One-hole motion in the two-dimensional frustrated t-J model

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(Received 2 October 1995; revised manuscript received 21 December 1995)

The influence of a frustration term in the exchange part of the t-J model onto the dispersion relation of one hole has been investigated. We have chosen two independent methods, namely, a variational ansatz which describes a magnetic polaron of minimal size and the exact diagonalization method of a 4×4 lattice. It has been found that the frustration shifts the minimum from the point $(\pi/2,\pi/2)$ to the point $(0,\pi)$ in k space. It has also been shown that the frustration term alone does not lead to the correct, experimentally observed flat dispersion region around $(0,\pi)$. A better agreement with the observed, extended saddle point singularity may be obtained by simulating the decrease of spin correlations due to a finite temperature.

I. INTRODUCTION

There exist already numerous studies of the single-hole motion in the two-dimensional (2D) t-J model. These studies are based on the exact diagonalization of small clusters,[1,2] the self-consistent Born approximation,[3,4] or a "string" ansatz for the hole wave function.[5] One can also start from a spin-rotational-invariant spin liquid state[6] instead of dealing with the two-sublattice Néel-type state[3–5] and obtain qualitatively the same result: The hole motion occurs mainly on one sublattice; i.e., the dispersion relation is dominated by an effective hopping to next nearest neighbors with the minimum of the dispersion at $(\pi/2,\pi/2)$. Throughout the present work we will choose the hole picture and we will set the lattice constant to unity $a=1$. It is generally believed that the t-J model describes qualitatively the hole spectrum of the CuO_2 plane in high-temperature superconductors. Recently, it has been possible to measure that dispersion directly in the insulating compound, namely, in the compound $Sr_2CuO_2Cl_2$, by angle-resolved photoemission.[7] In agreement with the theory of the t-J model, the minimum of the dispersion was found to be at $(\pi/2,\pi/2)$. But the energy at $(0,\pi)$ was found to be much higher in the experiment than in the calculations of the t-J model, such that it was nearly degenerate with the value at the Γ point (0,0). That shows already the necessity to extend the original t-J model. Furthermore, after doping the system, the experiment (see, e.g., Ref. 8) shows that the dispersion changes drastically: The energy value at $(0,\pi)$ goes down with respect to the Γ point such that a remarkable dispersion occurs along the line $(k_x,0)$. In the optimally doped compounds, the dispersion relation is characterized by a flat region close to the point $(0,\pi)$.[8,9] The energy value at the point (π,π) is even more affected by the doping than the energy value at $(0,\pi)$. As a result, it seems to be that the spectrum of the doped compounds resembles more a nearly free dispersion with effective nearest neighbor hopping and the photoemission data are usually interpreted in terms of a large Fermi surface.[9] Also numerical calculations on finite size systems indicate a large Fermi surface in the case of strong doping.[11]

The effect of doping can be simulated in several ways. The first possibility is a frustration term in the Hamiltonian as was proposed, for instance, in Ref. 10. Another possible way is the inclusion of a finite temperature. This brings about a decrease of the spin-spin correlation functions in a similar way as can be expected from the doping process. For very high temperatures one finds a dispersion which is dominated by an effective nearest neighbor hopping[6] which may explain the transition to a large Fermi surface. In the present work we will investigate the effect of frustration and temperature on the dispersion relation of one hole. We are interested in the question if the frustration or temperature has a similar effect as has the doping in the experiments. Especially, we will investigate if the energy value at $(0,\pi)$ goes down with respect to the other energies and if there occurs an extended saddle point in the vicinity of $(0,\pi)$.

We will choose two methods to investigate the effect of frustration on the dispersion of one hole, a variational method and the exact diagonalization of a 4×4 lattice. The variational ansatz describes the one-hole state as a magnetic polaron of minimal size and is an improvement of the ansatz used in Ref. 6. Within that method the dispersion is determined by static spin-spin correlation functions. These are calculated here in a spin-rotational-invariant Green's function method[12] (see also the zero-temperature version[13]). We describe the state of the magnetic subsystem as a spin liquid state in contrast to the widely used two-sublattice Néel-type state due to several reasons. At first, our choice gives the possibility to avoid the degeneracy of the hole spectrum between the points (0,0) and (π,π) which always occurs in the Néel-type state. Second, the spin liquid state does not contradict the Mermin-Wagner theorem[14] which forbids magnetic order in two dimensions for any finite temperature. So it gives the possibility to investigate one-hole motion at non-

zero temperatures. Of course, the variational ansatz corresponds to an approximate method. Therefore, it is reasonable to investigate the problem by the exact diagonalization method and to compare the results of two independent procedures. Let us remember, however, that also the exact diagonalization method has some shortcomings, such as finite-size effects, for instance. We will see that both methods complement each other.

The paper will be organized as follows. At first, in Sec. II we will present both methods, i.e., the variational ansatz and the exact diagonalization method. Then we show the results of both methods for zero-temperature and increasing frustration (Sec. III). We discuss also the influence of temperature on the dispersion relation in the frustrated and nonfrustrated cases. Finally we present our conclusions.

II. VARIATIONAL ANSATZ VS EXACT DIAGONALIZATION

We consider here the 2D t-J model on a square lattice with an exchange interaction that contains a frustration term,

$$H=H_t+H_J=-\sum_{ia\sigma} t_a X_i^{\sigma 0}X_{i+a}^{0\sigma}+\frac{1}{2}\sum_{ib} J_b \vec{S}_i\cdot\vec{S}_{i+b}, \quad (1)$$

where

$$t_a=\begin{cases} t_1>0 & \text{if } a \text{ is a nearest neighbor vector,}\\ 0 & \text{otherwise,}\end{cases} \quad (2)$$

and

$$J_b=\begin{cases} J_1>0 & \text{if } b \text{ is a nearest neighbor vector,}\\ J_2>0 & \text{if } b \text{ is a next nearest neighbor vector,}\\ 0 & \text{otherwise.}\end{cases} \quad (3)$$

The Hubbard operator $X_i^{0\sigma}=c_{i\sigma}(1-n_{i-\sigma})$ annihilates an electron with spin projection $S_i^z=\sigma/2$ at site i with no double occupancy and σ is a spin index $\sigma=+1$ or -1. Analogously, $X_i^{\sigma\sigma}=n_{i\sigma}(1-n_{i-\sigma})$, $X_i^{\sigma-\sigma}=c_{i\sigma}^{\dagger}c_{i-\sigma}$, and the spin operators are expressed as

$$S_i^{\sigma}=X_i^{\sigma-\sigma}, \quad S_i^z=\frac{1}{2}\sum_{\sigma}\sigma X_i^{\sigma\sigma}. \quad (4)$$

If each place is occupied by exactly one electron, also the completeness relation holds, $1=\Sigma_{\sigma}X_i^{\sigma\sigma}$. Without a hole, model (1) has already been investigated by many methods[12,13,15–17] and with increasing frustration J_2 several transitions from the antiferromagnetic to a spin liquid and the collinear stripe phase were found. Our following analytical calculation is based on the Green's function procedure[12] which has the advantage that it is spin rotational invariant and can be applied also at finite temperature.

Now, we look for the lowest state of (1) with one hole and a fixed momentum. We choose a variational ansatz which is constructed from the following five basis vectors $\phi_i^{a^{\dagger}}|\Psi_0)$ with $a=0,1,\ldots,4$. Here, the vector $|\Psi_0)$ denotes the spin-rotational-invariant singlet ground state of the pure spin system H_J without any hole. The corresponding five basis operators $\phi_i^{a^{\dagger}}$ are

$$\phi_i^0=X_i^{\sigma 0}, \quad \phi_i^a=\sum_s X_{i-a}^{\sigma s}X_i^{s0} \quad (a=1,\ldots,4), \quad (5)$$

where we will use the following notation hereafter: The small latin letter a denotes either a number between 0 and 4 or the corresponding lattice vector

$$\begin{aligned} 0\leftrightarrow(0,0) \quad 1\leftrightarrow(1,0) \quad 3\leftrightarrow(-1,0),\\ 2\leftrightarrow(0,1) \quad 4\leftrightarrow(0,-1),\end{aligned} \quad (6)$$

in a synonymous way. The set of operators (5) represents a magnetic polaron of minimal size. It may be seen that $\phi_i^{a^{\dagger}}|\Psi_0)$ corresponds to a one-hole state with a total spin 1/2 and with a spin-z projection $-\sigma/2$. We are interested in our variational approach only in states with total spin 1/2 since it is known that these states represent the bottom of the lowest band. The basis operator $\phi_i^{0^{\dagger}}$ corresponds to the creation of a hole on site i in the state $|\Psi_0)$ without any additional spin excitation. The remaining operators $\phi_i^{1^{\dagger}},\ldots,\phi_i^{4^{\dagger}}$ create a hole and an additional spin excitation at the neighboring site. They appear after acting with the kinetic energy operator on the state $\phi_i^{0^{\dagger}}|\Psi_0)$. A similar ansatz was already used in Ref. 6 where, however, only a fixed combination of $\phi_i^{1^{\dagger}},\ldots,\phi_i^{4^{\dagger}}$ was chosen. Treating them as independent states has the advantage that it gives correctly the limit $t_1=0$ where no dispersion should remain.

We will calculate the energy eigenvalues as in the Ritz variational procedure using the basis (5). For that we have to calculate the overlap matrix which is defined after Fourier transformation as

$$S^{ab}=\sum_j \langle \phi_l^a \phi_j^{b^{\dagger}}\rangle e^{ik(j-l)} \quad (a,b=0,\ldots,4), \quad (7)$$

where $\langle\cdots\rangle$ means the average with the ground state $(\Psi_0|\cdots|\Psi_0)$. It turns out that the overlap matrix does not depend on the momentum k, and its matrix elements are given by

$$\begin{aligned} S^{aa}&=1/2 \quad (a=0,\ldots,4),\\ S^{0a}&=Z_a \quad (a=1,\ldots,4),\\ S^{ab}&=D_{a,a-b} \quad (a,b=1,\ldots,4) \quad (a\neq b),\end{aligned} \quad (8)$$

where we introduced the abbreviations

$$Z_a=\sum_s \langle X_i^{\sigma s}X_{i+a}^{s\sigma}\rangle, \quad (9)$$

$$D_{a,b}=\sum_{s_1s_2} \langle X_i^{\sigma s_1}X_{i+a}^{s_1s_2}X_{i+b}^{s_2\sigma}\rangle, \quad (10)$$

and for further use we define, also,

$$V_{a,b,c}=\sum_{s_1s_2s_3} \langle X_i^{\sigma s_1}X_{i+a}^{s_1s_2}X_{i+b}^{s_2s_3}X_{i+c}^{s_3\sigma}\rangle. \quad (11)$$

The definitions (9)–(11) are only valid for noncoinciding lattice sites different from zero, $a\neq b\neq c\neq 0$. Note that the lattice sites $a-b$ which occur in (8) can be different from

nearest and next nearest neighbors. Using the spin-rotational-invariance we obtain from (9)–(11)

$$Z_a = \tfrac{1}{4} + S_a, \quad S_a = \langle \vec{S}_i \cdot \vec{S}_{i+a} \rangle, \tag{12}$$

$$D_{a,b} = \tfrac{1}{8} + \tfrac{1}{2}(S_a + S_b + S_{b-a}), \tag{13}$$

$$V_{a,b,c} = \tfrac{1}{16} + \tfrac{1}{4}(S_a + S_b + S_c + S_{b-a} + S_{c-a} + S_{c-b}) + \Sigma_{abc} - \Sigma_{bac} + \Sigma_{cab}, \tag{14}$$

where the following four-point spin-correlation functions appear:

$$\Sigma_{abc} = \langle (\vec{S}_i \cdot \vec{S}_{i+a})(\vec{S}_{i+b} \cdot \vec{S}_{i+c}) \rangle. \tag{15}$$

Next we determine the kinetic energy matrix

$$K^{ab}(k) = \sum_j \langle [\phi_l^a, H_t] \phi_j^{b\dagger} \rangle e^{ik(j-l)} \quad (a,b = 0,\ldots,4), \tag{16}$$

which depends explicitly on k. Here, we calculate the Hamilton matrix element not in the form $\langle \phi_i^a H \phi_j^{b\dagger} \rangle$, but by means of the commutator. Both definitions coincide if we assume a zero ground state energy of the pure spin Hamiltonian, i.e., of the state $|\Psi_0\rangle$. In other words, the variational ansatz gives the energy difference between the lowest state with one hole and a given momentum and the ground state energy without any hole. The matrix elements (16) are calculated to be

$$K^{00}(k) = \sum_{a=1}^{4} t_a Z_a e^{ika}, \tag{17}$$

$$K^{0a}(k) = \frac{1}{2} t_a e^{ika} + \sum_{c=1}^{4} \overline{\delta_{ac}} t_c D_{c,c-a} e^{ikc} \quad (a = 1,\ldots,4), \tag{18}$$

where we introduced $\overline{\delta_{ac}} = 1 - \delta_{ac}$ and $\delta_{ac} = 1$ for $a = c$ and zero elsewhere. Further, we obtain

$$K^{aa}(k) = t_a Z_a (e^{ika} + e^{-ika}) + \sum_{c=1}^{4} \overline{\delta_{ac}}\, \overline{\delta_{-a,c}} t_c V_{a,a+c,c} e^{ikc} \quad (a = 1,\ldots,4) \tag{19}$$

and for $a \neq b$ $(a,b = 1,\ldots,4)$

$$K^{ab}(k) = \overline{\delta_{-a,b}} t_b Z_a e^{ikb} + t_a Z_b e^{-ika} + t_{b-a} Z_{b-a} e^{ik(b-a)} + \sum_{c=1}^{4} \overline{\delta_{-a,c}}\, \overline{\delta_{bc}}\, \overline{\delta_{b-a,c}} t_c V_{a,a+c,a+c-b} e^{ikc}. \tag{20}$$

Analogously, we obtain the matrix of the exchange energy which does not depend on the momentum k like the overlap matrix $\underline{S}$,

$$E^{ab} = \langle [\phi_i^a, H_J] \phi_i^{b\dagger} \rangle = (J_1 + J_2) S^{ab} + \tilde{E}^{ab} \quad (a,b = 0,\ldots,4), \tag{21}$$

where the matrix elements $\tilde{E}^{ab}$ have the form

$$\tilde{E}^{00} = -\frac{1}{2} \sum_{c=1}^{8} J_c Z_c, \tag{22}$$

$$\tilde{E}^{0a} = -\sum_{c=1}^{8} J_c \left(\frac{\delta_{ac}}{4} + \frac{\overline{\delta_{ac}}}{2} D_{c,c-a} \right) \quad (a = 1,\ldots,4), \tag{23}$$

$$\tilde{E}^{aa} = -\sum_{c=1}^{8} J_c \left[\frac{\delta_{ac}}{2} Z_c + \overline{\delta_{ac}} \left(Z_c - \frac{Z_{c-a}}{2} \right) \right] \quad (a = 1,\ldots,4), \tag{24}$$

$$\tilde{E}^{ab} = \frac{1}{2} \sum_{c=1}^{8} J_c [-\delta_{bc} Z_{a-b} - \delta_{ac} Z_b + \delta_{c-a,-b} (Z_{a-b} - Z_a) - \overline{\delta_{ac}}\, \overline{\delta_{bc}} V_{a-c,a,a-b} + \overline{\delta_{ac}}\, \overline{\delta_{c-a,-b}} (V_{c,a,a-b} - V_{-c,a-c,a-c-b})] \quad (a \neq b) \quad (a,b = 1,\ldots,4). \tag{25}$$

Here, the summation c runs over nearest and next nearest neighbors. The Hamilton matrix is then given by $\underline{H} = \underline{K} + \underline{E}$ and the lowest eigenvalue of the diagonalization of $\underline{H}\,\underline{S}^{-1}$ gives the quasiparticle dispersion. Of course, our method cannot take into account the quasiparticle damping. The lowest eigenvalues, however, correspond to the coherent part of the spectrum which was found in Refs. 1–4. From Eqs. (12)–(15) one can see that in our method the Hamilton and overlap matrices are completely determined by static spin-spin correlation functions. In our calculation we will approximate the four-point spin correlation functions (15) as in a linear spin wave theory (see also Ref. 18), i.e.,

$$\Sigma_{abc} = S_a S_{c-b} + \tfrac{1}{3} S_b S_{c-a} + \tfrac{1}{3} S_c S_{b-a}. \tag{26}$$

As a result, the spectrum is completely determined by the static two-point spin-spin correlation functions. They have to be calculated from the Heisenberg model with frustration. We choose here the Green's function method.[12] As one can see, only the short-range magnetic order is important in our ansatz.

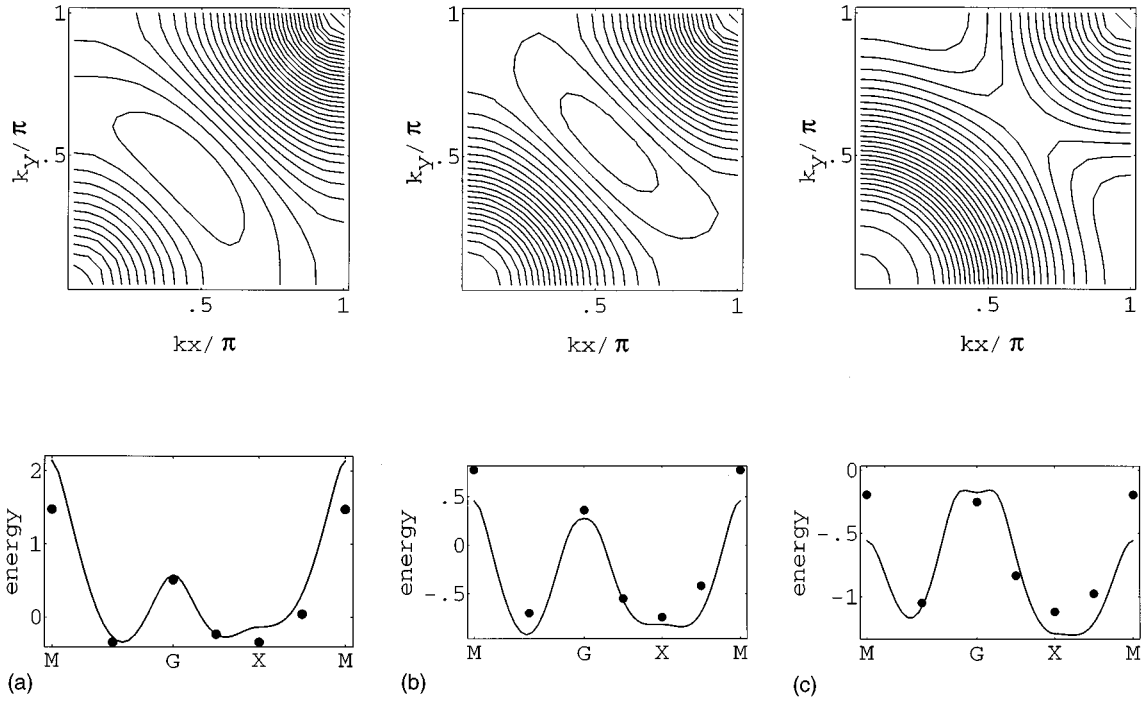

FIG. 1. Quasiparticle dispersion along the line M-G-X-M and contour plot for $J_1=t_1=1$, $T=0.085$, and increasing frustration: (a) $J_2=0$, (b) $J_2=0.2$, and (c) $J_2=0.4$. The points in k space mean $M=(\pi,\pi)$, $G=(0,0)$, and $X=(0,\pi)$. The circles are the result of the exact diagonalization of a 4×4 lattice at $T=0$ with total spin $S=1/2$.

The Lanczos exact diagonalization scheme is used as a complementary method to calculate the low-lying eigenstates for a square lattice of 4×4 sites (with periodic boundary conditions). These low-lying states are classified by momentum k and the total spin. Here we will concentrate on the band with total spin 1/2. There are only few exceptions [for the higher states with momentum (π,π) or $(0,0)$] where the lowest states have spin 3/2. It was already mentioned that the variational ansatz gives the energy difference between the lowest state with one hole for total spin 1/2 and fixed momentum and the ground state without any hole. The same energy difference is calculated for the 4×4 lattice and we will compare both methods in the next section.

III. NUMERICAL RESULTS

In Fig. 1 we show the influence of frustration on the one-hole motion at zero-temperature for $J_1=1$. In our calculations we will take t_1 as the unit of energy and we put $t_1=1$. One observes a quite reasonable agreement between the variational ansatz and the exact diagonalization data for these parameter values. And the important effect of the frustration, namely, that the energy at the point $X=(0,\pi)$ is decreased in comparison with the energy at $(\pi/2,\pi/2)$, is visible in both methods. That coincidence is understandable since for such large values of J_1 the magnetic energy stabilizes the size of the magnetic polaron and our concept of a polaron of small radius is justified. Let us note that for $J_1\ll t_1$ the bandwidth tends to be proportional to J_1.[1–5] In principle this result may also be obtained within our variational procedure if we enlarge the polaron size by taking into account more trial wave functions. However, the results for $J_1=1$ are already representative for the more realistic value $J_1=0.4$ if we scale the bandwidth by a factor of roughly 0.4. That is seen in Fig. 2 where we compare the exact diagonalization results for both values of J_1 dependent on J_2/J_1. For simplicity we did not subtract the ground state energy without a hole in Fig. 2 in contrast to the energy scales in Figs. 1 and 3.

Let us now discuss in more detail the results for zero-temperature and without frustration [Fig. 1(a)]. In that case the data of our exact diagonalization procedure coincide with that given by Dagotto *et al.*,[2] besides another sign of the hopping amplitude t_1 in Ref. 2. That can be compensated shifting by (π,π) in k space. Due to the special 4×4 size of the lattice, exact diagonalization leads to a degeneracy between $(\pi/2,\pi/2)$ and $(0,\pi)$ in the absence of frustration. The variational method gives the opportunity to clarify that the minimum of the spectrum is close to $(\pi/2,\pi/2)$. Nevertheless, also the variational method shows that $(\pi/2,\pi/2)$ and $(0,\pi)$ are very near in energy. In the corresponding contour plot one may easily observe a flat region around the minimum near $(\pi/2,\pi/2)$ in the direction of $(0,\pi)$.

If we increase the frustration, we can observe from Figs. 1(b) and 1(c) that the minimum and also the flat region are moved to a point of the line $(0,\pi)$-$(\pi/2,\pi)$. Also in the data of the exact diagonalization (Fig. 2) we see that the energy distance between the points $(\pi/2,\pi/2)$ and $(0,\pi)$ increases with frustration, whereas the distance between $(0,\pi)$ and $(\pi/2,\pi)$ decreases. For $J_2=0.5$ the last two points are even equal in energy. The flat dispersion region between $(0,\pi)$ and $(\pi/2,\pi)$ which can be observed in Fig. 1(c), resembles the flat dispersion region which may be observed in the photoemission experiment of the doped compound. But there it extends from $(0,\pi)$ into the direction of $(0,\pi/2)$. A second

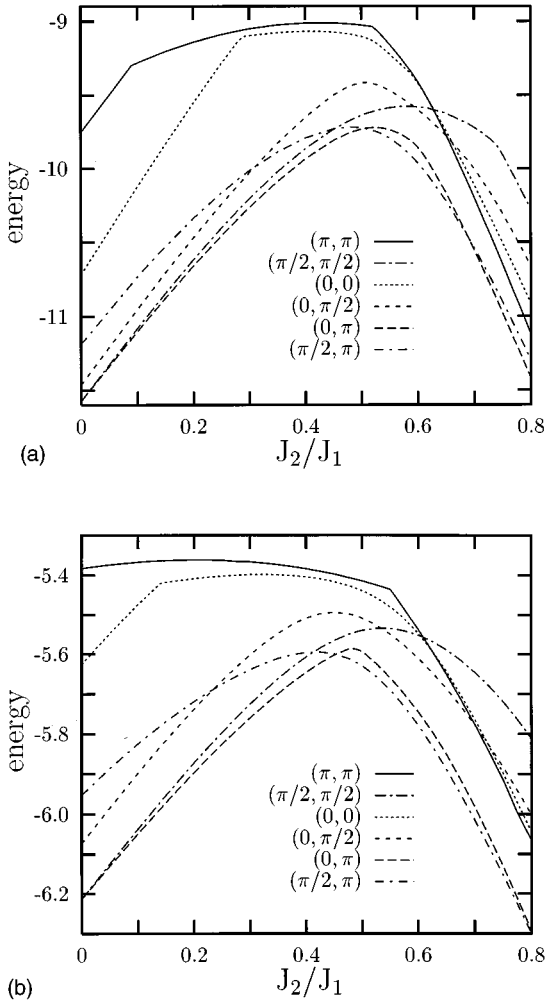

FIG. 2. The lowest-energy values of the 4×4 lattice for several momenta and total spin $S=1/2$ for (a) $J_1=t_1=1$ and (b) $J_1=0.4$, $t_1=1$ dependent on the frustration. Discontinuities in the slope are due to level crossings for the lowest state. In the region $J_2/J_1 \leq 0.2$ and for momentum (π,π) (in both cases) and (0,0) (only for $J_1=0.4$) there are even lower states with total spin $S=3/2$ which are not shown.

shortcoming of our data in comparison with experiment is the low-lying energy at $(0,\pi)$ without frustration. In the experiment one observes $(0,\pi)$ much higher in energy and, connected with that, a much more isotropic minimum around $(\pi/2,\pi/2)$. It may be that both features can be obtained due to the inclusion of a next nearest neighbor hopping term in our calculation. Such an additional term arises if we understand the t-J model as derived from the p-d model of the CuO_2 plane, taking into account direct oxygen-oxygen hopping.

In Fig. 2 we present the low-lying eigenstates of the 4×4 lattice with total spin 1/2 and several momenta for $J_1=1$ [Fig. 2(a)] and $J_1=0.4$ [Fig. 2(b)]. The similarity between both sets of curves is remarkable. Only the bandwidth is scaled. In both cases, the lowest state for $J_2/J_1 \leqslant 0.5$ has momentum $(0,\pi)$, and by increasing J_2/J_1 further, the state with momentum $(\pi/2,\pi)$ becomes the lowest one. There is a minor difference that the lowest state for $J_1=1$ and $J_2/J_1 \geqslant 0.7$ has momentum $(0,\pi)$. Such small differences,

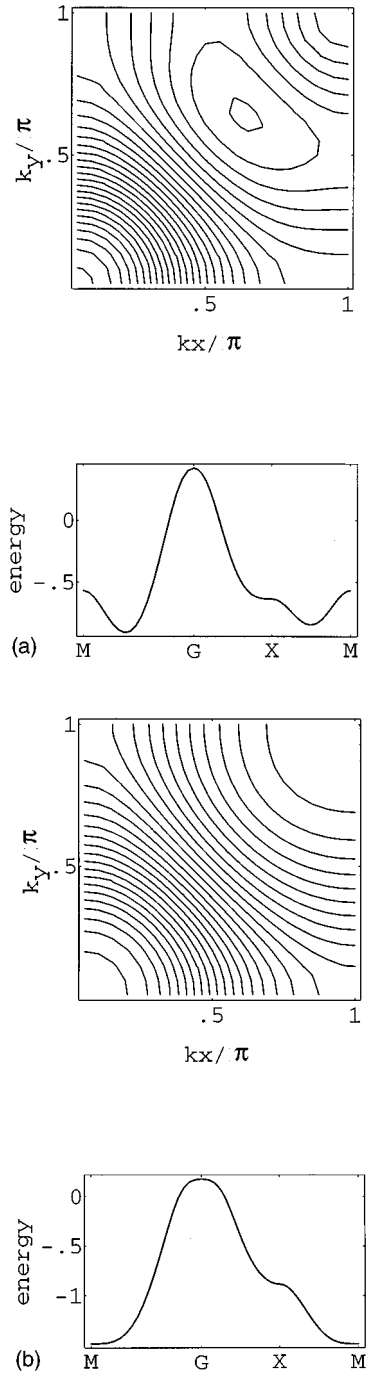

FIG. 3. Dispersion and contour plot for $J_2/J_1=0$ and different temperatures: (a) $T=0.8$ and (b) $T=1$. The other parameters are as in Fig. 1.

however, do not change the general statements. Level crossings between several bands with the same momentum and $S=1/2$ may be observed in Fig. 2 due to changes in the slope. Up to $J_2/J_1 \simeq 0.5$ the bandwidth of the $S=1/2$ band is diminished due to frustration. For still larger values of J_2 ($J_2/J_1>0.6$) there occurs a complete rearrangement of the spectrum. That is connected with the fact that for such large values of J_2 a completely new magnetic structure appears, close to the collinear stripe phase.[17] Of course, it is questionable whether such large values of J_2 may still be connected with the doping process.

TABLE I. Spin-spin correlation functions $S_a=\langle \vec{S}_i \cdot \vec{S}_{i+a}\rangle$ for the pure spin model H_J without any hole as obtained from the Green's function (GF) method for $T=0.085$ and by exact diagonalization of the 4×4 lattice for different frustration J_2/J_1 .

	$J_2/J_1=0$		$J_2/J_1=0.2$		$J_2/J_1=0.4$	
	GF	4×4	GF	4×4	GF	4×4
$S_{(1,0)}$	−0.352	−0.351	−0.282	−0.349	−0.208	−0.332
$S_{(1,1)}$	0.229	0.214	0.116	0.193	−0.002	0.141
$S_{(2,0)}$	0.200	0.214	0.091	0.194	0.047	0.151
$S_{(2,1)}$	−0.188	−0.202	−0.063	−0.165	0.007	−0.086
$S_{(2,2)}$	0.165	0.180	0.038	0.142	−0.004	0.058

Within the variational method, the one-hole dispersion will be determined by the two-point spin-spin correlations which act like parameters. Changing the spin-spin correlations also changes the dispersion. In Table I we compare the spin-spin correlations from the Green's function method[12] with the exact diagonalization of the 4×4 lattice. One needs more distant spin-spin correlation functions in the variational ansatz than are shown in Table I. In the exact diagonalization approach, due to the periodic boundary conditions of the finite lattice (4×4), the distant spin-spin correlation functions are traced back to that shown in Table I, i.e., $S_{(3,0)}=S_{(1,0)}, S_{(3,1)}=S_{(1,0)}, S_{(3,1)}=S_{(1,1)}, S_{(3,2)}=S_{(2,1)}$, and they do not decay with distance. The variational ansatz uses the results of the Green's function method[12] which is free from this shortcoming. One may observe that the data coincide quite well for $J_2=0$, but there are remarkable differences if we increase the frustration (see also Ref. 13). There may be several reasons for this discrepancy. On the one hand, the exact diagonalization has difficulties for large values of J_2/J_1 and especially in the limit $J_1=0$ when the lattice decouples into two noninteracting sublattices with only eight spins in each of them. The Green's function method describes this limit correctly; i.e., for instance, $S_{(2,2)}$ at $J_1=0$ coincides with $S_{(1,1)}$ at $J_2=0$.[13] On the other hand, it seems that the Green's function method overestimates the influence of frustration and leads to a rather wide region of the spin liquid state in the phase diagram. But as may be seen from Fig. 1, both sets of spin correlations lead qualitatively to a similar effect of frustration on the low-lying parts of the spectra.

Let us mention some additional points in the discussion. Without frustration [Fig. 1(a)] one may observe the variational property of our ansatz; i.e., its energy values are always higher than the exact diagonalization values. This property is destroyed for Figs. 1(b) and 1(c). That is due to the larger deviations of the spin-spin correlations (Table I) for the frustration values $J_2=0.2$ and 0.4. If we choose for the spin correlations in our variational ansatz the values from the exact diagonalization (Table I), the curves are shifted in such a way that the variational property will be restored. However, the overall agreement is not better than that shown in Figs. 1(b) and 1(c). Another point is that we have chosen $T=0.085$ instead of a zero-temperature in the numerical procedure[12] to calculate the spin-spin correlation function. The reason is that it is numerically simpler to deal with a small finite temperature. The results for S_a, however, are nearly not distinguishable from their values at $T=0$ (see Ref. 12).

It is seen from Fig. 1 that the frustration alone leads to a flat dispersion region but not to an extended saddle point which is experimentally observed. Therefore, it is interesting to investigate if such an effect may be obtained by increasing the temperature. It is clear that at very high temperatures the antiferromagnetic short-range order is destroyed and the spin-spin correlation functions are purely paramagnetic. In this case the spectrum is dominated by an effective nearest neighbor hopping with a saddle point at $(0,\pi)$ which is shown in Fig. 3(b). For a slightly lower temperature ($T=0.8$), namely if the magnetic correlation length is of the order of the magnetic polaron size,[6] one observes a very interesting dispersion relation [Fig. 3(a)]. As is seen, the spectrum has not only a flat dispersion region in the vicinity of the point $(0,\pi)$, but it also demonstrates the occurrence of an extended saddle point along the same direction as in the experiment. For lower temperatures $T\lesssim0.6$ the spectrum is very similar to the zero-temperature one [see Fig. 1(a)]. A similar destruction of the magnetic polaron due to temperature as in Fig. 3 was already observed in Ref. 6. But now we find a more pronounced extended saddle point feature [Fig. 3(a)] than in Ref. 6. That may be due to the larger basis in the present calculation.

Finally, we have also investigated the influence of a finite temperature in the frustrated case. As can be expected, one also observes for large enough temperature a dispersion which is dominated by nearest neighbor hopping. Surprisingly, the temperature which is needed to change the dispersion is only slightly reduced in the frustrated case in comparison with the nonfrustrated one. Then we obtain a dispersion similar to Fig. 3(b). An extended saddle point between the points $(0,\pi/2)$ and $(0,\pi)$ as in Fig. 3(a), however, was not obtained if we increase the temperature in the frustrated case. That is also the reason why we do not show further pictures.

IV. CONCLUSION

The experiment shows that the quasiparticle dispersion of the copper-oxygen plane is drastically changed by the doping process. One may observe two main features: First, the energy value at the point $(0,\pi)$ in k space is shifted downwards, and second, there occurs an extended saddle point singularity between $(0,\pi/2)$ and $(0,\pi)$. To simulate the effect of doping in a study of one-hole motion in a quantum antiferromagnet we have compared two possibilities, namely, the influence of frustration or a finite temperature.

It was found that the frustration shifts the minimum of the hole dispersion from $(\pi/2,\pi/2)$ to the point $(0,\pi)$. That was obtained within two different methods, namely, a variational ansatz where the spin-spin correlations in the frustrated Heisenberg model were calculated by a Green's function method[12] and the exact diagonalization of a 4×4 lattice. Both methods had a quite reasonable agreement where the variational method showed the effect in a more pronounced way. Furthermore, we have found flat dispersion regions in the nonfrustrated and frustrated cases. Without frustration, the flat region occurs around $(\pi/2,\pi/2)$, whereas for frustration $J_2/J_1\gtrsim0.4$ it occurs between $(0,\pi)$ and $(\pi/2,\pi)$. Such

a flat region is similar to the experiment, but there it occurs between $(0,\pi)$ and $(0,\pi/2)$. In addition, we have found that the frustration term alone produces only a flat region but no extended saddle point as in the experiment.

Interestingly, some similarities with the observed, extended saddle point singularity may be obtained by simulating the doping process by a finite temperature. A large enough temperature weakens the spin correlations to such an extent that the effective dispersion will be dominated by nearest neighbor hopping. A finite temperature, however, does not produce a downshift of the energy at $(0,\pi)$.

Of course, one cannot expect a complete coincidence between the present, quite simple investigation and all the experimental details. So there is already a difference between the measured dispersion of the undoped substance and the theoretical result of the pure t-J model without frustration or temperature. The experiment shows a much more isotropic minimum near $(\pi/2,\pi/2)$ and a higher energy at $(0,\pi)$. To obtain a better agreement it seems to be necessary to include additional hopping terms. It would be interesting to investigate if that gives also a better agreement in the doped case.

ACKNOWLEDGMENTS

We thank V.M. Beresovsky for use of his code to calculate the spin-spin correlation functions. One of the authors (A.F.B.) thanks Professor Eschrig and the Max-Planck Arbeitsgruppe in Dresden for hospitality where part of the work has been carried out. Furthermore, we acknowledge the financial support of the INTAS organization under project No. INTAS-93-285 and of the Deutsche Forschungsgemeinschaft project No. Ri 615/1-2.

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