Formation of ferromagnetic clusters around holes in the two-dimensional t-J model

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In the spin-wave approximation the energy spectrum of one-hole states of the two-dimensional t-J model is considered in the parameter range $0.01 \leq J/t \leq 1$, where J is the exchange constant and t the hopping-matrix element. Attention is focused on single-particle states (in contrast to hole-magnon continua) that form energy bands characterized by different values of the z component of the total spin S_z, corresponding to ferromagnetically ordered regions of different size around the hole. For an infinite lattice, the shapes and relative positions of the lowest bands are computed by means of the Lanczos method. The formation process of the ferromagnetically ordered region in the one-hole ground state is discussed. It is connected with a characteristic dependence of the band energy on J/t for different S_z. The shapes of the magnon cloud around the hole and the point symmetries of the eigenfunctions are determined for various points in the Brillouin zone and for different bands of interest.

I. INTRODUCTION

The Hubbard model and the related t-J model are the subject of an intense study because these models are supposed to describe the behavior of charge carriers in the CuO_2 planes of high-T_c cuprate superconductors.[1] However, there is still a number of unresolved problems with respect to the character of the elementary excitations in these models. One of the open questions concerns the nature of the one-hole low-energy excitations. The knowledge of their properties is essential, for example, for an understanding of various phenomena of relaxation and transport processes. It is the purpose of the present paper to present a detailed investigation of the one-hole excitations in the framework of the t-J model.

There are two different approaches to treat the problem in this model: One can either perform exact calculations for small clusters (see, e.g., Refs. 2–4) or employ various types of approximations which allow one to consider an infinite lattice (see, e.g., Refs. 5–7). Simple combinatorial arguments show that the size of the basis which is necessary for a straightforward numerical diagonalization of the t-J Hamiltonian increases extremely fast with the number of lattice sites considered. Therefore, clusters of not more than 20 sites can be taken into account by exact methods.[2–4] With respect to the infinite lattice this corresponds to an investigation of only a small number of points in the Brillouin zone. Therefore, the overall shapes of the energy bands cannot be determined precisely. Even more important is the influence of the cluster size on the eigenstates of the Hamiltonian. For small J/t (where as usual t is the hopping matrix element and J is the exchange constant) the low-energy one-hole excitations of the t-J Hamiltonian are characterized by the formation of a ferromagnetically ordered region around the hole (so-called ferron states).[8–11] It will be shown below in particular for parameter values presumably realized in cuprate perovskites that for some of these low-lying excited states the size of the ferrons is comparable with the size of the clusters used in the exact calculations mentioned. Accordingly, the results of the cluster investigations can be expected to suffer strongly from finite-size effects.

To avoid these problems it is necessary to consider an infinite lattice, which requires approximate methods. The main problem in this case is to take into account the transversal spin fluctuations described by the Heisenberg Hamiltonian. It is worth noting that previous considerations of the t-J model on an infinite lattice either did not consider ferron states (e.g., Refs. 5–7) or considered them without taking into account the transversal spin fluctuations (e.g., Refs. 8–11).

The fluctuations can be adequately considered in the framework of the spin-wave approximation, which appears natural in view of experimental observations of the long-range antiferromagnetic order in lightly doped samples of the cuprate perovskites at temperatures lower than the Néel temperature.[12] The spin-wave approximation is known to be remarkably accurate in determining the ground-state energy and the sublattice magnetization of the Heisenberg antiferromagnet[13] as well as a number of other properties of the undoped system.[14] Moreover, eigenenergies of small-spin one-hole excitations obtained with the help of this approximation for an infinite lattice[15] are in satisfactory agreement with the results of an exact diagonalization for the 4×4 cluster.[2,3] (Note that the energy is measured from the ground state of the undoped lattice, so that we can compare energy differences only.) The point symmetry of the eigenstates at those points of the Brillouin zone, which can be compared with the cluster, is the same in both studies, and the parameter values, for which the ferron states become the ground states, are also in close agreement. Thus, the spin-wave approximation can be supposed to be appropriate for the description of the energy spectrum and the eigenstates.

Accordingly, we employ the spin-wave approximation in the subsequent investigation. Here we extend the results of a previous paper[15] about the formation of ferrons in the one-hole ground state. For this purpose we study

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the eigenenergies for different values S_z of the z component of the total spin which is the integral of motion of the Hamiltonian in the spin-wave approximation. A larger value of S_z reflects a larger number of spins which are flipped with respect to the Néel state. The flipped spins form a ferromagnetically ordered region around the hole. The hole together with the surrounding flipped spins constitutes the quasiparticle, the ferron, so that the value of S_z characterizes the ferron size. Relative positions, shapes and widths of the lowest one-hole bands are computed for the parameter range $0.01 \le J/t \le 1$. The shapes of the ferromagnetic region around the hole and the point symmetries of the eigenfunctions are determined for the different bands in various points of the Brillouin zone. In particular, we analyze the dependence of the eigenenergy on the parameter J/t at certain points in the Brillouin zone. The slope of these curves grows monotonically with increasing S_z. We show that this behavior can be connected with the process of the formation of ferrons in the one-hole ground state.

II. THE SPIN-WAVE APPROXIMATION AND THE CALCULATION PROCEDURE

The two-dimensional t-J Hamiltonian can be represented in the following form:

$$H=-tP\sum_{l\mathbf{a}\sigma} a^{\dagger}_{l+\mathbf{a}\sigma}a_{l\sigma}P+\frac{J}{2}\sum_{l\mathbf{a}}(\mathbf{s}_{l+\mathbf{a}}\mathbf{s}_l-\gamma n_{l+\mathbf{a}}n_l)\ , \tag{1}$$

where P is the projection operator onto the subspace of states without doubly occupied sites, $a^{\dagger}_{l\sigma}$ creates an electron with spin label $\sigma=\pm 1$ on site l of a plane square lattice, $n_l=\sum_\sigma a^{\dagger}_{l\sigma}a_{l\sigma}$ is the density, and the spin operator $\mathbf{s}_l$ is composed from $s^z_l=\sum_\sigma \sigma a^{\dagger}_{l\sigma}a_{l\sigma}/2$ and $s^{\sigma}_l=s^x_l+i\sigma s^y_l=a^{\dagger}_{l\sigma}a_{l,-\sigma}$. The summation over $\mathbf{a}$ proceeds over nearest neighbors only. It is worth noting that the Hamiltonian (1) can be derived from the extended Hubbard Hamiltonian[16,17] which gives apparently the most realistic description of the CuO_2 planes of cuprate perovskites. In this picture, the operator $a_{l\sigma}P$ creates the hole state with a large admixture of the Zhang-Rice singlet state[17] for parameters presumably[18] realized in La_2CuO_4. For these parameters $\gamma\approx\frac{1}{4}$. Although the last term in Eq. (1) yields only some constant for the energy of one-hole states, it is worth noting that for $\gamma>0$ this term describes the static attraction of holes.[18]

The spin-wave approximation can be introduced with the help of the transformation[15]

$$\begin{aligned} &s^{+1}_l=\varphi_l b_l P^{+1}_l+b^{\dagger}_l\varphi_l P^{-1}_l,\quad s^{-1}_l=(s^{+1}_l)^{\dagger}\ ,\\ &s^z_l=e^{i\Pi\cdot l}(n_l/2-b^{\dagger}_l b_l),\quad \varphi_l=\sqrt{1-b^{\dagger}_l b_l}\ , \end{aligned} \tag{2}$$

where $P^{\sigma}_l=[1+\sigma\exp(i\Pi\cdot l)]/2$ and $\Pi=(\pi,\pi)$, the lattice constant is taken as a unit of length. The spin-wave operators b_l satisfy the following commutation relations:

$$[b_l,b^{\dagger}_{\mathbf{m}}]=\delta_{l\mathbf{m}}n_l,\quad [b_l,b_{\mathbf{m}}]=0\ . \tag{3}$$

One of the two Néel states $|N\rangle$ constitutes the vacuum with respect to these operators, i.e., $b_l|N\rangle=0$, and $h^{\dagger}_l=\sum_\sigma P^{\sigma}_l a_{l\sigma}$ creates a hole in the Néel state $|N\rangle$.

The spin operators $\mathbf{s}_l$ in the Hamiltonian (1) can be substituted by the spin-wave operators b_l according to the transformation (2). The essence of the spin-wave approximation is the neglect of the terms of third and higher orders in b_l. The remaining quadratic form obtained in this way contains nondiagonal terms describing transversal spin fluctuations. It can be diagonalized by the unitary transformation[15]

$$\begin{aligned} &\mathcal{U}=\exp\left[\sum_{\mathbf{k}}\alpha_{\mathbf{k}}(b_{\mathbf{k}}b_{-\mathbf{k}}-b^{\dagger}_{\mathbf{k}}b^{\dagger}_{-\mathbf{k}})\right],\\ &\alpha_{\mathbf{k}}=\frac{1}{8}\ln\left[\frac{1+\gamma_{\mathbf{k}}}{1-\gamma_{\mathbf{k}}}\right],\quad \gamma_{\mathbf{k}}=\frac{1}{4}\sum_{\mathbf{a}}\exp(i\mathbf{k}\cdot\mathbf{a})\ . \end{aligned} \tag{4}$$

In accordance with Eq. (3) the operators $b_{\mathbf{k}}=N^{-1/2}\sum_l b_l\exp(-i\mathbf{k}\cdot\mathbf{l})$ satisfy the boson commutation relations with an accuracy up to the order $O(n)$ where n is the number of holes per site.

Omitting terms which are unessential for the considered one-hole states the transformed Hamiltonian reads

$$\begin{aligned} \mathcal{H}=\mathcal{U}^{\dagger}H\mathcal{U}=t\sum_{l\mathbf{a}\mathbf{m}} h_l h^{\dagger}_{l-\mathbf{a}}[&(u_{\mathbf{m}-\mathbf{a}}+\nu_{\mathbf{m}})b_{l-\mathbf{m}}\\ &+(u_{\mathbf{m}}+\nu_{\mathbf{m}-\mathbf{a}})b^{\dagger}_{l-\mathbf{m}}]\\ &+\frac{J}{2}\sum_{\mathbf{k}}\omega_{\mathbf{k}}b^{\dagger}_{\mathbf{k}}b_{\mathbf{k}}\ . \end{aligned} \tag{5}$$

where u_l and ν_l are the Fourier transforms of $\cosh(2\alpha_{\mathbf{k}})$ and $-\sinh(2\alpha_{\mathbf{k}})$, and $\omega_{\mathbf{k}}=4\sqrt{1-\gamma^2_{\mathbf{k}}}$. A more detailed derivation of Hamiltonian (5) can be found in Ref. 15. Analogous Hamiltonians have been considered in Refs. 19 and 20.

Due to the fast decrease of $u_{\mathbf{m}-\mathbf{a}}+\nu_{\mathbf{m}}$ with growing $|\mathbf{m}|$, only the components of the sum in the kinetic term in Eq. (5) with $\mathbf{m}$ equal to one of the primitive translations are retained. [It can be exactly shown that $u_{\mathbf{m}-\mathbf{a}}+\nu_{\mathbf{m}}=0$ for $\mathbf{m}=(m_1,m_2)$ with $m_1+m_2=0,2,4,\ldots$.] Moreover, it is sufficient to consider the contributions of

$$\omega_{\mathbf{m}}=N^{-1}\sum_{\mathbf{k}}\exp(i\mathbf{k}\cdot\mathbf{m})\omega_{\mathbf{k}}$$

in the magnetic energy term with $\mathbf{m}=(0,0)$, $(\pm1,\pm1)$, $(\pm2,0)$, $(0,\pm2)$, because $\omega_{\mathbf{m}}$ also decreases fast with growing $|\mathbf{m}|$.

The energy spectrum of the one-hole states consists of single-particle levels and hole-magnon continua. The former yield energy bands characterized by different values of the z component of the total spin and different irreducible representations of the wave-vector group. The latter are composed of scattering states of single-particle excitations and one or more magnons. Excited single-particle states are thus immersed in the continua corresponding to lower bands and, consequently, are resonant states characterized by finite widths. In the present paper attention is focused on the lowest single-particle bands. Decay lifetimes and quasiparticle residues of the states are not determined here. But it is worth not-

ing that the residues can be small, especially for small values of J/t and large S_z corresponding to large ferrons. Accordingly, the single-particle excitations can effectively vanish in the surrounding scattering continuum. This is the reason why only the lowest states corresponding to a given wave vector $\mathbf{k}$ and z component of the total spin, which can be supposed to produce pronounced maxima in the density of states, are considered in the present paper.

For this purpose, approximate eigenfunctions and eigenvalues of the Hamiltonian (5) have been obtained with the help of the Lanczos algorithm.[21] In one step of this algorithm we determine a final state $|f\rangle$ from an initial state $|i\rangle$ according to the procedure

$$\langle i|i\rangle=1, \quad E_i=\langle i|\mathcal{H}|i\rangle, \quad V|f\rangle=(\mathcal{H}-E_i)|i\rangle \ . \quad (6)$$

Here V is a normalization constant which follows from $\langle f|f\rangle=1$. We note that the algorithm automatically ensures the orthogonalization $\langle f|i\rangle=0$. After one Lanczos step (6) the energy is minimized in the subspace of the states $|i\rangle$ and $|f\rangle$, and the corresponding optimized function is used as the initial function $|i\rangle$ in the next step of the Lanczos and optimization procedure, until a desired accuracy is reached.[22]

If the initial function $|i\rangle$ belongs to an irreducible representation of the space group, and has a definite spin component S_s, then the complementary function $|f\rangle$ possesses the same symmetry and the same S_z. Therefore, it is possible to obtain the lowest eigenvalues of $\mathcal{H}$ and the corresponding eigenstates of a given symmetry and a given spin by constructing starting states $|i\rangle$ with the desired properties, which can be easily achieved by an appropriate linear combination of a few spin waves.

In the general case an eigenstate contains an infinite number of components describing a magnon cloud around the hole. Consequently, the number of components in the approximate eigenstate will grow from step to step of the procedure described above. Usually, however, for an appropriate choice of a starting function, the most significant components with large amplitudes show up in the first few steps while smaller corrections appear in further steps. This indicates the way to overcome the bottle-neck of available computation time and necessary computer memory which is due to a fast growth of the number of spin waves taken into account in later steps of the procedure: After the energy minimization the expansion of the respective approximate eigenstate is restricted in each step to the j components with the largest amplitudes. After renormalization this restricted state becomes the initial state for the Lanczos procedure (6) in the next step of the recursion.

As usual the Lanczos algorithm yields the extreme eigenstate. Due to the discussed restriction to the largest j components, in the present case an upper bound of the ground-state energy for a given symmetry and spin is obtained. The accuracy of this approximation can be estimated by changing j. A detailed description of the calculational proceedings has been published elsewhere.[23]

In our calculations j was varied between 40 and 200. For the considered Hamiltonian and the investigated range of parameters $j=100$ was found to be sufficient to obtain the energy with an accuracy better than 2%. About 30 Lanczos steps were required for convergence if the point symmetry of the starting state coincides with that of the lowest state for the given k and S_z. The simple procedure of selecting the largest components in each recursion step may, however, change the point symmetry of the state so that even an initial state with the wrong symmetry will converge towards the respective ground-state approximation with the correct symmetry. But the convergence may be rather slow in this case and require sometimes up to more than a hundred steps. The selection procedure can be changed easily so that the symmetry of the starting function is preserved.[23] For our purpose the simplest restriction to the largest j components is sufficient because we are interested in the lowest state of arbitrary symmetry for a given $\mathbf{k}$ and S_z.

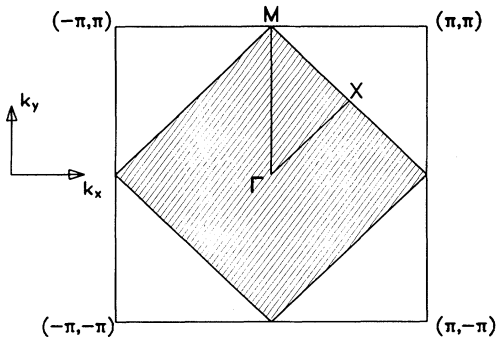

FIG. 1. The full and magnetic (shaded) Brillouin zones. Symmetry lines along which the energy is calculated are indicated. The wave vectors of the high symmetry points Γ, X, and M are $\mathbf{k}=(0,0)$, $(\pi/2,\pi/2)$, and $(0,\pi)$, respectively.

As explained above, the antiferromagnetic ordering is implied in the beginning. Therefore, the examination of the one-hole quasiparticles can be limited to wave vectors in the magnetic Brillouin zone shown in Fig. 1. To determine the correct symmetry of the lowest states in the high symmetry points Γ, X, M and along the symmetry lines connecting these points, we have used starting functions belonging to different representations of the wave-vector groups C_{4v}, C_{2v}, and C_s. We varied S_z between $\frac{1}{2}$ and $\frac{15}{2}$, and J/t in the range from 0.01 to 1. It should be noted that this interval comprises the value of J/t which is presumably realized[24] in La_2CuO_4, where the effective parameter J/t was estimated[18] to be in the range $0.1\leq J/t\leq 0.3$.

III. RESULTS AND DISCUSSION

As discussed in the previous section, we investigate in the present paper the lowest one-hole bands in dependence of J/t, but we do not study the hole-magnon continua, the quasi-particle residues and the lifetimes of the single-particle states. In the following we present in detail our results for the relative positions and the shapes of the lowest bands and show also the spatial extension of the corresponding ferromagnetic clusters which are formed around the hole.

For $J/t > 0.02$ the lowest two bands are those corresponding to $S_z = \frac{1}{2}$ and $\frac{3}{2}$. In Fig. 2 the general shape of these two bands is displayed for the moderate parameter value $J/t = 0.15$. The maximum of the band with $S_z = \frac{1}{2}$ is located at the Γ point while there are four equivalent minima on the edges of the magnetic Brillouin zone at the X points with $\mathbf{k} = (\pm\pi/2, \pm\pi/2)$, in agreement with previous investigations[2-7,15,19] of small clusters by exact diagonalization as well as infinite systems by approximate methods. Around these minima the band shows a quasi-one-dimensional behavior: The effective mass perpendicular to the boundary of the magnetic Brillouin zone is almost an order of magnitude smaller than the effective mass parallel to this boundary. A detailed analysis of the respective components of the effective mass tensor shows[25] that this behavior is typical for the $S_z = \frac{1}{2}$ band in the parameter range $J/t > 0.05$.

In contrast, the $S_z = \frac{3}{2}$ band displayed in Fig. 2(b) features degenerate maxima along the XM lines and a minimum at the center Γ of the Brillouin zone. Figure 2(b) shows that the curvature of the band around the minimum at the Γ point is nearly the same in every direction.

In Fig. 3 the dependence of the energies on the parameter J/t is shown for these two bands along the high-symmetry lines of the magnetic Brillouin zone. The overall shape of the band with $S_z = \frac{1}{2}$ does not change in the considered parameter range, except for very small J/t (< 0.05) for which the maximum of the band is somewhat shifted from the Γ point. We attribute this behavior to the crossover with another band which is characterized by a different symmetry. A detailed analysis of this question would require additional extensive computations, because as discussed above in the present investigation we have not attempted to preserve the symmetry of the initial function during the recursion procedure and we have not obtained solutions of a specific symmetry in the crossover region.

A close investigation shows that the band width of the $S_z = \frac{1}{2}$ band in Fig. 3(a) is not a monotonous function of J/t. The maximum of the band width is obtained for $J/t \approx 0.9$, and it is of the order of t in agreement with previous investigations.[6,15] In the high-symmetry points of the Brillouin zone the states of this band are transformed in a fully symmetric way under the operations of the corresponding point groups. The same behavior was obtained by the direct diagonalization[3] of the t-J Hamiltonian for a 4×4 cluster. The agreement with the cluster calculations[2-4] is also good with respect to the values of the band energies. For example, at $J/t = 0.25$ the energies counted from the ground state of the undoped system in the cluster[3] are 10–15 % higher than those in Fig. 3. This energy shift may be attributed to the restricted spatial extension of the magnon cloud in

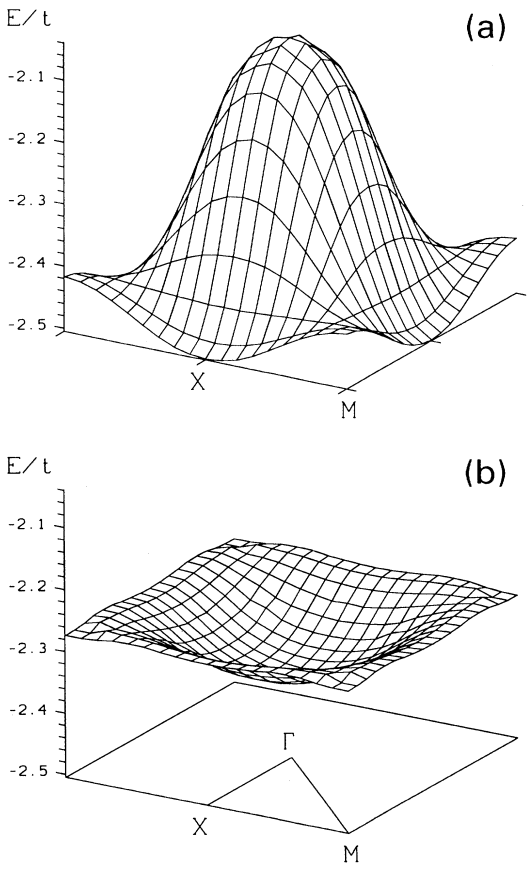

FIG. 2. The lowest-energy bands in the magnetic Brillouin zone at $J/t = 0.15$ corresponding to (a) $S_z = \frac{1}{2}$ and (b) $S_z = \frac{3}{2}$.

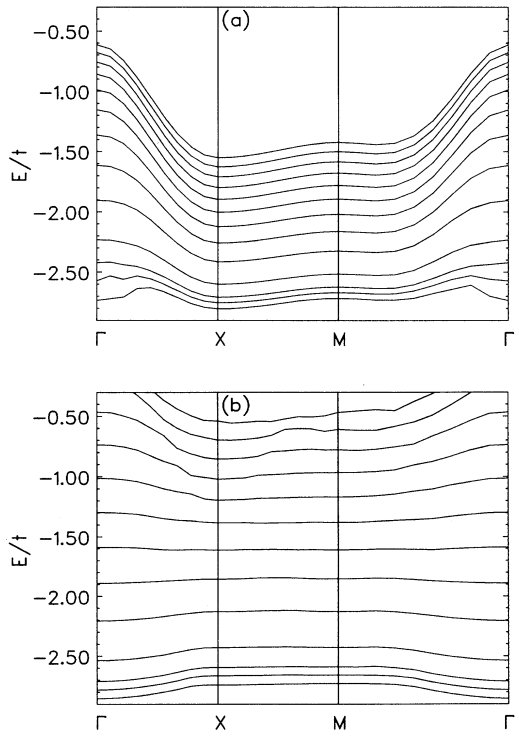

FIG. 3. The energy along the symmetry lines (compare Fig. 1) in the bands with (a) $S_z = \frac{1}{2}$ and (b) $S_z = \frac{3}{2}$ for $J/t = 0.01$, 0.03, 0.05, 0.1, 0.2, 0.3, 0.4, ... 1.0 (from bottom to top).

the cluster.

The behavior of the band with $S_z=\frac{3}{2}$ is qualitatively different, as can be seen in Fig. 3(b). This band changes its shape in dependence on J/t. For small J/t its shape is represented by Fig. 2(b). Near $J/t=0.35$ the overall appearance changes and for large J/t the shape of this band is similar to the $S_z=\frac{1}{2}$ band in Fig. 2(a). This means in particular that the position of the minima and maxima are exchanged. At the crossover $J/t\approx 0.35$ the bandwidth is very small, it is of the same order of magnitude as the numerical accuracy.

This drastic change of the overall shape is not connected to a change of symmetry in the corresponding wave function. Over the entire considered range of J/t wave functions of the lowest band with $S_z=\frac{3}{2}$ belong to the B_2 and E representations of the point group C_{4v} at the Γ and M points, respectively, and to the A_1 representation of the group C_{2v} at the X point. Along the ΓM symmetry line the wave functions are transformed according to the A'' representation of the C_s group, and along the two other symmetry lines in Fig. 1 they belong to the A' representation of the group C_s. In the 4×4 cluster calculation[3] the symmetry of the eigenfunctions for the band with $S_z=\frac{3}{2}$ has only been determined for the Γ point and the representation has been found to be B_2, in coincidence with our result.

In Fig. 4 the energies at the high-symmetry points are compiled for both bands, $S_z=\frac{1}{2}$ and $\frac{3}{2}$, for the entire range of the parameter J/t. Obviously the bands intersect in a wide range of J/t. Only for $J/t>0.92$ the ground-state energy is given by the $S_z=\frac{1}{2}$ band in the entire Brillouin zone. For smaller J/t the lowest energy in the center of the Brillouin zone is characterized by $S_z=\frac{3}{2}$. Near $J/t=0.053$ the overall ground-state changes from $\mathbf{k}=(\pm\pi/2,\pm\pi/2)$ and $S_z=\frac{1}{2}$ to $\mathbf{k}=(0,0)$ and $S_z=\frac{3}{2}$. This can be seen in more detail in Fig. 5, where the energies for all investigated bands are shown for small values of J/t. For $S_z=\frac{1}{2}$ and $\frac{3}{2}$ the positions of the minima and maxima are explicitly shown. With increasing S_z the band width decreases drastically, already for $S_z=\frac{5}{2}$ it is of the order of the numerical accuracy, so that it is sufficient to display an average energy for the bands with larger S_z. It is not surprising that these bands are so narrow, because a large value of S_z corresponds of a large ferron, i.e., a large number of flipped spins surrounding the hole. Accordingly the effective mass of the quasiparticle is large.

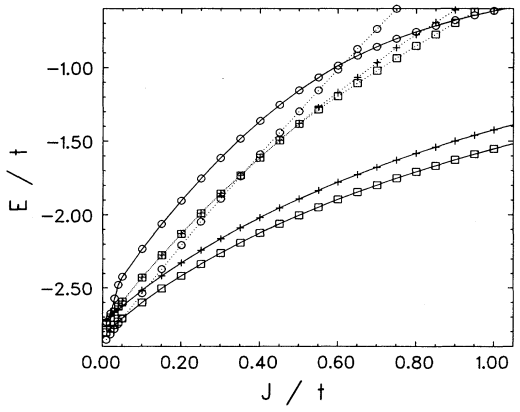

FIG. 4. The energy at high-symmetry points Γ (○), X (□), M (+) for the bands with $S_z=\frac{1}{2}$ (solid lines) and $S_z=\frac{3}{2}$ (dotted lines).

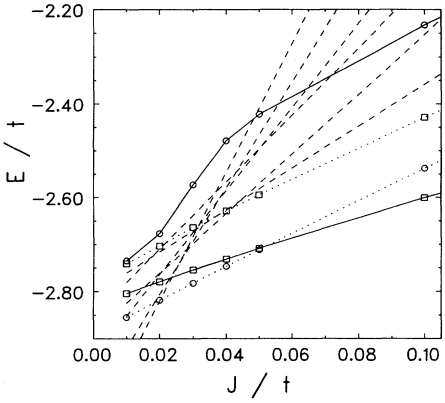

FIG. 5. Relative energies of the lowest bands. Positions are indicated at the high-symmetry points X (□) and Γ (○) for the bands with $S_z=\frac{1}{2}$ (solid lines) and $S_z=\frac{3}{2}$ (dotted lines). Due to the small bandwidth an average energy only is displayed for the bands with $S_z=\frac{5}{2}$, $\frac{7}{2}$, $\frac{9}{2}$, $\frac{11}{2}$, $\frac{13}{2}$, and $\frac{15}{2}$ (broken lines, from bottom to top for large J/t).

It can be seen in Fig. 5 that the lowest energy of the bands grows monotonously with increasing S_z for $J/t>0.053$. Thus the band with $S_z=\frac{1}{2}$ contains the ground state for larger values of the parameter J/t.

The energy varies linearly with J/t for small values of this parameter. This can be observed for all bands in Fig. 5, except for the maximum of the $S_z=\frac{1}{2}$ band at $\mathbf{k}=(0,0)$, as discussed above.

The steepness of the E/t–J/t curves in Fig. 5 grows monotonously with increasing S_z. As a consequence, for smaller values of J/t, the bands corresponding to larger values of S_z become lower in energy than those with smaller S_z, i.e., states with a more extended ferromagnetically ordered region around the hole become energetically more favorable. As discussed above, the one-hole ground states belong to the $S_z=\frac{1}{2}$ band for $J/t\geq 0.053$. In the range $0.02\leq J/t\leq 0.053$ the $S_z=\frac{3}{2}$ band yields the lowest energy while in the range $J/t\leq 0.02$ the ground state occurs for $S_z>\frac{15}{2}$. We did not check states with $S_z\geq\frac{17}{2}$ due to numerical difficulties, but the monotonous decrease of the energy with increasing S_z for small J/t suggests an even higher value of S_z for the ground state in this range. Thus, there is a large jump in the value of S_z in the ground state for $J/t\approx 0.02$. These pecularities of the energy structure provide an explanation for the spatial growth of the ferron in terms of the band picture because a more and more extended ferron becomes energetically more and more favorable for smaller J/t. A consideration of this rapid growth in small clusters is limited because the size of the ferron quickly reaches the

cluster size. Nevertheless, it is possible to compare the critical values of J/t at which the state corresponding to the smallest ferron size ($S_z=\frac{3}{2}$, one flipped spin) becomes the lowest one. For the 4×4 cluster this happens[2,3] at $J/t=0.075$, in reasonable agreement with $J/t\approx0.05$ observed above for the infinite lattice. It is obvious that for a small cluster the critical value should be larger because in the infinite system the surroundings prevent the ferron formation.

The previous discussion has been concerned with the eigenenergies of the one-hole states of the t-J Hamiltonian, and with the symmetry of these states. The obtained approximate eigenfunctions allow us to visualize the shape of the magnon cloud around the hole in different states. Figure 6 displays these clouds for several states including those of the lowest energy, thus showing different typical shapes of the ferromagnetic cluster. Contributions of the selected j spin configurations with largest amplitudes were used with their respective weight in obtaining the probabilities shown in this figure. The wave function contains components with a hole positioned either on the spin-up or on the spin-down sublattice of the Néel state. Corresponding magnon clouds are shown in separate plots. It can be seen from Figs. 6(a) and 6(b) that for fixed S_z the size of the magnon cloud grows with a decrease of J/t. Similarly, Figs. 6(b), 6(d), and 6(e) demonstrate the growing size of the ferron with an increase of S_z for a fixed J/t. In Fig. 6(c) an example for an asymmetric magnon cloud is displayed.

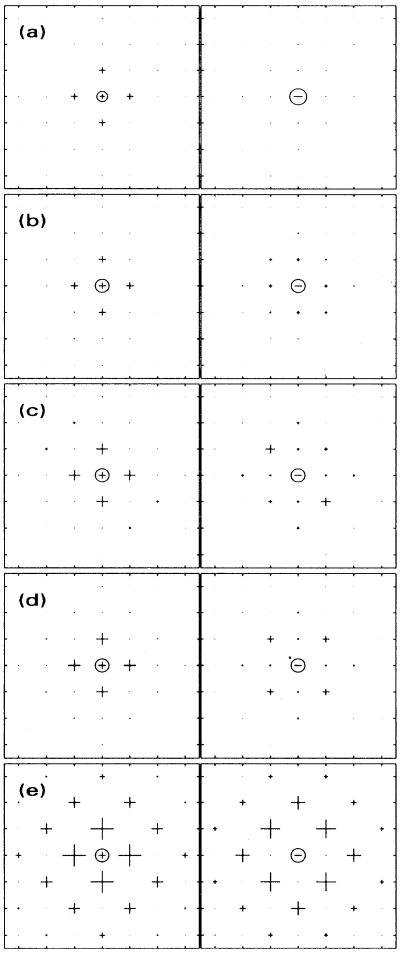

FIG. 6. Ferromagnetic clusters around the hole for (a) $S_z=\frac{1}{2}$, $J/t=0.8$ at the X point; (b) $S_z=\frac{1}{2}$, $J/t=0.05$ at X; (c) $S_z=\frac{3}{2}$, $J/t=0.05$ at X; (d) $S_z=\frac{3}{2}$, $J/t=0.05$ at Γ; (e) $S_z=\frac{15}{2}$, $J/t=0.02$ at Γ. The left and right panels show spin configurations of the wave-function components with the hole positioned on different sublattices of the Néel state. The circled sign in the center indicates the respective spin label σ of the removed electron. Circles and crosses show the relative positions of the hole and the spins that are flipped with respect to the Néel state. The size of the symbols is proportional to the probability of finding a flipped spin at the indicated distance and a hole on the indicated sublattice, respectively. The size of the symbols would equal the lattice constant (indicated by the ticks on the axes), if the probability were equal to unity.

In summary, within the framework of the spin-wave approximation the energy spectrum of the single-particle one-hole states of the two-dimensional t-J model has been considered in the parameter range $0.01\leq J/t\leq1$. The spectrum consists of bands characterized by different values of the z component of the total spin S_z and corresponding to different sizes of ferromagnetically ordered regions around the hole. The formation process of such a region in the ground state has been discussed. It can be attributed to a monotonous growth of the steepness of the $E/t-J/t$ curves with increasing S_z. The shapes of the magnon clouds around the hole and the point symmetries of the lowest eigenfunctions were determined for the different bands in various points of the Brillouin zone.

As mentioned above, the value of the parameter J/t for La_2CuO_4 is supposed to be in the range $0.1\lesssim J/t\lesssim0.3$ which is far from the critical value $J/t\approx0.05$ where the state corresponding to the smallest ferron ($S_z=\frac{3}{2}$) becomes the lowest one according to our calculation. Thus, the lowest hole state is characterized by $S_z=\frac{1}{2}$ and there is no ferromagnetic region around the hole. This fact, however, does not mean that ferron states will not be observable. It is clear that any relaxation process will include these states. A rather localized magnon distribution around the hole in some of these states implies that the lifetime with respect to a decay to a ferron with a smaller spin and a magnon can be large and the states can be observed as long-living metastable states. Due to their large spin these states are especially important for the magnetization processes. On the other hand, there are several classes of crystals characterized by anomalously small values of the effective parameter J/t, e.g., metamagnetics.[26] For such crystals the results obtained above and their straightforward extension to the 3D case give the quantitative description of the process of ferron formation in the ground state. Returning to cuprate perovskites it is worth noting that the above-mentioned quasi-one-dimensionality around the minima of the $S_z=\frac{1}{2}$ band effectively leads to a large sensitivity of the ferron state to the interaction with phonons. Accordingly the carrier transport is strongly anisotropic in this case.[27]

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