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SINGLE-HOLE STATE IN THE 2D t-J MODEL IN A TRANSVERSE MAGNETIC FIELD

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We have investigated the ground state of a single hole in the t-J model on a 2D square lattice in a transverse magnetic field using the coupled-cluster method. Here, we study the effects of the magnetic field on the system by considering the Zeeman interaction only. We obtain an analytical expression of the hole energy dispersion function $\epsilon(\vec{k})$ which in the small J limit reproduces several features consistent with earlier studies of the t-J model in zero magnetic field. As the magnetic field increases, the hole energy band is shifted downward around (π,π) and upward around (0,0), whereas comparatively small changes occur in the neighbourhood of the zone boundary.

In recent years the high-temperature superconductors have been widely studied, both theoretically and experimentally. It has been suggested that the nearly half-filled, 2D Hubbard model in the large Coulomb repulsion limit might be relevant to the physics of high-temperature superconductors.[1] In the strong coupling limit $t/U \ll 1$ and using second-order perturbation theory, the nearly half-filled Hubbard model can be further simplified to what is called the t-J model. This model has now become the focus of theoretical studies. An extensive effort has been made recently to study the properties of the ground state of a single hole by a number of authors both analytically and numerically.[2,3,4] In the present work, using the coupled-cluster method[5,6], we study the ground state of a single hole of the t-J model on a 2D square lattice in a transverse magnetic field. Here, we study the effects of the magnetic field on the system by considering the Zeeman interaction only. We obtain an analytical expression of the hole energy dispersion function $\epsilon(\vec{k})$; in the small J limit this dispersion function reproduces several features that have been found in earlier studies of the t-J model in zero magnetic field. As the magnetic field increases, the hole energy band is shifted downward around (π,π) and upward around $(0,0)$, whereas comparatively small changes occur in the neighbourhood of the zone boundary.

The basic idea of the coupled-cluster method can be outlined as follows: The ground state of a many-body Hamiltonian H can be expressed as

$$|\Psi>= exp(S)|\Phi_0> \tag{1}$$

with $|\Phi_0>$ being a starting wave function which is not orthogonal to the exact ground state. The Schrödinger equation

$$H|\Psi>= E_0|\Psi>, \tag{2}$$

can then be written as

$$\mathcal{H}|\Phi_0>\equiv exp(-S)Hexp(S)|\Phi_0>= E_0|\Phi_0>, \tag{3}$$

where

$$exp(-S)Hexp(S) = H + [H,S] + \frac{1}{2!}[[H,S],S] + \dots . \tag{4}$$

Since $|\Phi_0>$ is normalized, we may write

$$<\Phi_0|\mathcal{H}|\Phi_0>=<\Phi_0|exp(-S)Hexp(S)|\Phi_0>= E_0 , \tag{5}$$

and by projecting Eq. 3 onto the states $|\Phi_n>$ which are orthogonal to $|\Phi_o>$ we obtain

$$<\Phi_n|\mathcal{H}|\Phi_0>=<\Phi_n|exp(-S)Hexp(S)|\Phi_0>= 0 . \tag{6}$$

This orthogonality condition yields a series of nonlinear coupled equations, each of which contains a finite number of terms. The correlation operator S is determined by solving these equations. Once S is known, the ground-state energy and wave function can be obtained readily. Hence, the problem of finding the ground-state energy and wave function of the many-body system is reduced to computing the operator S. Nevertheless, this is a very formidable task, and we have to resort to some approximation to solve the coupled equations. In the following we will apply a successive coupled-cluster approximation scheme to investigate the ground state of a single hole of the 2D t-J model. This approximation was recently proposed by

Roger *et al.*[5] and has been successfully applied to both quantum spin systems and the Hubbard model on a square lattice.[5,7,8]

The Hamiltonian of the t-J model in a transverse magnetic field is given by

$$H = -t \sum_{(i,j),\sigma} (1 - n_{i\sigma}) C^{\dagger}_{i-\sigma} C_{j\sigma} (1 - n_{j-\sigma}) + \frac{J}{2} \sum_{(i,j)} \Big(\frac{S_i^{\dagger} S_j^{\dagger} + S_i^{-} S_j^{-}}{2} - S_i^z S_j^z \Big) - h \sum_i S_i^x \, . \tag{7}$$

Anticipating antiferromagnetism in the half-filled case, we have rotated the quantization axis at each site of one sublattice (down) into the direction of the local mean field, as evidenced by the $-\sigma$ subscript in Eq. 7. We choose the single-hole state with momentum $\vec{k}$ to be given by

$$exp(S)|\vec{k}> = exp(S) \frac{1}{\sqrt{N}} \sum_i exp(i\vec{k} \cdot \vec{r}_i) C_{i\uparrow} |Ne\acute{e}l> , \tag{8}$$

where the Neél state is taken to be the state with all spins 'up': $|Ne\acute{e}l> \equiv \prod_{i=1}^{N} C^{\dagger}_{i\uparrow} |vac>$ in this new basis. For the zeroth level of the coupled-cluster approximation (CCA), we simply choose the operator S equal to zero. Using this trivial correlation factor S, we obtain

$$\exp(-S) H \exp(S) |\vec{k}> = \{ E(\vec{k}) + F_1 \sum_{(i,j)} C^{\dagger}_{i\downarrow} C_{j\uparrow} (1 - n_{i\uparrow}) + F_2 \sum_{(i,j)} S_i^{-} S_j^{-} + F_3 \sum_i S_i^{-} \} |\vec{k}> , \tag{9}$$

where $E(\vec{k}) = -J(N/2 - 1)$, $F_1 = -t$, $F_2 = J/4$ and $F_3 = -h/2$. Then in the next level of approximation we also include in S the terms necessary to cancel the remaining terms of Eq. 9:

$$S = \alpha_1 \sum_{(i,j)} C^{\dagger}_{i\downarrow} C_{j\uparrow} (1 - n_{i\uparrow}) + \alpha_2 \sum_{(i,j)} S_i^{-} S_j^{-} + \alpha_3 \sum_i S_i^{-} \, . \tag{10}$$

Here the first and second terms represent the nearest neighbor hole-hopping and spin-exchange respectively, while the third is the single-site spin-flip term. After some straightforward algebra we find an expression similar to Eq. 9 with different $E(\vec{k})$ and F_i's, plus extra terms which are neglected at this level of approximation. By setting the coefficients to zero, the following set of three nonlinear coupled-cluster equations of the parameters α_i's are obtained:

$$\frac{5t\alpha_1^2}{2} + t\alpha_3^2 + \frac{3J\alpha_1}{2} + h\alpha_1\alpha_3 - t - \frac{J\alpha_1\alpha_3^2}{3} = 0 \tag{11}$$

$$\frac{J}{4} + 3J\alpha_2 - \frac{J\alpha_3^2}{2} + 2h\alpha_2\alpha_3 - 5J\alpha_2^2 - 3J\alpha_1\alpha_2 - \frac{h\alpha_1^2\alpha_3}{12} + \frac{2J\alpha_2\alpha_3^2}{3} = 0 \tag{12}$$

$$2J\alpha_3 + 8J\alpha_2\alpha_3 + \frac{h\alpha_3^2}{2} - \frac{h}{2} - 4h\alpha_2 - 2J\alpha_3^3 = 0\ . \tag{13}$$

These equations have no closed-form solution in general and need to be solved numerically. The hole energy $\epsilon(\vec{k})$ is given by

$$\epsilon(\vec{k}) = -4t\alpha_1 - J(\alpha_1^2 + 4\alpha_2 + 2\alpha_3^2 - 1) + \frac{h\alpha_3}{2} + \frac{1}{4}(J\alpha_1^2\gamma_{\vec{k}} + 4t\alpha_3 + 2h\alpha_1 - 6J\alpha_1\alpha_3)\gamma_{\vec{k}} \tag{14}$$

where $\gamma_{\vec{k}} \equiv \sum_{i(0)} \exp(i\vec{k}\cdot\vec{r}) = 2[\cos(k_x)+\cos(k_y)]$, and the sum denotes summation over nearest neighbor sites around the site 0. Note that only the terms involving hole-hopping and spin-flip are explicitly responsible for the dispersion of $\epsilon(\vec{k})$, and that along the direction $(\pi,0)$ to $(0,\pi)$ in the Brillouin zone the $\gamma_{\vec{k}}$ vanishes and the dispersion curve is flat.

For the case of zero magnetic field, we have $\alpha_3 = 0$ and the remaining two coupled-cluster equations, i.e. Eqs. 11 and 12, can be analytically solved to determine the α_1 and α_2:

$$\alpha_1 = \frac{3J}{10t}\{\sqrt{1 + \frac{40t^2}{9J^2}} - 1\} \tag{15}$$

$$\alpha_2 = -\frac{3(1-\alpha_1)}{10}\{\sqrt{1 + \frac{5}{9(1-\alpha_1)^2}} - 1\}\ . \tag{16}$$

The corresponding hole energy $\epsilon(\vec{k})$ is

$$\epsilon(\vec{k}) = -4t\alpha_1 + J(1 - \alpha_1^2 - 4\alpha_2) + \frac{J\alpha_1^2}{4}\gamma_{\vec{k}}^2\ . \tag{17}$$

In the small J limit, keeping terms up to the linear-order in J/t, Eq. 15 leads to: $\alpha_1 = \sqrt{2/5} - 3J/10t$ and $\alpha_2 = -0.13905 + 0.05020J/t$, and the hole energy is $\epsilon(\vec{k}) = -2.5298t + 2.3562J + 0.1J\gamma_{\vec{k}}^2$. It is clear that the hole energy dispersion function has a minimum value of $-2.5298t + 2.3562J$ at the zone boundary, which at this level of approximation is degenerate, and attains its maximum at $\vec{k} = (0,0)$ and (π,π). Thus, the hole energy bandwidth, defined as the difference between ϵ_{max} and ϵ_{min}, is given by $W = 1.6J$. Also, the effective mass of the hole is much smaller in the direction $(0,0)$ to (π,π) than in the direction $(0,\pi)$ to $(\pi,0)$. These results are in agreement with the qualitative statements made in previous studies of the t-J model.[2,3,4]

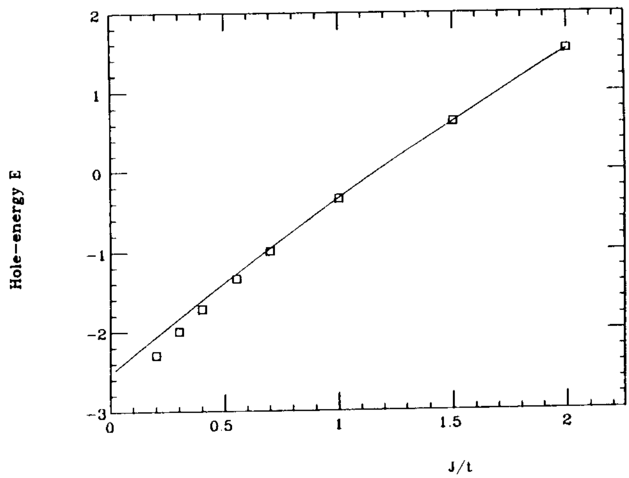

FIGURE 1 Hole energy E/t vs. J/t (at t=1). The solid line represents the results from coupled-cluster calculations. The squares refer to the exact diagonalization results of the $t-J$ model on a 4×4 lattice.

In Fig. 1 the hole energy E, identified as the bottom of the hole energy band, is plotted for $0 \leq J/t \leq 2$. Numerical results for the hole energy from exact diagonalization of the t-J model on a 4×4 lattice are shown as well.[4] Note that our results agree very well with the exact diagonalization results. Also, Fig. 2 compares results for the hole bandwidth. It is apparent that except for the small values of J/t, there exists a considerable discrepancy between the two sets of results. The difference may be due to the need for higher level corrections of the CCA to account for the dispersion. For the case of non-zero magnetic field, as mentioned above, the set of three nonlinear coupled-cluster equations has no closed-form solution, and thus we have to solve these equations numerically to determine the parameters α_i's for different values of J/t. With these numerical results we are able to calculate the hole energy dispersion function $\epsilon(\vec{k})$ in Eq. 14. Some typical results are shown in Fig. 3 for $J/t = 0.2$. For zero magnetic field our results for $\epsilon(\vec{k})$ are also consistent with previous studies of the t-J model. As the magnetic field increases, the hole energy band is shifted towards lower energy values around (π,π) whereas around (0,0) it is shifted upward. However, comparatively small changes occur in the neighbourhood of the zone boundary. These results are in qualitative agreement with those obained by a self-consistent perturbation approach which treats the spin-background in the linear spin-wave approximation, except that in the latter approach a decrease in energy around (0,0) is observed for small value of J.[9] This discrepancy may indicate the need for higher level corrections of the CCA.

In summary, we have investigated the ground state of a single hole of the 2D t-J model in a transverse magnetic field using the coupled-cluster method. We obtain an analytical expression of the hole energy dispersion function $\epsilon(\vec{k})$ which in the

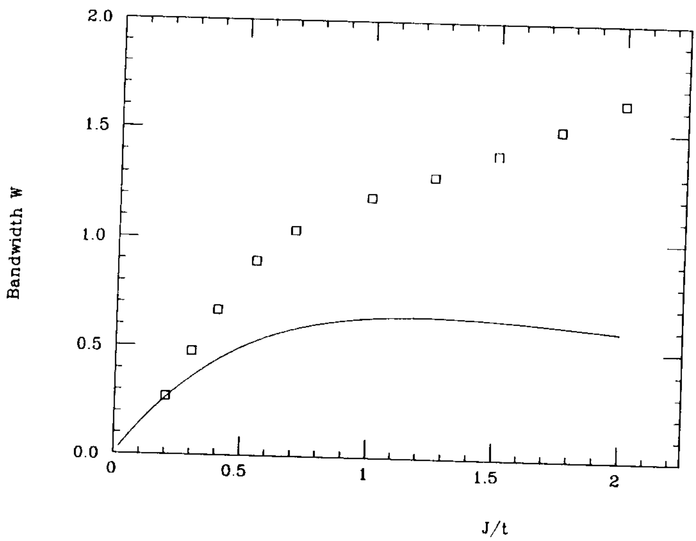

FIGURE 2 Bandwidth W/t vs. J/t. The solid line represents the results from coupled-cluster calculations. The squares refer to the exact diagonalization results of the $t-J$ model on a 4 × 4 lattice.

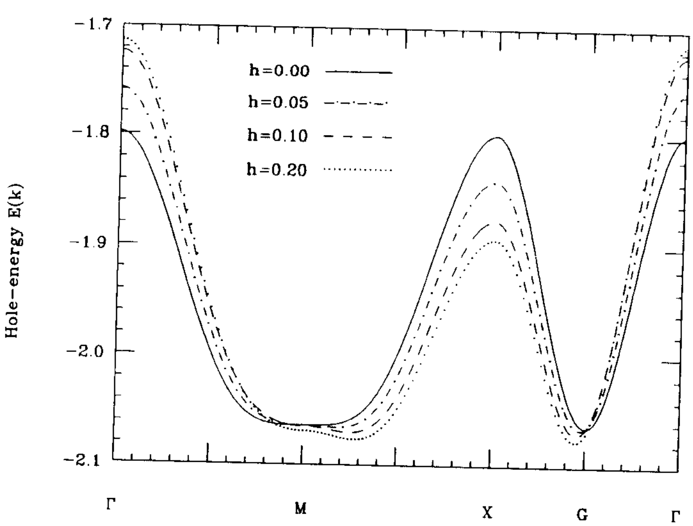

FIGURE 3 Dispersion curves, $E(\vec{k})/t$, plotted along the direction $\Gamma M X \Gamma$ for J/t=0.2 and various values of h/t: 0.0, 0.05, 0.1 and 0.2.

small J limit reproduces several features found in earlier studies of the t-J model in zero magnetic field. As the magnetic field increases, the hole energy band is shifted downward around (π,π) and upward around (0,0), whereas comparatively small changes occur in the neighbourhood of the zone boundary. We are in the process of studying the convergence of the CCA by including higher-order terms and a more detailed report will be presented elsewhere.

ACKNOWLEDGMENTS

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