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t-J MODEL. VERTEX FUNCTION FOR THE INTERACTION OF A HOLE WITH LONG WAVE LENGTH MAGNONS

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t-J Model. Vertex Function for the Interaction of a Hole with Long Wave Length Magnons

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ABSTRACT

We consider two-dimensional t-J model with a hole on the Neel background. The vertex function for the interaction of a hole with long wave length magnons is calculated.

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The investigation of two-dimensional t-J model is very popular now due to connection with high-T_c superconductors [1]. At a half filling the t-J model is equivalent to the Heisenberg model. It is well established that in this case there is Neel ordering in the ground state [2, 3, 4]. The problem is behaviour of a system under doping by the holes. To study the dynamics of the holes in doped antiferromagnet numerous approximations have been proposed, and some of the properties of a hole have been established. Calculations based on the moment method of Brincman and Rice [5] are carried out in the limit $t/J \to \infty$ [6, 7, 8]. The analytical spin-wave and variational methods were used in Refs. [9, 10, 11, 12, 13, 14]. Calculation of Trugman is an exact numerical diagonalization of Hamiltonian withing a retained portion of the Hilbert space [15, 16]. Approach of Refs. [17, 18, 19, 20] is based on numerical diagonalization of Hamiltonian on small lattices (see also the review paper [21]. It has been shown that one hole in the t-J model has a ground state with a momentum of either $\vec{k} = (\pm\frac{\pi}{2}, \pm\frac{\pi}{2})$ or $\vec{k} = (0, \pm\pi), (\pm\pi, 0)$. In any case the energy is almost degenerate along the line $cosk_x + cosk_y = 0$.

One of the problems connected with the t-J -model is melting of the long range Neel ordering which is observed in high -T_c superconductors. (Magnetic phase diagram for the compound $La_{2-x}Sr_xCuO_4$ is presented in the Ref. [22].) In the paper [23] we have demonstrated the quantum melting of Neel ordering at doping using variational method and numerical diagonalization. In the Ref. [23] we have used the anzats for trial wave-function convenient for both the Neel state and for the spin liquid state. This anzats was suggested in the work [24].

In the present work we use variational method as well. We suggest very simple anzats for the trial wave function of a hole which can be used only for the Neel background. Analytical expressions for the energy and for the

Hamiltonian

$$H = H_t + H_J = t \sum_{<ij>\sigma} (d^+_{i\sigma} d_{j\sigma} + h.c) + J \sum_{<ij>} \vec{S}_i \vec{S}_j \ . \quad (1)$$

where $d^+_{i\sigma}$ is the creation operator of a hole with spin σ at site i of a two-dimensional square lattice. The operator $d^+_{i\sigma}$ acts in the Hilbert space where there is no double electron occupancy. The spin variable is $S_i = \frac{1}{2} d^+_{i\alpha} \sigma_{\alpha\beta} d_{i\beta}$. $< ij >$ are the neighbour sites on the lattice. In further calculations we will set $J = 1$.

Let us denote by $|0>$ the background Neel state corresponding to half-filling. All our results are expressed in terms of spin correlators over this state.

$$\sigma = |<0|S^z_n|0>|, \qquad p = <0|S^z_n S^z_m|0>,$$
$$2q = <0|S^+_n S^-_m|0>, \quad \rho = p + 2q = <0|\vec{S}_n \vec{S}_m|0> . \quad (2)$$

p_1, q_1 and ρ_1 correspond to the neighbour sites n,m; and p_2, q_2, ρ_2 correspond to the next neighbour sites. For the Neel state the next neighbour correlators are practically independent on a path between the sites n and m. Numerical values of correlators for the Neel state are as follow

$$\sigma = 0.3, \quad p_1 = -0.17,\ p_2 = +0.1, \quad q_1 = -0.08,\ q_2 = 0.05. \quad (3)$$

Due to the work [11] the energy of a hole with respect to the background level is equal to

$$E(k) = \epsilon_0 + \epsilon(k), \qquad \epsilon(k) = \frac{\Delta}{2} - S(k), \quad (4)$$
$$S(k) = \sqrt{\Delta^2/4 + 4t^2(1+y) - t^2(x+y)(cosk_x + cosk_y)^2}.$$

The parameters here are as follow

$$\epsilon_0 = \frac{\sigma - 2\rho_1}{1/2+\sigma} \approx 1.2,$$
$$\Delta = \frac{\frac{1}{16} + \frac{11}{8}\sigma + \frac{9}{4}p_2 - \frac{1}{2}p_1(5+9\sigma) - 2q_1(2+3\sigma)}{1/4+\sigma-p_1} - \epsilon_0 \approx 1.33,$$
$$x = 1 - \frac{(g + 6(q_1+q_2)/g)^2}{1+6q_2} \approx 0.557, \quad (5)$$
$$y = \frac{(g - 2(q_1+q_2)/g)^2}{1-2q_2} - 1 \approx 0.138,$$

$$g = \sqrt{\frac{(1/4+\sigma-p_1)}{(1/2+\sigma)}} \approx 0.95.$$

Let us set $\lambda_n = +1$ for spin up sites of the Neel state and $\lambda_n = -1$ for spin down sites. The hole wave function derived in the Ref.[11] is of the form $\psi_\sigma(k) = h^+_{k\sigma}|0>$, where

$$h^+_{k\uparrow} = \nu(k)\hat{A}_{0\uparrow} + \sum_{\vec{\delta}} \xi_{\vec{\delta}}(k)\hat{A}_{\vec{\delta}\uparrow}, \qquad h^+_{k\downarrow} = \nu(k)\hat{A}_{0\downarrow} + \sum_{\vec{\delta}} \xi_{\vec{\delta}}(k)\hat{A}_{\vec{\delta}\downarrow},$$
$$\hat{A}_{0\uparrow} = \frac{1}{\sqrt{2N}} \sum_n (1-\lambda_n) d^+_{n\uparrow} e^{i\vec{k}\vec{r}_n}, \quad \hat{A}_{0\downarrow} = \frac{1}{\sqrt{2N}} \sum_n (1+\lambda_n) d^+_{n\downarrow} e^{i\vec{k}\vec{r}_n},$$
$$\hat{A}_{\vec{\delta}\uparrow} = \frac{1}{\sqrt{2N}} \sum_n (1+\lambda_n) d^+_{n\downarrow} S^+_{n+\vec{\delta}} e^{i\vec{k}\vec{r}_n},$$
$$\hat{A}_{\vec{\delta}\downarrow} = \frac{1}{\sqrt{2N}} \sum_n (1-\lambda_n) d^+_{n\uparrow} S^-_{n+\vec{\delta}} e^{i\vec{k}\vec{r}_n}. \quad (6)$$

Here $\vec{\delta}$ is the unit vector connecting the nearest-neighbour sites. The expansion coefficients are as follow

$$\nu(k) = \frac{1}{2}\sqrt{\frac{\Delta + 2S}{(1/2+\sigma)S}},$$
$$\xi_{\vec{\delta}}(k) = \frac{t}{\sqrt{(1/4+\sigma-p_1)S(\Delta+2S)}} \times$$
$$\times \left((1+v)e^{i\vec{k}\vec{\delta}} - \frac{1}{2}(u+v)(cosk_x + cosk_y) \right), \quad (7)$$

where

$$u = 1 - \frac{g + 6(q_1+q_2)/g}{1+6q_2} \approx 0.416,$$
$$v = \frac{g - 2(q_1+q_2)/g}{1-2q_2} - 1 \approx 0.124. \quad (8)$$

Besides the hole wave function we need the wave function of a magnon. Let a^+_n be the spin flip operator at the site n

$$a^+_n = \frac{1+\lambda_n}{2} S^-_n + \frac{1-\lambda_n}{2} S^+_n \ . \quad (9)$$

sites n,m. For the Neel state the next and the next next neighbour correlators are practically independent on a path between the sites n and m. Numerical values of correlators for the Ising background (background without quantum fluctuations: $S_n^z = \pm 1/2$) and for the Neel one are as follow

$$\begin{aligned} I:\sigma &= 1/2,\ p_1=-1/4,\ p_2=+1/4,\ p_3=-1/4,\quad q_i=0\ . \\ N:\sigma &= 0.3,\ p_1=-0.17,\ p_2=+0.1,\ p_3=-0.09\ , \\ q_1 &= -0.08,\ q_2=0.05,\ q_3=-0.04\ . \end{aligned} \tag{8}$$

Note that due to the Eqs.(6) the basis set (5) is orthonormalized for the Ising background.

Next is calculation of the Hamiltonian matrix. Let us consider at first the H_J. One should use the commutation relations

$$[H_J, d^+_{n\uparrow}] = \frac{1}{2}\sum_{\vec\delta}\left(d^+_{n\uparrow}S^z_{n+\vec\delta} + d^+_{n\downarrow}S^+_{n+\vec\delta}\right), \qquad [H_J, S^\alpha_n] = i\sum_{\vec\delta}\epsilon_{\alpha\beta\gamma}S^\beta_n S^\gamma_{n+\vec\delta}\ . \tag{9}$$

For example

$$\begin{aligned} <1|H_J|1> &= \frac{1}{N}\sum_n (1-\lambda_n) <0|d_{n\uparrow}\left([H_J, d^+_{n\uparrow}] + d^+_{n\uparrow}H_J\right)|0>= \\ &= (\sigma - 2\rho_1) + E_0 <1|1>\ . \end{aligned} \tag{10}$$

Here E_0 is the energy of background: $H_J|0>= E_0|0>$. Full H_J matrix is as follow (we omit the terms $E_0 <i|j>$):

$$\begin{aligned} <1|H_J|1> &= (\sigma - 2\rho_1), \quad <1|H_J|i>=0, \quad i,j=2,3,4,5\ , \\ <i|H_J|i> &= \frac{1}{16} + \frac{11}{8}\sigma + \frac{9}{4}p_2 - \frac{1}{2}p_1(5+9\sigma) - 2q_1(2+3\sigma)\ , \\ <i|H_J|j> &= q_1(\sigma - 1/2 - 4q_2) + 2q_2(2\sigma - p_1 + 3p_2) + B(\sigma - 2p_1)\ , \\ & \quad i \neq j\ . \end{aligned} \tag{11}$$

Here $B = 3q_3$ if i+j is even and $B = q_1 + 2q_3$ if i+j is odd. In calculation we have used the ground state factorization. For example:

$$\begin{aligned} &<0|\lambda_n S^z_n S^-_{n+\vec\delta} S^+_{n+\vec\delta+\vec\delta'}|0>\approx \\ &\approx <0|\lambda_n S^z_n|0><0|S^-_{n+\vec\delta}S^+_{n+\vec\delta+\vec\delta'}|0>= 2q_1\sigma\ , \\ &<0|S^z_n S^z_{n+\vec\delta} S^-_{n+\vec\delta'} S^+_{n+\vec\delta'+\vec\delta''}|0>\approx \\ &\approx <0|S^z_n S^z_{n+\vec\delta}|0><0|S^-_{n+\vec\delta'}S^+_{n+\vec\delta'+\vec\delta''}|0>= 2q_1p_1\ . \end{aligned} \tag{12}$$

This is rather crude estimation, but in any case uncertainty in the estimation is very small numerically.

The energy of a hole at t=0 is equal to

$$\epsilon_0 = \frac{<1|H_J|1>}{<1|1>} = \frac{\sigma - 2\rho_1}{1/2+\sigma} = \begin{cases} 1 & \text{for I-state} \\ 1.2 & \text{for N-state} \end{cases}\ . \tag{13}$$

Relaxation of the background is neglected in this equation. Let us estimate this effect. It is due to the admixture of the states with more complicated structure to the wave function $|1>$ (Eqs. (4),(5)). The most important that are double spin-flip excitations

$$|b>= \frac{1}{\sqrt{2N}}\sum_n (1-\lambda_n) d^+_{n\uparrow} S^-_{n+\vec\delta} S^+_{n+\vec\delta+\vec\delta'} e^{i\vec k\vec r_n}|0>\ . \tag{14}$$

Calculations similar to that described above give the matrix elements:

$$\begin{aligned} <b|b> &= (\frac{1}{2}+\sigma)(\frac{1}{4} - p_1) + \frac{1}{2}\sigma - \frac{1}{2}p_1 + \frac{1}{2}p_2\ , \\ <1|b> &= 2q_1(1/2+\sigma)\ , \\ <b|H_J|b> &\approx 2.3, \qquad <1|H_J|b>= q_1(-1/4+\sigma-3\rho_1)\ . \end{aligned} \tag{15}$$

There are 12 states $|b>$ corresponding to the different orientations of $\vec\delta, \vec\delta'$ in Eq.(14), and therefore total correction to the hole energy is equal to

$$\delta\epsilon_0 = 12 \times \frac{(<b|H_J|1> - \epsilon_0 <b|1>)^2}{<1|H_J|1><b|b> - <b|H_J|b><1|1>} \approx -0.05\ . \tag{16}$$

We have used here the parameters of Neel state from Eq.(8). (We remind the reader that we set J=1) Other contribution to the background relaxation is due to the state

$$|c>= \frac{1}{\sqrt{2N}}\sum_n (1-\lambda_n) d^+_{n\downarrow} S^+_{n+\vec\delta} e^{i\vec k\vec r_n}|0>\ . \tag{17}$$

There is no such a state for the Ising background ($|c>\equiv 0$), but for the Neel one due to the quantum fluctuations it is a real state. Simple calculations show that the hole energy correction connected with the states $|c>$ is equal to $\delta\epsilon_0 \approx -5\times 10^{-3}$. Thus the background relaxation is due mainly to double spin-flip excitations (16), but the effect is very small and can be neglected.

Let us come back to the case of nonzero t. It is convenient to shift the energy level in such a way that the hole energy to be zero at t=0. To do it we should subtract

$$<\alpha|H_J|\beta>\rightarrow<\alpha|\tilde H_J|\beta>=<\alpha|H_J|\beta> - \epsilon_0 <\alpha|\beta>\ . \tag{18}$$

Here $E(k)$ is the hole energy (4), and E_0 is the energy of the Neel background. It is obvious that the contribution proportional to E_0 in the second term of Eq.(12) exactly cancels that in the first term. Therefore further we set $E_0 = 0$.

In the off-diagonal matrix element $< 0|h_{k+q\downarrow} H h^+_{k\uparrow} c^+_q|0 >$ let us consider at first the contribution of H_J. The H_J does not change position of a hole. Therefore this contribution is proportional to $\nu \times \xi$ (see Eq.(6)). Using the commutation relations

$$[H_J, d^+_{n\uparrow}] = \frac{1}{2}\sum_{\vec{\delta}}\left(d^+_{n\uparrow}S^z_{n+\vec{\delta}} + d^+_{n\downarrow}S^+_{n+\vec{\delta}}\right), \qquad (20)$$

$$[d_{n\downarrow}, H_J] = \frac{1}{2}\sum_{\vec{\delta}}\left(-d_{n\downarrow}S^z_{n+\vec{\delta}} + d_{n\uparrow}S^+_{n+\vec{\delta}}\right)$$

we find

$$< 0|h_{k+q\downarrow} H_J h^+_{k\uparrow} c^+_q|0 >=$$

$$= \frac{1}{N}\sum_{n\vec{\delta}} e^{-i\vec{q}\vec{r}_n} < 0|\Big\{(1+\lambda_n)\nu^*(k+q)\xi_{\vec{\delta}}(k)[d_{n\downarrow}, H_J]d^+_{n\downarrow}S^+_{n+\vec{\delta}} +$$

$$+(1-\lambda_n)\nu(k)\xi^*_{\vec{\delta}}(k+q)d_{n\uparrow}S^+_{n+\vec{\delta}}\left([H_J, d^+_{n\uparrow}] + d^+_{n\uparrow}\omega_q\right)\Big\} \approx \qquad (21)$$

$$\approx -\frac{t}{2S}\frac{1/4-\sigma+3\rho_1}{\sqrt{(1/2+\sigma)(1/4+\sigma-\rho_1)}}(1+u+2v)Z .$$

Let us remind once more that the terms proportional to $cosk_x + cosk_y$ are neglected.

Calculation of the H_t contribution is not complicated as well. The H_t changes the position of a hole. Therefore there are two parts in this contribution: The first part is proportional to $\sim \nu \times \nu$, and the second one $\sim \xi \times \xi$ (see Eqs. (6)). Calculation of the $\nu \times \nu$ contribution is trivial

$$\nu \times \nu : \quad < 0|h_{k+q\downarrow} H_t h^+_{k\uparrow} c^+_q|0 > \to -t\frac{\Delta + 2S}{2S}Z . \qquad (22)$$

Calculation of the $\xi\times\xi$ contribution is also straightforward, but more cumbersome

$$\xi\times\xi : \quad < 0|h_{k+q\downarrow} H_t h^+_{k\uparrow} c^+_q|0 > \to -\frac{t^3}{S(\Delta+2S)}(6+34v+8u(1+v))Z . \qquad (23)$$

Summing the contributions (21), (22), (23), (18), (19) we get the hole magnon vertex

$$\begin{aligned} \Gamma_0 &= f(t)Z, \quad \text{where} \\ f(t) &= -t\Big(\frac{\Delta+2S}{2S} + \frac{1}{2S}(1+u+2v)(1+v+\Delta-2S) + \\ &+ \frac{t^2}{S(\Delta+2S)}(6+34v+8u(1+v))\Big) . \end{aligned} \qquad (24)$$

Function $f(t) \approx -3.4t$ at $t \ll \Delta/4$ and $f(t) \approx -0.87t$ at $t \gg \Delta/4$.

The vertex function (24) corresponds to the normalization (10): one magnon in the volume. More convenient normalization is $2\omega_q$ magnons in the volume. At this normalization a magnon Green function is $1/(\omega^2 - \omega_q^2)$, and the vertex is $\Gamma = \sqrt{2\omega_q}\Gamma_0$ From the Eqs.(24), (18), (11) we get

$$\Gamma(k,q) = \frac{1}{\sqrt{N}}(q_x sink_x + q_y sink_y)f(t) \qquad (25)$$

Thus in the present paper we have calculated the hole-magnon vertex function for long wave magnons ($q \ll 1$) near the bottom of the hole band ($cosk_x + cosk_y \ll 1$). First of all this interaction gives self-energy correction to the hole energy (4). The vertex (25) vanishes at the points $\vec{k} = (0, \pm\pi), (\pm\pi, 0)$, and it is maximal at $\vec{k} = (\pm\frac{\pi}{2}, \pm\frac{\pi}{2})$. Just due to this reason the bottom of the band is at $\vec{k} = (\pm\frac{\pi}{2}, \pm\frac{\pi}{2})$. Surely the long wave limit is not enough to calculate the energy correction. However for estimation one can cut the integral over q at $q \sim 1$. This procedure gives the value of correction which agrees with that obtained from numerical calculations (see Table in Ref.[11]). Much more important to our view is calculation of the magnon polarization operator and of the magnon dispersion relation. This question will be considered elsewhere.

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t-J Модель. Взаимодействие дырки с длинноволновыми магнонами

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