HOLE MOTION IN A QUANTUM ANTIFERROMAGNET UNDER THE INFLUENCE OF THE ZEEMAN INTERACTION

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We study the effects of the coupling of a magnetic field with the spin background through the Zeeman interaction on the band-structure of a single-hole in a quantum antiferromagnet. We include effects of exchange anisotropies and we consider both cases where the direction of the external field is parallel and perpendicular to the direction of the staggered magnetization. We use a self-consistent perturbation approach which treats the spin-background in the linear spin-wave approximation. We calculate the effects of the magnetic field on the hole spectral-function, energy-band and residues of the lowest energy peaks. We find that states around the points $\vec{k} = (\pi, \pi)$ and $\vec{k} = 0$ of the Brillouin-Zone are substantially affected by the interaction of the spin background with the magnetic field.

I. INTRODUCTION

Certain features of the problem of strongly correlated electrons can be understood within the $t - J$ model and in particular it is believed that it may capture aspects of the charge motion in the cuprate superconductors.[1] This model combines an antiferromagnetic (AF) exchange coupling and a hole hopping term. The strong on-site Coulomb repulsion is taken into account approximately by restricting the Hilbert space in the subspace of singly occupied Wannier states. This restriction demands that the hole motion is strongly correlated with the motion of the other degrees of freedom. Let us consider the following Hamiltonian

$$H_{t-J} = -t \sum_{<ij>,\sigma} (\tilde{c}^{\dagger}_{i\sigma}\tilde{c}_{j\sigma} + h.c) + J \sum_{<ij>} \left((S^z_i S^z_j - \frac{1}{4} n_i n_j) + \lambda (S^x_i S^x_j + S^y_i S^y_j) \right). \quad (1)$$

The isotropic $t - J$ model is obtained by setting $\lambda = 1$ in Eq. (1), and we have allowed for exchange anisotropies ($\lambda \neq 1$). Here, $\tilde{c}^{\dagger}_{i\sigma}$ creates electrons only on empty sites, thus the double occupancy is avoided.

In the case where there is one electron per site (e.g, the case of the stoichiometric La_2CuO_4) the model (1) and the spin-1/2 Heisenberg antiferromagnet are equivalent. Studies of the latter model indicate that several magnetic properties of the cuprous oxides can be understood within this simple model.[2]

Most of the features of the motion of a single-hole in the $t - J$ model have been revealed by a number of approaches.[3-10] A hole added to the spin-1/2 quantum antiferromagnet becomes a rather well defined excitation which corresponds to a sharp low energy peak in the spectral function. The minimum of the hole energy band is at $\vec{k} = (\pm\frac{\pi}{2}, \pm\frac{\pi}{2})$ and the hole acquires an effective mass that is strongly dependent on the specific crystallographic direction of the square lattice. For the purpose of our convenience we would like to single out one approach introduced by Schmitt-Rink, Varma, and Ruckenstein[3](SVR) and by Kane, Lee, and Read[4] (KLR). This is a self-consistent perturbative treatment of the model where, along the spirit of spin-wave approximation, one expresses the standard spin-operators in terms of spin-deviation operators and keeps up to quadratic terms in these operators. The coupling between the spin-degrees of freedom and the hole motion is due to the fact that the hole-hopping creates spin-deviations. The hole Green's function in this approach was studied[3,4] within self-consistent perturbation theory where one neglects the vertex corrections. More recently, Liu and Manousakis[5] solved the self-consistent equation numerically on finite but large-size lattices and studied the contribution of vertex corrections. By comparing their results with available results obtained by exact diagonalization[6] (on small lattices) they found that this method is reasonably accurate in the physical region ($t >> J$).

In this paper we shall use the method of Ref. 5 to study the effects of maqnetic field through the Zeeman interaction on the band-structure of a single-hole created inside an antiferromagnet using the $t - J$ model. The usual approach of taking the effects of an external magnetic field on a system of interacting electrons is to neglect the influence of the field on their band structure. In our case, however, the spin-background is coupled to the hole-motion in an intimate way which produces a band-structure which is qualitatively different from the non-interacting case. In this paper, we wish to study the indirect effects on the hole band-structure of the fact that the background is altered by the external field. When a hole is introduced in a quantum antiferromagnet, the order parameter around the hole is twisted.[7,8,10] The form of the distortion depends on the momentum of the excitation and, generally speaking, it involves a long-range dipolar distortion of the staggered magnetization and a ferromagnetic moment localized around the hole with direction perpendicular to the staggered magnetization. The induced ferromagnetic moment around the hole couples to the external magnetic field and the magnitude of the moment is momentum dependent; thus, we expect to find that the effects of the external field depend on the hole crystal momentum.

We need to distinguish two different possibilities depending on the relative directions of the staggered magnetization vector and the direction of the external magnetic field. First, let us discuss what happens in a pure antiferromagnet with an exchange anisotropy ($\lambda \neq 1$) and with the field applied parallel to the direction of the staggered magnetization. Within spin-wave theory, as long as $h < 2Ja\sqrt{1-\lambda^2}$ (a is the lattice spacing) the system stays antiferromagnetically ordered in a direction parallel to the external field. For $h > 2Ja\sqrt{1-\lambda^2}$ the system develops staggered magnetization in a direction perpendicular to the external field and a magnetization parallel to the field, which for small fields is given by $M_z = \chi_\perp B$ where $\chi_\perp$ is the perpendicular susceptibility. If there are no exchange anisotropies the stable configuration is the one where the direction of the staggered magnetization and that of the external field are perpendicular.

In the next section, we consider the case where the magnetic field and the staggered magnetization are perpendicular and we study the hole Green's function, the hole energy-band and the residue of the lowest energy peaks. In the case where the field is applied in a direction parallel to the staggered magnetization, we introduce an exchange anisotropy to avoid the instability of the system towards a global rotation of the staggered magnetization. In this case, the exchange anisotropy ($\lambda < 1$) favors the development of AF order in the direction of the applied field. This case is studied in the last section.

II. PERPENDICULAR FIELD

Here, we study the effects of the coupling of a magnetic field B with the spin background through the Zeeman interaction on the band-structure of a single-hole in the $t-J$ model and on the square lattice:

$$H = H_{t-J} - h \sum_i S_i^x , \tag{2}$$

where $h = g_0 \mu_B B$, g_0 is the electron gyromagnetic ratio.

We write the hopping Hamiltonian using a fermion operator $f_i^\dagger = c_{i\uparrow}$ which creates holes and a hard-core boson operator $b_i^\dagger = S_i^-$ on the up-sublattice and $f_j^\dagger = c_{j\downarrow}$ and $b_j^\dagger = S_j^+$ on the down-sublattice. In the linear spin-wave approximation, one keeps terms only up to quadratic in the hard-core boson operators in both the Heisenberg and hopping terms of Eq. (2). In this approximation the Hamiltonian (2) takes the following form:

$$H = \frac{tz}{\sqrt{N}} \sum_{\vec{k},\vec{q}} \left(\gamma_{\vec{k}} f_{\vec{k}}^\dagger f_{\vec{k}+\vec{q}} b_{\vec{q}}^\dagger + \gamma_{\vec{k}-\vec{q}} f_{\vec{k}}^\dagger f_{\vec{k}-\vec{q}} b_{\vec{q}} \right) + H_{LSW}(\{b_{\vec{k}}^\dagger, b_{\vec{k}}\}) - \frac{1}{2} h \sqrt{N} (b_0 + b_0^\dagger), \tag{3}$$

where H_{LSW} is the Heisenberg term in the linear spin-wave approximation and $\gamma_{\vec{k}} = \sum_{\vec{\delta}} e^{i\vec{k}\cdot\vec{\delta}}/z$. We then shift the boson operators by a constant $b_{\vec{k}} = a_{\vec{k}} + c_0 \delta_{\vec{k},0}$, and we select the constant c_0 in such a way to eliminate terms linear in Boson operators, i.e., $c_0 = \frac{h}{8dJS}\sqrt{N}$. We obtain:

$$H = \frac{t}{J} h \sum_{\vec{k}} \gamma_{\vec{k}} f_{\vec{k}}^\dagger f_{\vec{k}} + \frac{tz}{\sqrt{N}} \sum_{\vec{k},\vec{q}} \left(\gamma_{\vec{k}} f_{\vec{k}}^\dagger f_{\vec{k}+\vec{q}} a_{\vec{q}}^\dagger + \gamma_{\vec{k}-\vec{q}} f_{\vec{k}}^\dagger f_{\vec{k}-\vec{q}} a_{\vec{q}} \right)$$
$$+ H_{LSW}(\{a_{\vec{k}}^\dagger, a_{\vec{k}}\}) - \frac{h^2}{16dSJ} N. \tag{4}$$

Then, following the standard approach of spin-wave theory for antiferromagnets, one diagonalizes H_{LSW} using the Bogoliubov transformation. We find:

$$H = \sum_{\vec{k}} e_h(\vec{k}) f_{\vec{k}}^\dagger f_{\vec{k}} + \frac{tz}{\sqrt{N}} \sum_{\vec{k},\vec{q}} f_{\vec{k}+\vec{q}}^\dagger f_{\vec{k}} \left(\alpha_{\vec{q}} (u_{\vec{q}} \gamma_{\vec{k}} - v_{\vec{q}} \gamma_{\vec{k}+\vec{q}}) + \alpha_{-\vec{q}}^\dagger (v_{\vec{q}} \gamma_{\vec{k}} + u_{\vec{q}} \gamma_{\vec{k}+\vec{q}}) \right) + h.c + \sum_{\vec{k}} \Omega_{\vec{k}} \alpha_{\vec{k}}^\dagger \alpha_{\vec{k}} + E_0 - \frac{h^2}{16dSJ} N, \tag{5}$$

where E_0 is the ground state energy of an antiferromagnet in the linear spin-wave theory and $e_h(\vec{k}) \equiv \frac{t}{J} h \gamma_{\vec{k}}$. Here $u_{\vec{k}}^2 = \frac{1}{2}\left(\frac{1}{\sqrt{1-\lambda^2\gamma_{\vec{k}}^2}} + 1\right)$, $v_{\vec{k}}^2 = \frac{1}{2}\left(\frac{1}{\sqrt{1-\lambda^2\gamma_{\vec{k}}^2}} - 1\right)$, and z is the number of the nearest-neighbors. The α's are spin-wave operators related to the a's via the Bogoliubov transformation $a_{\vec{k}} = u_{\vec{k}} \alpha_{\vec{k}} + v_{\vec{k}} \alpha_{-\vec{k}}^\dagger$ with dispersion relation $\Omega_{\vec{k}} = JzS\sqrt{1-\lambda^2\gamma_{\vec{k}}^2}$. Namely, the hole at the unperturbed level is placed in a band with bandwidth linear in the field h.

In the limit $t >> J$, using the self-consistent perturbation approach where only non-crossing diagrams are summed,[3,4,5] one obtains the following expression for the hole propagator:

$$G(\vec{k},\omega) = \frac{1}{\omega - e_h(\vec{k}) - \sum_{\vec{q}} |f(\vec{k},\vec{q})|^2 G(\vec{k}-\vec{q}, \omega - \Omega_{\vec{q}})}, \tag{6.a}$$

where

$$f(\vec{k},\vec{q}) \equiv zt(\gamma_{\vec{k}-\vec{q}} u_{\vec{q}} + \gamma_{\vec{k}} v_{\vec{q}})/\sqrt{N}. \tag{6.b}$$

Here, we iterate Eq. (6) on finite clusters of size $N = L \times L$ starting from

$$G^{(0)}(\vec{k},\omega) = \frac{1}{\omega - e_h(\vec{k}) + i\epsilon}, \tag{7}$$

assuming that the output of the n^{th} iteration $G^{(n)}(\vec{k},\omega)$ has both real and imaginary parts $G^{(n)}(\vec{k},\omega) = G_R^{(n)}(\vec{k},\omega) + iG_I^{(n)}(\vec{k},\omega)$, where $G_R^{(n)}(\vec{k},\omega)$ and $G_I^{(n)}(\vec{k},\omega)$ are the results of the n^{th} iterations of coupled equations derived from Eq. (6).

The spectral function $A(\vec{k},\omega) = -\frac{1}{\pi} G_I^{(\infty)}(\vec{k},\omega)$ is obtained after the convergence is achieved for a given lattice and given value of ϵ.

The results obtained in the case of $J/t = 0.2$ and $h = 0, 0.1, 0.2$, $\epsilon = 0.05$ and for a 16^2 lattice are shown in Fig. 1. In Ref. 5, the significance of finite-size and finite ϵ effects has been studied for the case of zero magnetic field. In Fig. 1(a) the spectral function is shown for $\vec{k} = (\frac{\pi}{2}, \frac{\pi}{2})$. In Fig. 1(b) the spectral function is given for $h = 0.1$ and $\vec{k} = (\pi,\pi)$ (dashes) and for $\vec{k} = 0$ (dots). For

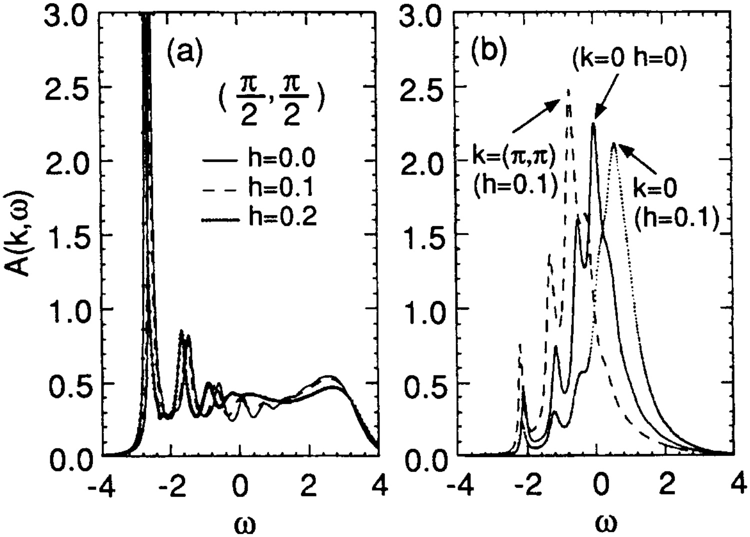

FIGURE 1 (a) The hole spectral-functions $A(\vec{k} = (\frac{\pi}{2}, \frac{\pi}{2}), \omega)$ for magnetic field strengths $h = 0, 0.1, 0.2$ and direction perpendicular to the direction of the staggered magnetization. (b) The spectral functions for $h = 0$ and $\vec{k} = 0$ (solid line), for $h = 0.1$ and $\vec{k} = (\pi, \pi)$ (dashed line) and $\vec{k} = 0$ (dotted line).

$h = 0$, the spectral functions for these two states are identical and they are shown by the solid line in Fig. 1(b). We note that the most significant effects of the magnetic field occur on the higher energy peaks of the spectral function for $\vec{k} = (\pi, \pi)$ and $\vec{k} = 0$. In particular the higher energy peaks, which can be interpreted as excited states ("string" excitations) arising from the hole motion in a nearly linear potential, are most dramatically affected. This was expected since in these states there is a ferromagnetic moment around the hole, with direction perpendicular to the staggered magnetization, which couples to the external field. Notice that the main peak in the spectral function for $\vec{k} = (\pi, \pi)$ is shifted at lower energy for $h \neq 0$, while that for $\vec{k} = 0$ towards higher energy. The lowest peak in both spectral functions which has very small weight shifts towards lower energy.

We found that the residue of the lowest peak in the case of $\vec{k} = (\frac{\pi}{2}, \frac{\pi}{2})$ is not significantly affected by the external field of the magnitude used while the residue

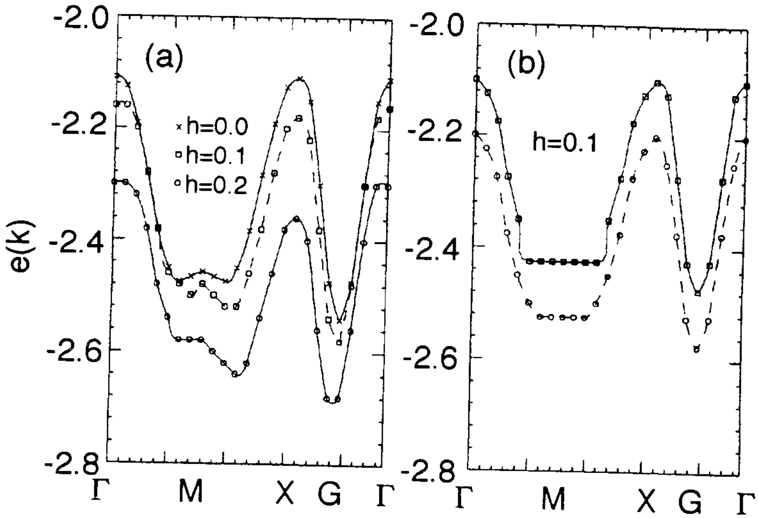

FIGURE 2 (a) The hole energy-band for external field perpendicular to the staggered magnetization and $h = 0, 0.1, 0.2$. (b) The hole energy-band for the anisotropic $t-J$ model with $\lambda = 0.1$ and magnetic field parallel to the staggered magnetization and $h = 0.1$. The two curves correspond to holes from different sublattices.

of the lowest peak for $\vec{k} = (0,0)$ is seriously affected. In addition, the main peaks of $A(\vec{k} = 0, \omega)$ are shifted by an amount large compared to h.

The hole energy-band along the high symmetry path $\Gamma M X \Gamma$ of the Brillouin-Zone (in our notation $\Gamma \equiv (0,0)$, $M \equiv (\pi, 0)$, $X \equiv (\pi,\pi)$ and $G \equiv (\frac{\pi}{2}, \frac{\pi}{2})$) is shown in Fig. 2(a). Notice that while the minimum of the band occurs at $\vec{k} = (\frac{\pi}{2}, \frac{\pi}{2})$ as in the case without field a new pocket appears at a point between the M and X. In addition, the states $\vec{k} = 0$ and $\vec{k} = (\pi,\pi)$ (X point) are no longer degenerate, the latter having lower energy. In a fully ferromagnetically aligned background the hole energy band has its minimum at $\vec{k} = (\pi,\pi)$. Thus, the magnetic field is expected to lower the energy of this state. The state $\vec{k} = 0$ is also lower from the case without a magnetic field for this value of $J/t = 0.2$. This may be explained by the fact that when the hole is in this state, it creates a ferromagnetic moment around it in a direction perpendicular to the staggered magnetization and in this case parallel to the external field; thus for certain range of J/t the field can lower the energy of the hole state for $\vec{k} = 0$. As mentioned earlier, however, these states have very small weight in the spectral function where the main peaks for $\vec{k} = (\pi,\pi)$ and $\vec{k} = 0$

move to opposite directions. We notice that, crudely speaking, the hole energy-band is uniformly shifted by the Zeeman term towards lower energy values without significantly affecting the bandwidth or the residues of the lowest-energy quasi-hole peak. Similar features of the hole band in the presense of a transverse field is found in Ref. 11 where the coupled-cluster method was applied.

III. PARALLEL FIELD

As discussed in the introduction the isotropic Heisenberg antiferromagnet without anisotropies develops AF order always in a direction perpendicular to the field. Thus, we can apply a field parallel to the staggered magnetization only if there is an anisotropy which creates a gap in the spin-wave excitation spectrum. Let us consider the $t-J$ model with exchange anisotropy

$$H = H_{t-J} - h \sum_i S_i^z , \tag{8}$$

where H_{t-J} is given by Eq. (1) with $\lambda < 1$. In this case the above Hamiltonian in the linear spin-wave approximation takes the following form:

$$\begin{aligned} H = & \frac{tz}{\sqrt{N}} \sum_{\vec{k},\vec{q}} f^\dagger_{\vec{k}+\vec{q}} h_{\vec{k}} \Big(\alpha_{\vec{q}} (u_{\vec{q}} \gamma_{\vec{k}} - v_{\vec{q}} \gamma_{\vec{k}+\vec{q}}) + \beta^\dagger_{\vec{q}} (v_{\vec{q}} \gamma_{\vec{k}} + u_{\vec{q}} \gamma_{\vec{k}+\vec{q}}) \Big) + h.c \\ & + \sum_{\vec{k}} \Big(\Omega^\alpha_{\vec{k}} \alpha^\dagger_{\vec{k}} \alpha_{\vec{k}} + \Omega^\beta_{\vec{k}} \beta^\dagger_{\vec{k}} \beta_{\vec{k}} \Big) + E_0, \end{aligned} \tag{8}$$

where α and β are spin-wave operators creating spin-waves in each separate sublattice and $f^\dagger$ and $h^\dagger$ are hole creation operators for each sublattice. Here:

$$\Omega^\alpha(\vec{k}) = \Omega(\vec{k}) - h, \tag{9.a}$$

$$\Omega^\beta(\vec{k}) = \Omega(\vec{k}) + h. \tag{9.b}$$

At this point, it becomes evident that if $h > \Omega(\vec{k})$ for any value of $\vec{k}$ the system becomes unstable. For $\vec{k} = 0$, this occurs for $h > 2J\sqrt{1-\lambda^2}$. This means that the direction of the staggered magnetization will rotate in a direction perpendicular to the external field and the treatment is similar to that of the previous section. In the case of small fields, so that this instability does not occur, the problem can be solved as follows. Holes in different sublattice have different Green's functions. The equations for the Green's function of the hole are given by the following coupled equations:

$$G^\alpha(\vec{k},\omega) = \frac{1}{\omega - \sum_{\vec{q}} |f(\vec{k},\vec{q})|^2 G^\beta(\vec{k}-\vec{q}, \omega - \Omega^\alpha_{\vec{q}})}, \tag{10.a}$$

$$G^\beta(\vec{k},\omega) = \frac{1}{\omega - \sum_{\vec{q}} |f(\vec{k},\vec{q})|^2 G^\alpha(\vec{k}-\vec{q}, \omega - \Omega^\beta_{\vec{q}})}. \tag{10.b}$$

In the case of no anisotropy as we discussed Ω^α becomes negative for $\vec{k} = 0$ and any finite field. This shows the instability towards alignment of the staggered magnetization in a direction perpendicular to the external field. In Fig. 3 we present results obtained in the presence of an exchange anisotropy for $\lambda = 0.1$ and for $h = 0.1$. The dashed and solid lines represent the spectral function for holes in different sublattices. We notice that the shifts in the energy peaks of the spectral function of the hole for both $\vec{k} = (\frac{\pi}{2}, \frac{\pi}{2})$ and $\vec{k} = 0$, are uniform and of the order of the Zeeman splitting. Thus, in this case the Zeeman term separates the energy bands (see Fig. 2(b)) of the holes from opposite sublattices by an energy shift of order of the Zeeman splitting, while most of the other features of hole spectral functions remain nearly unaffected.

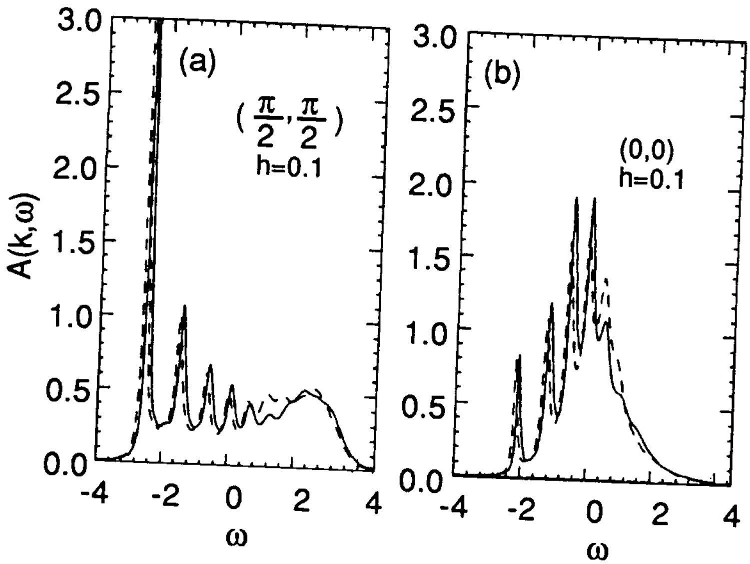

FIGURE 3 (a) The hole spectral-functions $A(\vec{k} = (\frac{\pi}{2}, \frac{\pi}{2}), \omega)$ for magnetic field parallel to the direction of the staggered magnetization and $h = 0.1$. The dashed and solid lines correspond to holes in different sublattices. (b) Same as (a) for $A(\vec{k} = 0, \omega)$ and $h = 0.1$.

IV. ACKNOWLEDGEMENTS

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