This is supported by the experimental data obtained by inelastic neutron scattering for $La_{1.85}Sr_{0.15}CuO_4$.[4] In that work authors studied the dispersion of optical phonons at low temperatures (10 K) and obtained a spectrum that has a discontinuous step at one half of the Brillouin zone along (100) indicating cell doubling. However, no superlattice peaks suggesting cell doubling was observed and the discontinuity in the phonon dispersion is diffuse. Therefore the cell doubling must be dynamic and short range. Simple spring model calculations reproduce the observed dispersion quite well if one assumes that there exists a dynamic charge ordering on every other row of oxygen in the CuO_2 plane that could be produced by the Cu half-breathing mode. This discontinuity is limited to low temperatures, and was not observed at room temperature in the earlier work by Pintschovius.[2] This suggests that the dynamic cell doubling may be a consequence of the Cu breathing mode coupling to hole pairs, confirming our present conclusion.

The origin of this coupling may come from the tendency of doped holes to segregate from the antiferromagnetic background, which is well known for the t-J model.[29] The charge stripes on every other row of oxygens created by the Cu $(\pi,0)$ mode are characterized by larger values of transfer integral (t). Since the stripes are broad enough to accommodate the hole pair, it lowers the GS energy by increasing the kinetic motion of the pair. At the same time, the values of t between the stripes are diminished, which reduces the corresponding superexchange interaction and induces the dimerization of Cu-Cu bonds in the direction perpendicular to the stripes. In their recent work[30] White and Scalapino explicitly showed that such dimerization is favorable when a hole pair is present in a cluster, therefore the dimerization induced by the Cu $(\pi,0)$ mode is expected to lower the GS energy further. The O ''half-breathing'' mode, on the other hand, creates almost one-dimensional Cu-O chains which may be too ''narrow'' for the pair to move effectively. This is confirmed by analyzing the direction of hole hopping, which can be carried out by dividing the kinetic part (t term) of the Hamiltonian into two parts: along the distortion and across it. Then one can see that in the case of the O distortion the paired holes actually prefer to move *across* the stripes, while for Cu mode they rather move along. As mentioned in the beginning of this section, the strong effect of Cu $(\pi,0)$ mode is primarily due to the nonlocal part of electron-lattice coupling. Since this coupling represents the Su-Schrieffer-Heeger model, our results show that this model can produce important differences as compared to the more widely studied Holstein model. The substantial increase in the hole pairing force obtained in the presence of Cu half-breathing distortion also conforms with the idea of singular quasiparticle interactions arising in the proximity of charge-density-wave instability proposed by Castellani, Di Castro, and Grilli.[31] These authors argue that the presence of a quantum critical point due to formation of incommensurate charge-density waves accounts for basic features of the high-temperature superconductivity.

IV. CONCLUSION

In this paper we proposed an effective two-band Hamiltonian suited to describe strongly correlated electrons and their interaction with phonons in the CuO_2 planes of cuprates. The Hamiltonian was studied by exact diagonalization on the square $Cu_{16}O_{32}$ cluster. Our results can be summarized as follows:

(1) For the one-doped hole the GS properties are in general in close agreement with those obtained in the regular t-J model.

(2) For two-doped holes the GS was found to be a doublet with $\mathbf{k}=(\pi,0)$ in the strong-correlation regime ($J/t>0.11$) and a single state with $\mathbf{k}=(0,0)$ for $J/t<0.11$. This is different from the results of the t-J model where the GS momentum is $\mathbf{k}=(0,0)$ in the whole range of J/t ratio. In the strong-correlation regime a two-hole bound state is formed with the maximum of the hole-hole correlation density in the configuration where the two holes are in the second-nearest oxygen sites along the same Cu-O chain.

(3) Some phonon modes studied in the adiabatic approximation are shown to couple strongly to the doped holes. Specifically, the O half-breathing mode is shown to couple to a single doped hole GS. On the other hand, the Cu half-breathing mode couples strongly to hole pairs, increasing the hole-hole correlation and binding energy. The dynamic doubling of a unit cell in $La_{1.85}Sr_{0.15}CuO_4$ that has been recently observed at low temperatures can be a manifestation of this phenomenon.

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[1] T. Egami and S. J. L. Bilinge, *Physical Properties of High-Temperature Superconductors V*, edited by D. Ginsberg (World Scientific, Singapore, 1996), p. 265.
[2] L. Pintschovius and W. Reichardt, *Physical Properties of High-Temperature Superconductors IV*, edited by D. Ginsberg (World Scientific, Singapore, 1994), p. 295.
[3] M. Braden *et al.*, J. Supercond. **8**, 595 (1995).
[4] R. J. McQueeney, Y. Petrov, T. Egami, M. Yethiraj, G. Shirane, and Y. Endoh (unpublished).
[5] M. Nohara, T. Suzuki, Y. Maeno, T. Fujita, I. Tanaka, and H. Kojima, Phys. Rev. Lett. **70**, 3447 (1993).
[6] M. Nohara, T. Suzuki, Y. Maeno, T. Fujita, I. Tanaka, and H. Kojima, Phys. Rev. B **52**, 570 (1995).
[7] D. Mihailovic, T. Mertelj, B. Podobnik, J. Demsar, P. Canfield, Z. Fisk, and C. Chen, Physica B (to be published).
[8] B. Tanner and T. Timusk, in *Physical Properties of High Temperature Superconductors III*, edited by D. Ginsberg (World Scientific, Singapore, 1992), p. 363.
[9] T. Egami, W. Dmowski, R. J. McQueeney, T. R. Sendyka, S. Ishihara, M. Tachiki, H. Yamauchi, S. Tanaka, T. Hinatsu, and S. Uchida, Proc. SPIE **2158**, 27 (1994).
[10] B. H. Toby, T. Egami, J. D. Jorgensen, and M. A. Subramanian, Phys. Rev. Lett. **64**, 2414 (1990).
[11] H. Fehske, H. Röder, A. Mistriotis, and H. Büttner, J. Phys.: Condens. Matter **5**, 3565 (1993).
[12] G. Wellein, H. Röder, and H. Fehske, Phys. Rev. B **53**, 9666 (1996).
[13] J. Bonca, P. Prelovsek, and I. Sega, Phys. Rev. B **39**, 7074 (1989).
[14] Y. Hasegawa and D. Poilblanc, Phys. Rev. B **40**, 9035 (1989).
[15] T. Itoh, M. Arai, and T. Fujiwara, Phys. Rev. B **42**, 4834 (1990).
[16] F. C. Zhang and T. M. Rice, Phys. Rev. B **37**, 3759 (1988).
[17] M. Ogata and H. Shiba, J. Phys. Soc. Jpn. **57**, 3074 (1988).
[18] V. J. Emery and G. Reiter, Phys. Rev. B **38**, 4547 (1988).
[19] E. Dagotto, Rev. Mod. Phys. **66**, 763 (1994).
[20] G. Fano, F. Ortolani, and A. Parola, Phys. Rev. B **46**, 1048 (1992).
[21] R. Eder, K. W. Becker, and W. H. Stephan, Z. Phys. B **81**, 33 (1990).
[22] P. Fulde, *Electron Correlations in Molecules and Solids* (Springer-Verlag, Berlin, 1993), p. 363.
[23] The space symmetry of the lowest energy state for the one-hole-doped cluster is different from the symmetry of the state for the undoped cluster at these points. This agrees with the results for the one-band Hubbard model (Ref. 18).
[24] W. Harrison, *Electronic Structure and the Properties of Solids* (Dover, New York, 1989), p. 482.
[25] W. P. Su, J. R. Shrieffer, and A. J. Heeger, Phys. Rev. Lett. **42**, 1698 (1979).
[26] T. Holstein, Ann. Phys. (N.Y.) **8**, 325 (1959).
[27] S. Ishihara, T. Egami, and M. Tachiki, Phys. Rev. B **55**, 3163 (1997).
[28] The GS wave function of the distorted cluster converges smoothly without a change of symmetry to the GS wave function of the undistorted cluster, as distortion goes to zero.
[29] S. R. White and D. J. Scalapino, Phys. Rev. Lett. **80**, 1272 (1998).
[30] S. R. White and D. J. Scalapino, Phys. Rev. B **55**, 6504 (1997).
[31] C. Castellani, C. Di Castro, and M. Grilli, cond-mat/9702112 (unpublished).