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HOLE ENERGY AND WAVE FUNCTION IN THE THREE-DIMENSIONAL t–J MODEL

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ABSTRACT

A hole is considered by variational method in the t-J model at half filling in a simple cubic lattice with Néel ordering. Analytical expressions for hole energy and wave function are derived. Interaction with magnetic excitation is calculated. Role of dimensions is discussed.

The $t-J$ model (equivalent at $t \ll J$ to the Hubbard model) is widely used to describe correlation effects. The two-dimensional $t-J$ model is now very extensively studied as a model describing electronic structure of high-temperature superconductors. Much attention is paid to the one-dimensional model [1]–[5]. However, much information on the problem can also be obtained from three-dimensional studies. For example, comparison with two-dimensional results will make possible to distinguish correlation effects from geometry effects.

In two dimensions, the most popular approach is numerical cluster calculations (a review is presented in [7]). However, such calculations in three dimensions are much more complicated. Calculations on only 8-site cubic clusters have been reported [8]–[12]. First works calculated ground state energy if the Hubbard model with infinite [8] and finite [9] interaction without periodic boundary conditions. Symmetry properties of the ground state in the t-t'-J model for several lattices were studied in [11]. Finally, spectral weight function of a hole oi the cubic Hubbard model is presented in [12]. Obviously, small cluster size limits possibilities of obtaining details of the three-dimensional band structure by numerical calculations. In contrast, the variational method, which has proved to be successful in two dimensions [13]–[16], is easily generalized to three dimensions. In this paper, we variationally calculate hole dispersion and wave function in a simple cubic lattice. Using the obtained wave function, we calculate the vertex function for interaction of holes with long wave length magnons.

The model is defined by the Hamiltonian

$$H = H_t + H_J = t \sum_{<nm>\sigma} (d^\dagger_{n\sigma} d_{m\sigma} + \text{H.c.}) + J \sum_{<nm>} \mathbf{S}_n \cdot \mathbf{S}_m, \qquad (1)$$

where $d^\dagger_{n\sigma}$ and $d_{n\sigma}$ are the creation and destruction operators for a hole of spin σ ($\sigma = \uparrow, \downarrow$) on site n. The spin operators are $\mathbf{S}_n = \frac{1}{2} d^\dagger_{n\alpha} \vec{\sigma}_{\alpha\beta} d_{n\beta}$. $< nm >$ implies summing over all nearest neighbors in a simple cubic lattice. The Hamiltonian (1) is supplemented by the constraint of no double electron occupancy. For convenience, we set $J = 1$ in further calculations. The system at half filling (one electron per site) is a Heisenberg antiferromagnet. Its ground state has Néel ordering (see [6] for a review).

Let us consider a hole added to a half filled system with Néel ordering (we may also consider a background with Ising ordering, *i.e.*, an antiferromagnet without quantum fluctuations). We assume the wave function to be of the form

$$|\psi_{\mathbf{k}\uparrow}>= \left\{ A^\dagger_0 + \sum_\delta \xi_\delta A^\dagger_\delta \right\} |0>,$$

$$A^\dagger_0 = (2N)^{-1/2} \sum_n (1 - \lambda_n) d^\dagger_{n\uparrow} \exp(i\mathbf{k} \cdot \mathbf{r}_n), \qquad (2)$$

$$A^\dagger_\delta = (2N)^{-1/2} \sum_n (1 + \lambda_n) d^\dagger_{n\downarrow} S^+_{n+\delta} \exp(i\mathbf{k} \cdot \mathbf{r}_n),$$

where $|0>$ is the background state, $\lambda_n = 1$ for the spin-up sublattice and $\lambda_n = -1$ for the spin-down sublattice, δ is a unit vector corresponding to one step in the lattice, and $\mathbf{k}$ is the wave vector. The trial wave function (2) includes spin-up holes on the spin-down sublattice (operator $A^\dagger_0$) and spin-down holes on the spin-up sublattice with nearest neighbor spin flip (operators $A^\dagger_\delta$). In other words, we consider states with one simple hole and one possible hopping (given by applicaton of H_t). This assumpsion is quite natural at $t \ll J$. However, it turns out that in two dimensions this ansatz gives reasonable results [16] even for $t/J \approx 5$. In three dimensions we expect a similar range of validity since neither coordination number nor background are changed drastically as compared to two dimensions. An important advantage of the ansatz (2) is that it leads to simple *analytical* expressions for dispersion and wave function which enable one to perform further calculations, *e.g.*, of interaction between holes.

For calculations, we denote the basis states of the wave function (2) as

$$|1>= A^\dagger_0|0>,$$

$$|2>= A^\dagger_x|0>, \qquad |3>= A^\dagger_{-x}|0>,$$

$$|4>= A^\dagger_y|0>, \qquad |5>= A^\dagger_{-y}|0>,$$

$$|6>= A^\dagger_z|0>, \qquad |7>= A^\dagger_{-z}|0> . \qquad (3)$$

The basis (3) is not orthogonal. The normalization matrix is

$$\begin{aligned} <1|1> &= A, \qquad <1|i>= 0, \qquad i,j = 2, ..., 7; \\ <i|j> &= B\delta_{ij} + 2A(1-\delta_{ij})[q_{20}\delta^{23}_{ij} + q_{11}(1-\delta^{23}_{ij})]; \\ A &= \frac{1}{2} + \sigma, \qquad B = \frac{1}{4} + \sigma - p_1; \qquad (4) \\ \delta^{23}_{ij} &= \begin{cases} 1, & \text{if } \{i,j\} = \{2,3\}, \{4,5\}, \{6,7\}; \\ 0, & \text{otherwise.} \end{cases} \end{aligned}$$

Here and hereafter the following characteristics of the background are used

$$\begin{aligned} p_1 &= <0|S^z_n S^z_{n+\delta}|0>, \qquad q_1 = \frac{1}{2} <0|S^+_n S^-_{n+\delta}|0>, \\ p_{11} &= <0|S^z_n S^z_{n+\delta+\delta'}|0>, \qquad q_{11} = \frac{1}{2} <0|S^+_n S^-_{n+\delta+\delta'}|0>, \\ p_{20} &= <0|S^z_n S^z_{n+2\delta}|0>, \qquad q_{20} = \frac{1}{2} <0|S^+_n S^-_{n+2\delta}|0>, \qquad (5) \\ \sigma &= |<0|S^z_n|0>|, \quad \rho_1 = p_1 + 2q_1 =<0|\mathbf{S}_n \cdot \mathbf{S}_{n+\delta}|0>, \quad \delta \perp \delta'. \end{aligned}$$

For the Ising state, the correlators (5) are trivial. For the Néel state, using the spin-wave theory (see, *e.g.*, [6]) we obtained the following numerical values

$$\begin{aligned} \sigma &= 0.422, \qquad \rho_1 = -0.299, \\ p_1 &= -0.194, \qquad p_{11} \approx p_{20} = p_2 = 0.179; \\ q_1 &= -0.052, \qquad q_{11} = 0.020, \qquad q_{20} = 0.013; \\ A &= 0.922, \qquad B = 0.866. \qquad (6) \end{aligned}$$

To make the theory self-consistent, we took $q_1 = \frac{1}{2}(\rho_1 - p_1)$. Results close to (6) can be obtained by other methods [6].

We will calculate the energy with respect to the background level E_0: $H|0>= H_J|0>= E_0|0>$. Therefore, we make a shift $H_J \to H_J - E_0$. Now the Hamiltonian matrix is

$$< 1|H|1 >= \frac{3}{2}(\sigma - 2\rho_1), \quad i,j = 2,...,7, \quad i \neq j,$$

$$< 1|H|i >= -t\Big\{Be^{-i\mathbf{k}\delta_i} + 2A(q_1+q_{20})e^{i\mathbf{k}\delta_i} + 2A(q_1+q_{11})\sum_{\delta' \perp \delta_i} e^{i\mathbf{k}\delta'}\Big\},$$

$$< i|H|i >= \frac{1}{16} + \frac{17}{8}\sigma - 4p_1 + \frac{15}{4}p_2 - 6q_1 - \frac{15}{2}\sigma p_1 + 10\sigma q_1, \quad (7)$$

$$< i|H|j >= q_1(\sigma - 1/2) + q_{20}(7\sigma - 4p_1 + 10p_2 - 8q_1) + (\sigma - 2p_1)q_1\delta_{ij}^{23}.$$

In order to simplify formulas, ground state factorization has been used in calculations of the matrix elements (7). Complicated correlators were treated as, *e.g.*,

$$< 0|\lambda_n S_n^z S_{n+\delta}^+ S_{n+2\delta}^-|0 > \approx < 0|\lambda_n S_n^z|0 >< 0|S_{n+\delta}^+ S_{n+2\delta}^-|0 >= 2q_1\sigma. \quad (8)$$

These terms play a negligable role in the final results. Therefore, inroduced small errors can be safely ignored.

When $t=0$ (*i.e.*, $H = H_J$ and there is no hopping) the hole energy is

$$\epsilon_0 = \frac{< 1|H|1 >}{< 1|1 >} = \frac{3}{2}\cdot\frac{\sigma - 2\rho_1}{1/2+\sigma} = \begin{cases} 3/2 & \text{for Ising state,} \\ 1.7 & \text{for Néel state.} \end{cases} \quad (9)$$

Simple estimations show that the correction to the energy (9) is $\delta\epsilon_0 \approx -0.1$. This correction comes from appearing in the wave function states with more complicated structure (relaxation of the background). The most important states are those with double hopping $d_{n\uparrow}^\dagger S_{n+\delta}^- S_{n+\delta+\delta'}^+|0>$. Their contribution can be estimated a perturbation.

The set of basis functions (3) can be orthonormalized by the following transformation

$$\begin{aligned}
|\tilde{1}> &= \alpha_1|1>,\\
|\tilde{2}> &= \alpha_2(|2>-|3>),\\
|\tilde{3}> &= \alpha_2(|4>-|5>),\\
|\tilde{4}> &= \alpha_2(|6>-|7>),\\
|\tilde{5}> &= \alpha_3(|2>+|3>-|4>-|5>),\\
|\tilde{6}> &= \alpha_4(|2>+|3>+|4>+|5>-2|6>-2|7>),\\
|\tilde{7}> &= \alpha_5(|2>+|3>+|4>+|5>+|6>+|7>), \quad (10)\\
\alpha_1 &= A^{-1/2},\\
\alpha_2 &= [2(B-2q_{20}A)]^{-1/2},\\
\alpha_3 &= [4(B-2(2q_{11}-q_{20})A)]^{-1/2},\\
\alpha_4 &= [6(B-2(2q_{11}-q_{20})A)]^{-1/2},\\
\alpha_5 &= [6(B+(8q_{11}+2q_{20})A)]^{-1/2}.
\end{aligned}$$

The variational procedure leads (for the Néel state) to a fourth degree equation. In order to obtain an approximate solution, we assume correlators q_{11} and q_{20} to be equal. So we substitute $q_{20}, q_{11} \to q_2 = \frac{4}{5}q_{11} + \frac{1}{5}q_{20} = 0.018$. The coefficients for q_{11} and q_{20} are chosen taking into account how often they appear in (4) and (7). The small role of q_{11} and q_{20} in final results justifies this approximation.

Now the variational procedure yields the energy of a hole

$$\epsilon_\mathbf{k} = \epsilon_0 + \frac{\Delta}{2} - S_\mathbf{k}, \quad S_\mathbf{k} = \left[\frac{\Delta^2}{4} + 6t^2(a - b\gamma_\mathbf{k}^2)\right]^{1/2}, \quad (11)$$

where

$$\gamma_\mathbf{k} = \frac{1}{3}(\cos k_x + \cos k_y + \cos k_z), \quad \Delta = \frac{< i|H|i >}{< i|i >} - \epsilon_0,$$

$$a = \frac{[g - 2(q_1+q_2)/g]^2}{1 - 2q_2/g}, \quad b = a - \frac{[g + 10(q_1+q_2)/g]^2}{1+10q_2/g}, \quad g = \left(\frac{A}{B}\right)^{1/2}.$$

For the Ising state, $\Delta = 5/2$, $a = 1$, $b = 0$, and $g = 1$. In the absense of quantum fluctuations, a hole can propagate only in a spiral way by tunneling through string barrier [13, 14]. This process is neglected in the ansatz (2). Therefore, we have results with no dispersion. For the Néel state, the dominating process is motion as allowed by quantum fluctuations with $\Delta = 1.94$, $a = 1.12$, $b = 0.80$, and $g = 0.97$. In the strong interaction limit ($t \gg J$), the total band width is $2t\sqrt{6a} = 5.2t$, which agrees well with $5.4t$ presented in [12]. Unfortunately, absolute values of band parameters are not given in [12].

The normalized wave function has the form

$$|\psi_{\mathbf{k}\uparrow}>= h^\dagger_{\mathbf{k}\uparrow}|0>= \left(\frac{\Delta + 2S_\mathbf{k}}{8AS_\mathbf{k}N}\right)^{1/2} \times$$

$$\times \sum_n \left\{(1-\lambda_n)d^\dagger_{n\uparrow} + (1+\lambda_n)\sum_\delta \xi_\delta d^\dagger_{n\downarrow}S^+_{n+\delta}\right\}|0> \exp(i\mathbf{k}\cdot\mathbf{r}_n), \qquad (12)$$

where

$$\xi_\delta = \frac{2t}{g(\Delta+2S_\mathbf{k})}[(1+v)\exp(i\mathbf{k}\cdot\delta) - (u+v)\gamma_\mathbf{k}],$$

$$u = 1 - \frac{g + 10(q_1+q_2)/g}{1+10q_2/g}, \qquad v = \frac{g - 2(q_1+q_2)/g}{1-2q_2/g} - 1.$$

For the Ising state, $u = v = 0$. For the Néel state, $u \approx 0.48$ and $v \approx 0.08$. In another notation, the wave function is

$$|\psi_{\mathbf{k}\uparrow}>= \left(\frac{\Delta + 2S_\mathbf{k}}{8AS_\mathbf{k}N}\right)^{1/2} \times$$

$$\times \sum_n (1-\lambda_n)\left\{1 - \sum_\delta \xi_\delta \exp(-i\mathbf{k}\cdot\delta)d^\dagger_{n-\delta\downarrow}d_{n\downarrow}\right\}d^\dagger_{n\uparrow}|0> \exp(i\mathbf{k}\cdot\mathbf{r}_n). \quad (13)$$

Obviously, the wave function of a spin-down hole can be obtained by taking the sums in (12) or (13) over the other sublattice and inverting spin indeces.

The bottom of the band (11) is located at the surface $\gamma_\mathbf{k} = 0$

$$\epsilon_b = \epsilon_0 + \frac{\Delta}{2} - \left[\frac{\Delta^2}{4} + 6at^2\right]^{1/2}. \qquad (14)$$

Taking into account the difference between q_{20} and q_{11}, we found the following correction to dispersion along the surface $\gamma_\mathbf{k} = 0$,

$$\delta\epsilon = \begin{cases} -0.09t^2(\sin^2 k_x + \sin^2 k_y + \sin^2 k_z) & \text{for } t \ll 0.4, \\ -0.012t(\sin^2 k_x + \sin^2 k_y + \sin^2 k_z) & \text{for } t \gg 0.4. \end{cases} \qquad (15)$$

Thus, we have the band bottom at $\mathbf{K}_0 = (\pm\pi/2, \pm\pi/2, \pm\pi/2)$. The same effect exists in the two-dimensional case. Assuming $q_{11} = q_{20}$, the band bottom is at the line $\cos k_x + \cos k_y = 0$ [16]. After taking into account the difference between q_{11} and q_{20}, the band bottom is at $\mathbf{K} = (\pm\pi/2, \pm\pi/2)$, in agreement with results of other methods [7]. The energy correction along the line $\cos k_x + \cos k_y = 0$ is

$$\delta\epsilon = \begin{cases} -0.22t^2(\sin^2 k_x + \sin^2 k_y) & \text{for } t \ll \Delta/4, \\ -0.004t(\sin^2 k_x + \sin^2 k_y) & \text{for } t \gg \Delta/4. \end{cases} \qquad (16)$$

Holes are defined within the Brillouin zone which is the same as that for fcc lattice with lattice constant 2. There are $N/2$ states for spin-up holes and the same number for spin-down holes. Under doping at zero temperature the zone occupied by holes has the form of 8 semiellipsoids in the neighborhood of the points of minimum energy. The Fermi energy ϵ_F is connected with the doping concentration x by the equation

$$\epsilon_F = \frac{3\pi}{4}\left(\frac{\pi}{6}\right)^{1/3} \beta_\parallel^{1/3}\beta_\perp^{2/3}x^{2/3}, \qquad (17)$$

where $\beta_\perp$ and $\beta_\parallel$ are the hole reciprocal masses at the bottom ($\beta_\perp$ is for the direction towards the origin and $\beta_\parallel$ for the perpendicular plane). According to (11) and (15),

$$\beta_\parallel = \frac{2bt^2}{(6at^2+\Delta^2/4)^{1/2}} \approx \begin{cases} 1.65t^2 & \text{for } t \ll 0.4, \\ 0.62t & \text{for } t \gg 0.4; \end{cases} \qquad (18)$$

$$\beta_\perp \approx \begin{cases} 0.025t^2 & \text{for } t \ll 0.4, \\ 0.18t & \text{for } t \gg 0.4. \end{cases}$$

The knowledge of the wave function (12) enables one to calculate the interaction of holes with long wave length magnons. Short wave length magnetic excitations are effectively included in the ansatz (2) and do not need more consideration. In the spin wave approximation (see [6]), the magnon dispersion is $\omega_\mathbf{q} = 3(1-\gamma^2_\mathbf{q})^{1/2}$. In the long wave length limit ($q \ll 1$) it reduces to $\omega_\mathbf{q} = \sqrt{3}q$. The explicit form of the magnon creation operator is

$$c^\dagger_\mathbf{q} = N^{-1/2}\sum_n(\cosh\theta_\mathbf{q}\, a^\dagger_n - \sinh\theta_\mathbf{q}\, a_n)\exp(i\mathbf{q}\cdot\mathbf{r}_n), \qquad (19)$$

where

$$\tanh 2\theta_\mathbf{q} = \gamma_\mathbf{q}, \qquad a^\dagger_n = \frac{1+\lambda_n}{2}S^-_n + \frac{1-\lambda_n}{2}S^+_n.$$

We consider hole-magnon interaction by the perturbation theory. In the unpertured Hamiltonian we include simple excitations (12) and (19)

$$H_0 = E_0 + \sum_{\mathbf{k}\sigma}\epsilon_\mathbf{k} h^\dagger_{\mathbf{k}\sigma}h_{\mathbf{k}\sigma} + \sum_\mathbf{q}\omega_\mathbf{q} c^\dagger_\mathbf{q} c_\mathbf{q}, \qquad (20)$$

where the second sum is restricted to small q, and we treat the remaining part of the Hamiltonian as perturbation $V = H - H_0$. The interaction is then characterized by the vertex function

$$\Gamma(\mathbf{k}\downarrow; \mathbf{k}-\mathbf{q}\uparrow, \mathbf{q}) = <0|h_{\mathbf{k}\downarrow} V h^\dagger_{\mathbf{k}-\mathbf{q}\uparrow} c^\dagger_\mathbf{q}|0>. \qquad (21)$$

Neglecting terms propotional to magnon energy we come to

$$\Gamma(\mathbf{k}\downarrow;\mathbf{k}-\mathbf{q}\uparrow,\mathbf{q}) =$$
$$=< 0|h_{\mathbf{k}\downarrow}(H-E_0)h^{\dagger}_{\mathbf{k}-\mathbf{q}\uparrow}c^{\dagger}_{\mathbf{q}}|0> -\epsilon_{\mathbf{k}} < 0|h_{\mathbf{k}\downarrow}h^{\dagger}_{\mathbf{k}-\mathbf{q}\uparrow}c^{\dagger}_{\mathbf{q}}|0> . \qquad (22)$$

Calculation of the vertex function (21) is quite similar to the corresponding two-dimensional calculation presented in [17]. It is performed by commutation of operators and asumes ground state factorization. For $\gamma_{\mathbf{k}} = 0$ and $q \ll 1$, we obtained

$$\Gamma(\mathbf{k}\downarrow;\mathbf{k}-\mathbf{q}\uparrow,\mathbf{q}) = -\left(\frac{3}{N}\right)^{1/2} f(t)(q_x \sin k_x + q_y \sin k_y + q_z \sin k_z), \qquad (23)$$

where

$$f(t) = A_1 t + A_2 \frac{t}{S_{\mathbf{k}}} + A_3 \frac{t^3}{S_{\mathbf{k}}(\Delta + 2S_{\mathbf{k}})},$$

$A_1 = 0.69, A_2 = -3.58$, and $A_3 = -21.8$. Approximately,

$$f(t) = \begin{cases} 3.0t & \text{for } t \ll 0.4, \\ 0.9t + 1.1 & \text{for } t \gg 0.4. \end{cases}$$

The structure of the vertex (23) supports that the band bottom lies at the points $\mathbf{K}_0 = (\pm\pi/2, \pm\pi/2, \pm\pi/2)$ because interaction with magnons, which reduces energy, is maximum at these points. Not small value of the vertex function indicates that spin waves may play an important role in behavior of electrons.

The results obtained in this paper are quite analogous to those of the two-dimensional model. This suggests that one-particle properties are determined by correlation effects and are not specific in the two-dimensional geometry.

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