Exact-diagonalization study of the effective model for holes in the planar antiferromagnet

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The effective single-band Hamiltonian for holes in the two-dimensional quantum antiferromagnet, relevant for the CuO_2 layers in copper-oxide superconductors, is studied by the exact diagonalization of a finite-size system with 16 cells. Single- and two-hole ground-state properties are calculated. Pair-binding-energy and hole-density correlation functions indicate that two holes bind for moderate exchange interactions, even in the case of the extreme anisotropic-Ising limit.

I. INTRODUCTION

At present there exists well-established experimental evidence that copper-oxide-based superconductors (SC) behave as strongly correlated electronic systems.[1] Relevant properties are mainly controlled by CuO_2 layers, where charge carriers are holes introduced by doping the reference substance, e.g., La_2CuO_4, being a magnetic insulator with long-range antiferromagnetic (AFM) order. Several microscopic models based on a single-band[2,3] or multiple-band[4-6] Hubbard Hamiltonian have been proposed for the description of electrons in CuO_2 layers. The simplest prototype model, which contains at least some important features of this strongly correlated system, is the effective single-band model

$$H=-t\sum_{\langle i,j\rangle s}(c_{is}^{\dagger}c_{js}+c_{js}^{\dagger}c_{is})+J\sum_{\langle i,j\rangle}(\mathbf{S}_i\cdot\mathbf{S}_j-\tfrac{1}{4}n_in_j)\ , \tag{1}$$

which describes hopping of electrons in the presence of a finite concentration of holes in the magnetic (AFM) insulator, as represented by the Heisenberg exchange model. Here $c_{is}^{\dagger}(c_{is})$ are projected fermionic operators $c_{is}^{\dagger}=\bar{c}_{is}^{\dagger}(1-\bar{n}_{i,-s})$, taking into account the strong correlation requirement that no double occupancy of sites is allowed. $\mathbf{S}_i=\frac{1}{2}\sum_{ss'}\boldsymbol{\sigma}_{ss'}c_{is}^{\dagger}c_{is'}$ are corresponding local spin operators. Summations $\langle ij\rangle$ extend over all pairs of nearest-neighbor sites on a square lattice, as relevant for CuO_2 layers.

The effective Hamiltonian [Eq. (1)] has been introduced[2,3] in connection with CuO_2 layers as the representation of a single-band Hubbard model for Cu d orbitals with a large on site Coulomb repulsion U, where $J=4t^2/U$. Even the two-band Hubbard model has been mapped in the relevant parameter regime onto the hole-spin models[7] and finally onto the same restricted basis set[8] as in Eq. (1) with three states per cell, i.e., $|\uparrow\rangle$, $|\downarrow\rangle$, and $|0\rangle$. In the latter case, $|0\rangle$ takes the role of a local singlet, formed by a spin in the Cu d orbital and a hole in the symmetrized O p orbital. Nevertheless, the reduction leads, in general, to higher-order invariants not included in Eq. (1). They are different for single- and multiple-band Hubbard models. Thus we omit a three-site term (see, e.g., Refs. 9 and 10) connected with next-nearest-neighbor hopping, as obtained by a straightforward reduction of a single-band Hubbard model.

The effective model [Eq. (1)] has been studied for a small density of holes in the quantum AFM state by several authors. The Brinkman-Rice[11] approach to the problem of a single-hole motion in the limiting case $J/t\to 0$ has been applied[12-14] to the calculation of the single-hole and two-hole ground states for the square lattice and finite J/t. Although different analytical treatments[9,15-17] and numerical calculations[18] have been presented, some crucial aspects still remain to be settled. The nature of the *spin polaron,* a hole in the AFM background, is not yet clarified, whether spin distortions around a hole are more of the ferromagnetic (FM) type[19] or of the singlet spin-liquid[3] type, etc. The possibility of long-range dipolar distortions has also been considered.[16] With respect to a possible hole binding, analytical results are controversial,[12-14] mainly not being in favor of hole binding. Numerical studies seem to indicate that in the single-band Hubbard model SC pairing is not possible,[20] while in the two-band case some evidence for the binding of holes has been presented.[21]

Spin fluctuations are very pronounced in the isotropic Heisenberg model with $J_{\alpha\alpha}=J$, $\alpha=x$, y, and z. The ground state of the spin model without holes still shows a long-range AFM order on a square lattice,[22,23] hence it is not clear to what extent single- and two-hole properties are governed by large spin fluctuations,[13,14,16] the latter being specific to the isotropic case, but not to anisotropic models, as in the Ising limit $J_{zz}=J_{\parallel}\gg J_{xx}=J_{yy}=J_{\perp}$.

In this paper we study the effective model [Eq. (1)] by performing an exact diagonalization of a small-size system, our calculations restricted to $4\times 4=16$ cells with periodic boundary conditions. In comparison with approximate analytical treatments,[1,12-14] which had relied on rather restricted basis sets, our method with a complete set for a finite system yields some essentially different results. This is particularly true of the nature of the interaction between holes, and in a brief account of this work we presented evidence that binding of (two) holes can occur.[24] On the other hand, as far as numerical

calculations are concerned, the model [Eq. (1)] has advantage over the single-band Hubbard model due to only three basis states per cell. Still only few numerical calculations for the model [Eq. (1)] have been performed.[18,25]

In Sec. II we present our modified Lanczos method used in the calculation of the ground states for one and two holes in the model [Eq. (1)]. Results for a single-spin polaron are presented in Sec. III. The energy spectra and the character of spin distortions around the hole are examined. Section IV is devoted to results for two holes. The binding energy and different correlation functions are calculated, which point to the existence of hole pairing. We also examine the case of the extreme anisotropic spin exchange, in order to discuss the influence of spin fluctuations on the hole binding and other properties. We summarize our results in Sec. V.

II. NUMERICAL METHOD

Due to the smallest possible number of basis states, i.e., three per cell, the effective model Eq. (1) allows a numerical study of larger size systems than in the case of Hubbard models[20,21] and coupled hole-spin models.[26] We choose a single size, i.e., a very symmetric system of 16 cells, which in the case of two holes represents our present computational limit.

Essentially we are using the Lanczos procedure defined by the iteration

$$H|\Phi_n\rangle = b_{n-1}|\Phi_{n-1}\rangle + a_n|\Phi_n\rangle + b_n|\Phi_{n+1}\rangle \ , \quad (2a)$$

$$a_n = \langle \Phi_n|H|\Phi_n\rangle, \quad b_{n-1} = \langle \Phi_{n-1}|H|\Phi_n\rangle \ , \quad (2b)$$

which generates a set of orthonormal basis functions $|\Phi_n\rangle$ under the appropriate initial choice of the function $|\Phi_0\rangle$ and $b_{-1}=0$. Diagonalizing the tridiagonal matrix of elements $\{a_n\},\{b_n\}$ we obtain energies (eigenvalues) and corresponding eigenfunctions expressed in terms of $|\Phi_n\rangle$. We are interested only in the lowest-energy states $|\Psi_0\rangle$ for a given symmetry. In all cases considered this can be achieved with less than 40 Lanczos steps. In contrast to usual implementations of the Lanczos method,[27] we use as basis states those of blocks $j=1,\ldots,4$, i.e., in our case of the 2×2 lattice (see Fig. 1). These block states $|\varphi_l^j\rangle$, $l=1,\ldots,81$ are characterized by several quantum numbers: the number of holes n_h^j, spin S^j, S_z^j, and reflection symmetries m_x^j, m_y^j.

The Hamiltonian (1) can be written as a sum of block diagonal and interblock terms:

$$H = \sum_{j=1}^{4} H_{jj} + H_{12} + H_{23} + H_{34} + H_{41} \ , \quad (3)$$

and interblock matrix elements are, e.g.,

$$h^{12}_{lk,l'k'} = \langle \varphi_l^1|\langle \varphi_k^2|H_{12}|\varphi_{k'}^2\rangle|\varphi_{l'}^1\rangle \ . \quad (4)$$

Due to the conservation of $n_h^j + n_h^{j'}$ and $S_z^j + S_z^{j'}$, as well as of $m_x^j m_x^{j'}$ and $m_y^j m_y^{j'}$, the number of nonzero elements is strongly reduced. We thus store as arrays only nonzero elements h and their indices $lkl'k'$. The Lanczos procedure is then performed using the product basis

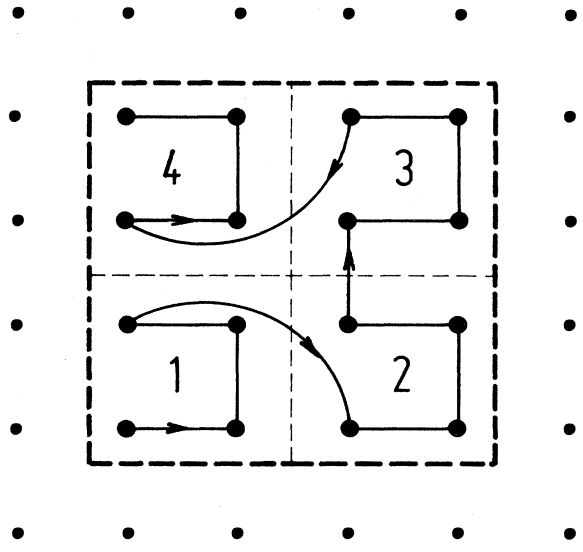

FIG. 1. Cluster of 16 sites with periodic boundary conditions on a square lattice used in this calculation. The four blocks, each containing four sites, are shown. The oriented thin line defines the ordering of fermions on the lattice.

$$|\phi_{lkhp}\rangle = |\varphi_l^1\rangle|\varphi_k^2\rangle|\varphi_h^3\rangle|\varphi_p^4\rangle \ . \quad (5)$$

Since the initial $|\Phi_0\rangle$ is chosen to have good quantum numbers $N_h = \sum_j n_h^j$, $S_z = \sum_j S_z^j$ and reflections $M_{x,y} = \prod_j m_{x,y}^j$, we can find an appropriate subset of states $\{lkhp\}$, where all states can be directly indexed and easily accessed. It should be pointed out that simple rules for the sign problem are obtained if fermions are counted in the sequence of blocks (see Fig. 1).

The method as described above has several advantages.

(a) The Lanczos iteration is very fast due to prestored matrix elements. Since on a square lattice the dimension required for the product basis $\{lkhp\}$ is roughly equal to the number of nonzero matrix elements (4), the computation time is optimally distributed among the calculation of matrix elements and simple Lanczos iterations (2a) and (2b). For typical cases studied, i.e., $N_h=2$, $S_z=0$ on $N=16$ sites, the relevant basis set dimension is $N_{st}\sim 100\,000$ and the convergence requires a computation time of ~ 2 h on a VAX 8650.

(b) Since the block basis $|\varphi_l^j\rangle$ has good S^j, one can easily construct symmetrized initial $|\Phi_0\rangle$ having good total spin $S_{\rm tot}$. This is especially straightforward for small $S_{\rm tot}$, e.g., $S_{\rm tot}=0$ being mainly of interest. Thus $S_{\rm tot}$ is directly controlled and conserved during the procedure, which is not the case for the usual Lanczos methods in the site-product or q-product basis. On the other hand, q is not a good quantum number in our procedure. It is, however, determined by inspection from the block symmetries m_x^j, m_y^j and their symmetrization in the initial $|\Phi_0\rangle$.

(c) At least in the regime of rather localized holes, simple initial $|\Phi_0\rangle$ can be constructed, which retain substantial weight in the final $|\Psi_0\rangle$. In this sense the method is

well adapted to generalizations of real-space renormalization procedures as used in one-dimensional systems, as well as to the study of larger systems with additional blocks but with a truncated basis.

III. SPIN POLARON PROPERTIES

Although single-hole states were studied by a number of authors,[12–17] several aspects regarding the energy spectra as well as the ground-state properties of the spin polaron still require clarification. We are using much larger basis sets $N_{st} \sim 20\,000$ as compared to analytical approaches,[12–14] which also relied, basically, on the Lanczos procedure.

Low-energy states for a single hole have been investigated in the whole regime of physically interesting values of J/t, that is for $J/t \lesssim 1$.

(a) We found that for $J/t \gtrsim 0.088$, the ground state has $S=\frac{1}{2}$ and is in our $N=16$ system, in addition, degenerate for all $\mathbf{q}$ lying on the edges of the reduced AFM Brillouin zone, i.e., at $\mathbf{q}_{1-4}=(\pm\pi/2,\pm\pi/2)$, $\mathbf{q}_5=(0,\pi)$, and $\mathbf{q}_6=(\pi,0)$ (note that we choose $a_0=1$). The ground state is thus a sixfold degenerate spin doublet. The energy of the spin polaron, defined relative to the AFM ground state $E_0(N_h=0)$ as

$$\Delta E_1 = E_0(N_h=1) - E_0(N_h=0) ,$$

is shown in Fig. 2. An approximate degeneracy of single-hole states for two nonequivalent $\mathbf{q}$, e.g., $\mathbf{q}_1$ and $\mathbf{q}_5$, has been reported also by other authors.[13,14,16] An exact degeneracy, however, is likely to be specific to a very symmetric $N=16$ lattice with periodic boundary conditions. It can also be traced back to the exactly equal values of spin correlations $C(\mathbf{R})=\langle \mathbf{S}(0)\cdot\mathbf{S}(\mathbf{R})\rangle$ at nonequivalent distances $R=\sqrt{2}$ and 2 from the pure isotropic Heisenberg model. (The same phenomenon has also been reported in Ref. 18.) The necessary condition seems to be that the random walks associated with each of the above correlations are, term by term, of equal length. This is indeed the case for the 4×4 lattice considered in this work.

(b) The theorem of Nagaoka[19] requires that as $J/t \to 0$ the ground state should become ferromagnetic, i.e., with $S=\frac{15}{2}$ in our system. The crossover to the FM polaron occurs at quite low J/t. The ferromagnetic state is found to be stable for $J/t < J_c/t \cong 0.088$, while $S=\frac{1}{2}$ remains the ground-state spin value for $J/t \gtrsim 0.088$. At $J/t \cong 0.075$ we obtain $S=\frac{3}{2}$, whereas below this value a rapid crossover to $S=\frac{15}{2}$ occurs, presumably over all intermediate S values. This seems to be consistent with results obtained by other authors.[28] We did not pursue these fine-scale effects any further numerically. We also note that for $J/t \gg 1$, e.g., $J/t=4.5$, the character of the ground state is also found to change over to a doubly degenerate spin doublet with $\mathbf{q}=\mathbf{q}_{5,6}$.

(c) The lowest-energy states at other $\mathbf{q}$ in the Brillouin zone are easily calculated by using the initial $|\Phi_0\rangle$ of the corresponding symmetry. In the most interesting regime $0.1 \lesssim J/t \lesssim 1$ we investigate the bandwidth of the lowest $E_0(\mathbf{q})$ branch. At $\mathbf{q}=(\pi,\pi)$, however, we find that $E_0(\mathbf{q})$ corresponds to $S=\frac{3}{2}$, which cannot be interpreted as a simple excited hole state but rather as a spin excitation above the single-hole ground state. On the other hand, at $\mathbf{q}=0$ the lowest state is $S=\frac{1}{2}$, so we define the bandwidth as $W=E_0(\mathbf{q}=0)-E_0(\mathbf{q}_1)$. We plot W versus J/t in Fig. 3, where W is found to scale almost linearly with J in the intermediate J/t regime. Clearly, one might associate W to the mass of the mobile quasiparticle as $m^* \propto 1/W$, hence $m^* \propto t^2/J$.[13,14,17] However, as already noticed, the single-hole excited states could be predominantly magnonlike, which makes the relation of W to m^* somewhat ambiguous. We have also calculated the single-hole states in the anisotropic case $J_\parallel=J$, $J_\perp=0$ and found that, in contrast to the isotropic case, the lowest-energy states now have $\mathbf{q}=(0,0)$ and $\mathbf{q}=(\pi,\pi)$.

The character of the spin polaron, associated with a hole in the AFM background is of even greater interest.

(a) The hole gains, through nearest-neighbor hopping, in kinetic energy $E_{\rm kin}$. Strong correlations built in the

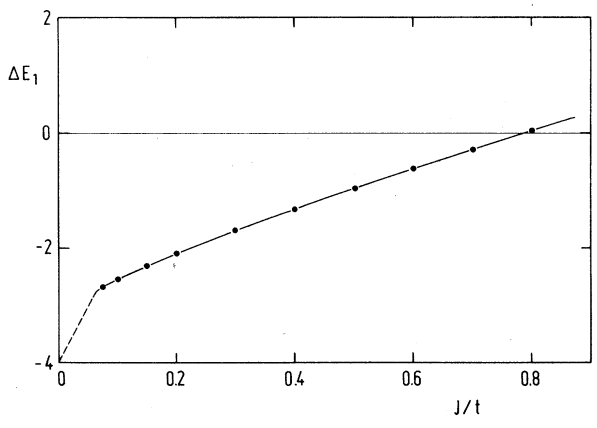

FIG. 2. Ground-state energy ΔE_1 (in units of t) of one hole relative to the AFM ground state vs J/t. Here and in all subsequent figures the thin lines connecting the points are guides to the eye only. Note, however, that the dashed part of the line is an exact result.

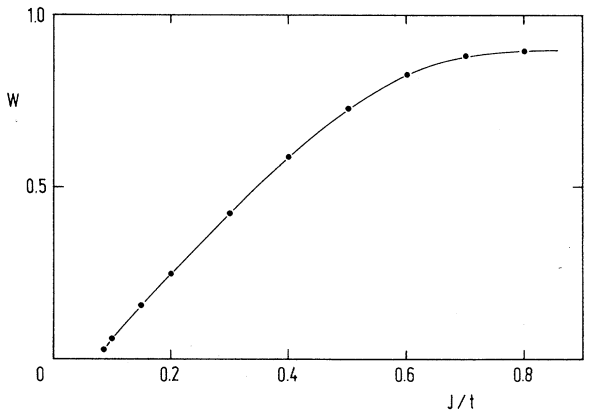

FIG. 3. Quasiparticle bandwidth W vs J/t.

model [Eq. (1)] do not significantly reduce $E_{\rm kin}$ with respect to the maximum uncorrelated value $E_{\rm kin}^{\rm max}=-4t$. We find that for $N=16$ and in the region where the ground state has $S=\frac{1}{2}$, the ratio $\eta=E_{\rm kin}/E_{\rm kin}^{\rm max}$ is only weakly dependent on J, i.e., approximately linear, $\eta\approx 0.775-0.2J/t$ for $0.1<J/t<0.6$. This kinetic energy gain is large when compared, e.g., to the result $\eta=0.63$, obtained for the Hubbard model in the $U\rightarrow\infty$ limit by using the projected, i.e., generalized, Gutzwiller trial wave functions,[9] but smaller than the analytical result $\eta=\sqrt{3}/2\cong 0.866$ obtained in Ref. 11.

(b) The nature of the spin configuration around the hole can be tested only indirectly, via several correlation functions. A direct analysis of the ground state is to some extent complicated by the fact that $\mathbf{q}\neq 0$ there. Since the spin polaron has $S_z=\pm\frac{1}{2}$, a nontrivial quantity is the distribution of the magnetization

$$s(\mathbf{R})=\sum_i \langle\Psi_0|n_h(\mathbf{R}_i)S_z(\mathbf{R}_i+\mathbf{R})|\Psi_0\rangle\ , \tag{6}$$

where we denote the hole density by $n_h(\mathbf{R}_i)=1-n(\mathbf{R}_i)$. In the same manner one can study the modified spin correlations in the vicinity of the hole

$$\tilde{C}(\mathbf{R}_1,\mathbf{R}_2)=\sum_i \langle\Psi_0|n_h(\mathbf{R}_i)\mathbf{S}(\mathbf{R}_i+\mathbf{R}_1)\cdot\mathbf{S}(\mathbf{R}_i+\mathbf{R}_2)|\Psi_0\rangle\ . \tag{7}$$

Results for $s(\mathbf{R})$, plotted in Fig. 4 for all nonequivalent distances R, show that in the region of $J/t<0.5$ the extra magnetization is distributed over a large number of surrounding sites, thus implying a substantial radius of the spin polaron. It is only for larger values of $J/t>0.5$ that a redistribution of excess S_z is in favor of nearest neighbors and of lattice sites within one AFM sublattice, i.e., $R=1$ and $\sqrt{5}$, whereas the gain on the other sublattice can even be of the opposite sign. Note that spin correlations $\tilde{C}(\mathbf{R}_1,\mathbf{R}_2)$ explicitly depend on both vectors $\mathbf{R}_1,\mathbf{R}_2$. In Fig. 5 we present the three lowest correlations. These values should be compared to the AFM state without holes, where for $N=16$

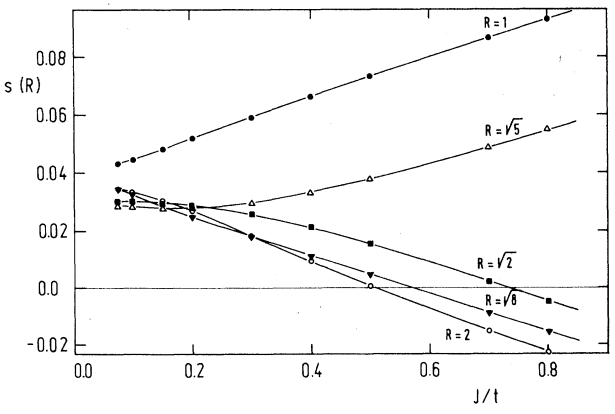

FIG. 4. Distribution of excess magnetization $s(R)$ vs J/t, plotted for all nonequivalent distances R on a 16-site cluster.

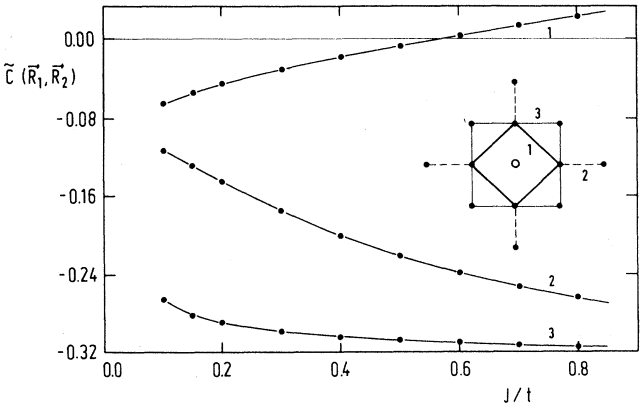

FIG. 5. Modified spin-spin correlation function $\tilde{C}(\mathbf{R}_1,\mathbf{R}_2)$ vs J/t. The numbers 1–3 label the three nonequivalent pairs of $\mathbf{R}_1$ and $\mathbf{R}_2$ given in the insert, where the hole is represented by the open circle.

$$C(R_{12}=1)=-0.3509\ ,$$

$$C(R_{12}=\sqrt{2})=0.2137\ ,$$

$\mathbf{R}_{12}=\mathbf{R}_1-\mathbf{R}_2$. The effect of a hole on nearest-neighbor correlations with $R_{12}=1$ is the reduction of them. The radial correlation, with $\mathbf{R}_1=(0,1)$, $\mathbf{R}_2=(0,2)$ is found to be more suppressed, while the azimuthal ones, with, e.g., $\mathbf{R}_1=(0,1)$ and $\mathbf{R}_2=(1,1)$, are less affected. The correlations between next-nearest neighbors, e.g., with $R_{12}=\sqrt{2}$, are also depressed or even change sign (see curve 1 in Fig. 5). These results indicate that the spin configuration is strongly perturbed in the vicinity of the hole. It is not easy to interpret our results in terms of several analytical approaches[13–16] to spin polaron configurations. Since azimuthal nearest neighbors $R_{12}=1$ are not significantly affected and second-neighbor $R_{12}=\sqrt{2}$ correlations are essentially zero in the relevant range of J/t, an approximate description can be given in terms of a ring of singlets surrounding the hole. We should stress, however, that since the translational invariance of the ground state is broken, due to $\mathbf{q}\neq 0$, the interpretation of the correlation function data becomes less straightforward.

IV. BINDING OF HOLES

Our calculations of eigenstates for two holes $N_h=2$ are not as extensive as for one hole since the computational requirements are substantially higher. On the other hand, contrary to the $N_h=1$ case, the ground state does not seem to change the quantum numbers with J/t. In the whole regime we investigated, the two-hole ground state was found to be a spin singlet $S=0$ and doubly degenerate, corresponding to $\mathbf{q}_1=(0,\pi)$ and $\mathbf{q}_2=(\pi,0)$. The latter conclusion already differs from the results of other authors.[13,14] These differences might be attributed to the much smaller basis sets used in previous calculations.[13,14]

Our results on the effective binding energy of the hole pair, defined through

$$\Delta = E_0(N_h=2) + E_0(N_h=0) - 2E_0(N_h=1) , \quad (8)$$

are presented in Fig. 6. They show that for the isotropic exchange Δ is negative in the whole regime of $J/t > J_c/t$. This is an indication of the existence of the attractive interaction between holes where the binding approximately scales with J. In order to check the importance of quantum spin fluctuations on Δ, we also performed the calculation in the limit $J_\perp = 0$ for four values of $J_\parallel = J$. These data are also plotted in Fig. 6 and show that one still has $\Delta < 0$ for $J/t \gtrsim 0.4$, where the reduced value of Δ can be, to some extent, attributed to lower effective J in this limit. Thus our results show that quantum spin fluctuations enhance the binding, in contrast to some analytical arguments.[13]

$\Delta < 0$ by itself cannot be used as a reliable test for the occurrence of binding since we are comparing states with different quantum numbers, specifically with different S at $N_h = 0, 1, 2$. An additional test is the hole-density correlation function

$$g(\mathbf{R}) = \sum_i \langle \Psi_0 | n_h(\mathbf{R}_i) n_h(\mathbf{R}_i + \mathbf{R}) | \Psi_0 \rangle . \quad (9)$$

In the case of the hole attraction, $g(\mathbf{R})$ shows a maximum at small distances R, while for repulsive holes the maximum will shift to largest possible R. As shown in Fig. 7(a) our results are consistent with the former case, at least for large J/t. For $J/t > 0.5$, $g(\mathbf{R})$ is largest for nearest neighbors, $R = 1$. In the intermediate region $0.2 < J/t < 0.5$, the preference is on next-nearest (diagonal) neighbors $R = \sqrt{2}$, while for $J/t < 0.15$ the repulsion between holes becomes evident through the enhanced occupation of most distant sites. Our observation that $g(R = \sqrt{2}) > g(R = 1)$ seems to be consistent with recent Monte Carlo results[29] for the single-band Hubbard model. We also tested the anisotropic case $J_\perp = 0$. The behavior is found to be qualitatively similar [see Fig. 7(b)], except that the transition to the repulsive regime occurs at higher $J/t \sim 0.5$.

Results for the spin correlations

$$C(\mathbf{R}) = \sum_i \langle \Psi_0 | \mathbf{S}(\mathbf{R}_i) \cdot \mathbf{S}(\mathbf{R}_i + \mathbf{R}) | \Psi_0 \rangle \quad (10)$$

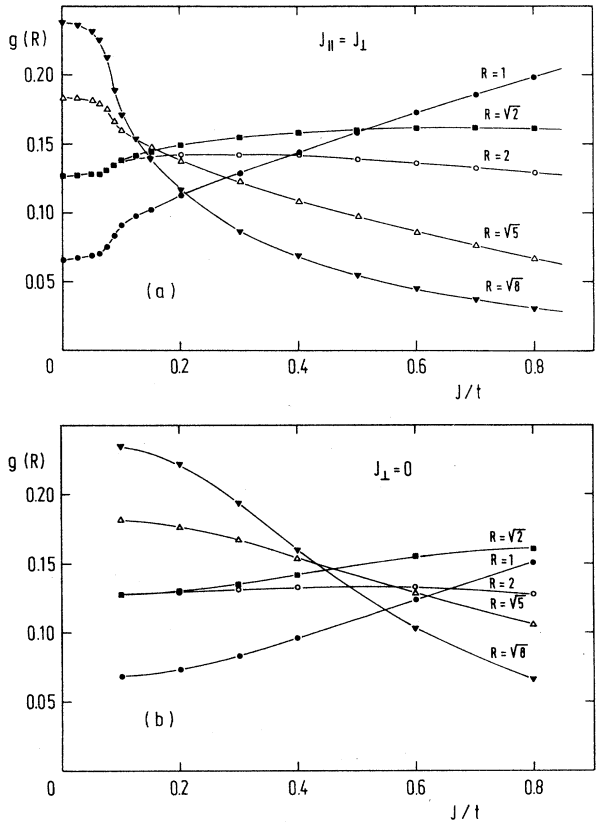

FIG. 7. (a) Hole-density pair-correlation function $g(R)$ vs J/t in the isotropic case. (b) Same as in (a), but for $J_\perp = 0$.

in the presence of two holes $N_h = 2$ are plotted in Fig. 8. In the region $J/t > 0.15$, the computed $C(\mathbf{R})$ are somewhat reduced but otherwise not qualitatively different from those in the AFM state without holes. A gradual change to an entirely different state happens below $J/t < 0.1$. The nearest-neighbor correlation $C(R = 1)$ becomes FM-like, while most distant spins, i.e., those at

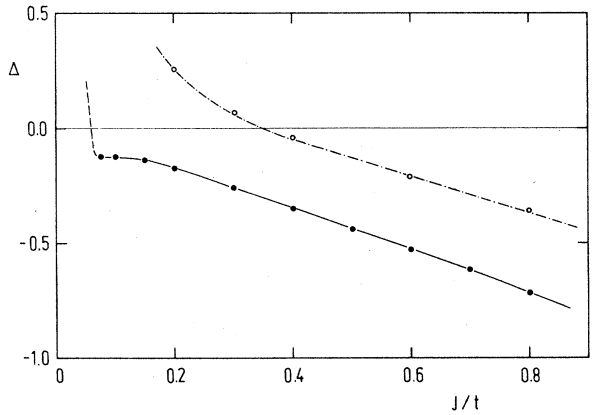

FIG. 6. Effective binding energy Δ of two holes (in units of t) vs J/t. Also shown are some results for the extreme anisotropic case $J_\perp = 0$ (dashed line).

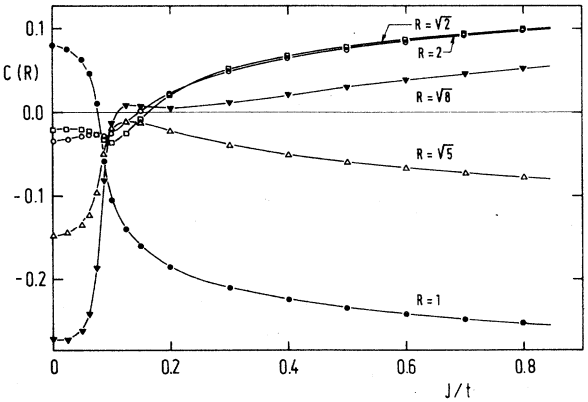

FIG. 8. Spin-pair-correlation function $C(R)$ vs J/t in the presence of two holes.

TABLE I. Some of the pairing correlation functions $Z_{lR,lR'}$ for two values of J/t. The type of pairing l is indicated in the first row. All entries should be multiplied by the factor 10^{-2}. No entries are given for p pairing when either R or R' is equal to 2, since in our case this pairing is identically zero.

				$J/t=0.4$						
l		s		p_x		p_y		d		
R \ R'	1	$\sqrt{2}$	2	1	$\sqrt{2}$	1	$\sqrt{2}$	1	$\sqrt{2}$	2
1	1.694	−1.256	−0.215	1.417	−1.080	1.417	0.938	7.381	0.181	−1.494
$\sqrt{2}$	−1.256	1.261	0.226	−1.080	1.812	0.938	1.491	0.181	0.543	0
2	−0.215	0.226	2.108					−1.494	0	2.108
				$J/t=0.8$						
1	1.978	−1.519	−0.295	1.641	−1.080	1.641	0.917	11.612	0.114	−1.459
$\sqrt{2}$	−1.519	1.427	0.264	−1.080	1.654	0.917	1.392	0.114	0.439	0
2	−0.295	0.264	1.755					−1.459	0	1.755

$R=\sqrt{8}$, prefer antiparallel orientation. Such situations, also observed in other models,[26] can be simply explained by the formation of two oppositely polarized FM-spin polarons that repel each other. This interpretation is consistent with the attractive-repulsive transition observed in $g(\mathbf{R})$ at $J/t\sim 0.15$.

In order to test the character of hole-pair wave functions, we also calculate several pairing correlation functions:

$$Z_{rr'}=\langle\Psi_0|\Delta_r^\dagger\Delta_{r'}|\Psi_0\rangle\ , \tag{11}$$

where Δ_r are hole-pair operators

$$\Delta_r=\frac{1}{\sqrt{N}}\sum_{\mathbf{k}} f_r(\mathbf{k})c^\dagger_{\mathbf{k}\uparrow}c^\dagger_{-\mathbf{k}\downarrow} \tag{12}$$

relating to the wave functions $f_r(\mathbf{k})$ and corresponding to different point symmetries and total spin. We consider only the set of Δ_r which tests the holes being at smallest distances $R=1$, $\sqrt{2}$, and 2. The nonequivalent orthogonal functions $f_r(\mathbf{k})$ for the square lattice can be then classified as $r=s\mathbf{R}$-, $d\mathbf{R}$-, or $p\mathbf{R}$-type, where $\mathbf{R}=(n,m)$ denotes the radial vector between holes, and

$$f_{s\mathbf{R}}(\mathbf{k})=\cos(k_x n+k_y m)+\cos(k_x m-k_y n)\ , \tag{13a}$$

$$f_{d\mathbf{R}}(\mathbf{k})=\cos(k_x n+k_y m)-\cos(k_x m-k_y n)\ , \tag{13b}$$

$$f_{p\mathbf{R}}(\mathbf{k})=\sqrt{2}\sin(k_x n+k_y m)\ . \tag{13c}$$

If the ground state would be a $\mathbf{q}=0$ spin singlet state, s-, p-, and d-wave pairing correlations would not mix. In addition one would also have $Z_{d1,d\sqrt{2}}=0$, where we characterize $\mathbf{R}$ just be the distance $R=(n^2+m^2)^{1/2}$. Since our $|\Psi_0\rangle$ for two holes is degenerate due to $\mathbf{q}\neq 0$, some of these mixed correlations remain nonzero, but they do not seem to be essential. In Table I we present results for some of the largest diagonal and offdiagonal pairing functions $Z_{rr'}$ for two values of J/t. It is evident that the largest correlation is $Z_{d1,d1}$, which increases relative to other components with increasing J/t. This indicates that the largest coherent contribution comes from hole pairs being in the d state on nearest neighbors. Still, this contribution exhausts only a smaller part of $|\Psi_0\rangle$, since $Z_{d1,d1}\ll 1$. Namely, the value for ideal $d1$ pairs would be $Z_{d1,d1}=1$. From these data we also see that all other pairing functions, with the exception of some offdiagonal $Z_{r,r'}$ that are small, are roughly of the same value and do not change appreciably with J. However, for $R=\sqrt{2}$, which in the intermediate J/t regime is the preferential distance [as deduced from the hole density-density correlations $g(\mathbf{R})$], the pairing character is quite uniformly distributed over the s and p waves, whereas d pairing is suppressed. We also calculated the $Z_{s1,d1}$ pairing function and found it to be small, i.e., $\lesssim 10^{-3}$ so that there is almost no mixing of $s1$ and $d1$ waves.

One can as well look for a normalized $\tilde{\Delta}$,

$$\tilde{\Delta}=\sum_r \alpha_r\Delta_r,\quad \sum_r|\alpha_r|^2=1\ , \tag{14}$$

which would maximize $\tilde{Z}$:

$$\tilde{Z}=\langle\Psi_0|\tilde{\Delta}^\dagger\tilde{\Delta}|\Psi_0\rangle\ . \tag{15}$$

$\tilde{\Delta}$ can then be interpreted as the best effective two-particle representation of the many-body wave function $|\Psi_0\rangle$ for a bound hole pair. Our results show that in the regime of bound holes, the optimal $\tilde{\Delta}$ still corresponds to the d wave.

V. CONCLUSIONS

In the paper we presented numerical results for the ground-state properties of a single hole and two holes in a quantum AFM. We restricted our calculations to the system of 16 cells. At least for $J/t>0.4$, perturbations due to a single-spin polaron as well as for a hole pair seem to be quite localized, so one may expect that conclusions would remain qualitatively similar for larger systems. The very symmetric 4×4 system with periodic boundary conditions used in our calculations has, however, some consequences: It leads to a large, i.e., sixfold, degeneracy with respect to $\mathbf{q}$ of the single-hole ground state, which is expected to remain only approximate in an infinite system.[13,14] To some extent quite substantial binding energy of two holes may also be attributed to specific nesting conditions of our lattice.

Our results clearly indicate that bound pairs could be stable in the effective model in a wide range of $J/t > 0.1$. The situation is thus essentially different from the corresponding model (1) on a chain,[25] where $g(R)$ was found to increase with R in the whole regime of J, being an evident indication against hole-hole attraction. However, the interpretation of the binding mechanism in our two-dimensional system is less straightforward. The fact that we found a weak binding $\Delta < 0$ even in the Ising limit, seems to support a simple interpretation in terms of broken exchange bonds.[12–15] Namely, assuming that both holes are entirely localized, they would prefer to be on adjacent sites in the Néel AFM state, gaining an energy $J/2$. This argument is, however, oversimplified since holes were found to be correlated over a substantially larger distance $R > 1$, while the binding energy is even enhanced in the Heisenberg exchange case, i.e., $|\Delta| \sim J$. This is an indication that spin fluctuations[16] contribute substantially to the formation of the bound-hole pairs. The interpretation of these results is, however, complicated by the fact that the two-hole ground state is degenerate, corresponding to $\mathbf{q} \neq 0$. The coherent character of the bound-pair wave function is found to be predominantly that of the d-wave type, with holes being on the adjacent sites. Still this component does not by far exhaust the many-body two-hole wave function. Thus contributions from other pairing functions, even those with $\mathbf{q} \neq 0$, are expected to remain substantial. Which of these components could possibly lead to SC pairing still remains to be shown.

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