ИЯФ

ИНСТИТУТ ЯДЕРНОЙ ФИЗИКИ СО АН СССР

O.P. Sushkov

t-J MODEL. DISPERSION RELATION AND WAVE FUNCTION OF A HOLE ON THE NEEL BACKGROUND

PREPRINT 92-13

НОВОСИБИРСК

t-J Model. Dispersion Relation and Wave Function of a Hole on the Neel Background

O.P.Sushkov

Budker Institute of Nuclear Physics
630090, Novosibirsk 90, USSR

ABSTRACT

on the Neel background. The energy and the wave function is calculated analytically using variational method. Comparison with computer simulation justifies suggested approximation at least at $t/J \leq 4-5$. However it is possible that this approximation is valid for larger t as well.

It is widely agreed that two-dimensional t-J model describes the high-temperature superconducting Cu-O materials. The phase diagram for the compound $La_{2-x}Sr_xCuO_4$ is presented in the Ref. [1]. At x=0 it is insulator with long range antiferromagnetic ordering (Neel state). At $x \geq$ ≥ 0.03 $La_{2-x}Sr_xCuO_4$ becomes a metal without long range magnetic order. The structure at x=0 is well understood in frameworks of the t-J model. Actually, 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]. Structure of the metallic state which arises from the doping of the insulating state remains a puzzle. Still some of the properties of one hole are by now established. It has been shown analytically [5, 6, 7, 8, 9, 10, 11] and numerically [12, 13, 14, 15, 16, 17, 18, 19] 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 $cosk_x + cosk_y = 0$. In the papers [19] (numerical diagonalization on small lattice) and [18] (variational method with numerical diagonalization) melting of the Neel order at doping has been demonstrated.

In the Ref.[11] we considered the dynamics of a hole on the Neel background. The analytical variational solution for the hole dispersion relation and for the wave function was obtained. Only short range correlations were included into the wave function. In this approach the Neel state instability as well as relatively small correction to the hole energy is due to the residual interaction of a hole with long wave length magnons. To consider these effects one need the vertex function for the interaction of a hole with long wave length magnon. In the present work we calculate this vertex.

We consider the t-J model with less than half-filling. It is defined by the wave function of a hole are derived. Comparison with the results of numerical calculations is presented. In this approach the Neel state instability as well as relatively small correction to the hole energy is due to the residual interaction of a hole with long wave length magnons. This question will be considered elsewhere [25].

Let us consider the t-J model with less than half-filling. It is defined by the Hamiltonian (see e.g. [26])

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

where $d^+_{i\sigma}$ creates a hole of spin σ at site i of a two-dimensional square lattice, $n_{i\sigma} = d^+_{i\sigma} d_{i\sigma}$ is the number operator. 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. Sometimes it is convenient to write down the Hamiltonian of t-J model in more simple form, but with additional constraint.

$$H = H_t + H_J = t \sum_{<ij>\sigma} (d^+_{i\sigma} d_{j\sigma} + h.c) + J \sum_{<ij>} \vec{S}_i \vec{S}_j \ . \qquad (2)$$

The constraint is that $d_{i\sigma}$ acts in the Hilbert space where there is no double electron occupancy.

Due to the Eqs.(1),(2) the holes in an antiferromagnet cannot move freely, but couple strongly with spin excitations. The idea to write down trial wave function of a hole as a polynomial in d^+, d acting on the background state $|0>$ is quiet natural. The state $|0>$ corresponds to a half-filling. This representation was used for example in the Refs. [9, 20]. In the work [23] we have used similar anzats with the combinations $d^+_n d_n$ expressed in the terms of spin operator $\vec{S}$:

$$\begin{aligned} \psi_\uparrow(k) \ \sim \ & \sum_n e^{i\vec{k}\vec{r}_n} \Big\{ \alpha d^+_{n\uparrow} + \sum_{\vec{\delta}} \Big(\beta_{\vec{\delta}} d^+_{n\uparrow} S^z_{n+\vec{\delta}} + \gamma_{\vec{\delta}} d^+_{n\downarrow} S^+_{n+\vec{\delta}} \Big) + \\ + \ & \sum_{\vec{\delta}\vec{\delta}'} \Big(\mu_{\vec{\delta}\vec{\delta}'} d^+_{n\uparrow} S^z_{n+\vec{\delta}+\vec{\delta}'} + \nu_{\vec{\delta}\vec{\delta}'} d^+_{n\downarrow} S^+_{n+\vec{\delta}+\vec{\delta}'} + \qquad (3) \\ + \ & \xi_{\vec{\delta}\vec{\delta}'} d^+_{n\uparrow} S^z_{n+\vec{\delta}} S^z_{n+\vec{\delta}+\vec{\delta}'} + \zeta_{\vec{\delta}\vec{\delta}'} d^+_{n\uparrow} S^-_{n+\vec{\delta}} S^+_{n+\vec{\delta}+\vec{\delta}'} + \\ + \ & \theta_{\vec{\delta}\vec{\delta}'} d^+_{n\downarrow} S^z_{n+\vec{\delta}} S^+_{n+\vec{\delta}+\vec{\delta}'} \Big) \Big\} |0> . \end{aligned}$$

Here $\vec{\delta}, \vec{\delta}'$ are the unit vectors connecting the nearest-neighbour sites. The representation (3) can be used for both the Neel background and for the spin-liquid background. However it can be simplified for the Neel state. There

are two sublattices. Let $\lambda_n = 1$ for spin up sublattice and $\lambda_n = -1$ for spin down one. Obviously $S^z_n|0>= \frac{1}{2}\lambda_n|0> + quantum\ fluctuation\ correction.$ The fluctuation correction can be absorbed into the higher terms in (3). Thus all S^z_n in the Eq.(3) one can replace by the λ_n with corresponding renormalization of the coefficients. Carring out calculation in the Ref.[23] we have observed that the hole wave function is very close to rather simple one:

$$\begin{aligned} \psi_\uparrow(k) \ &= \ \Big\{ \nu(k)\hat{A}_0 + \sum_{\vec{\delta}} \xi_{\vec{\delta}}(k) \hat{A}_{\vec{\delta}} \Big\} |0>, \\ \hat{A}_0 \ &= \ \frac{1}{\sqrt{2N}} \sum_n (1-\lambda_n) d^+_{n\uparrow} e^{i\vec{k}\vec{r}_n}, \qquad (4) \\ \hat{A}_{\vec{\delta}} \ &= \ \frac{1}{\sqrt{2N}} \sum_n (1+\lambda_n) d^+_{n\downarrow} S^+_{n+\vec{\delta}} e^{i\vec{k}\vec{r}_n}. \end{aligned}$$

The $\hat{A}_0$ creates additional spin up hole only on the spin down sites. The $\hat{A}_{\vec{\delta}}$ creates additional spin down hole on the spin up sublattice and flips the spin at the neighbour site. The wave function (4) is quiet natural for $t \ll J$. However our numerical calculation [23] with rather wide anzats (3) shows that the hole wave function is close to the (4) at large t as well. This is valid at least at $t \leq (4-5) \times J$, where the calculation [23] is carried out.

In the present work we will calculate analytically the energy and the wave function of a hole basing on the anzats (4). In the further calculations we will set $J = 1$. There are five basis states in the trial function (4)

$$\begin{aligned} |1> \ &= \ \hat{A}_0|0>, \quad |2>= \hat{A}_x|0>, \quad |3>= \hat{A}_y|0>, \qquad (5) \\ |4> \ &= \ \hat{A}_{-x}|0>, \quad |5>= \hat{A}_{-y}|0> . \end{aligned}$$

They are not orthonormalized. Calculation of the normalization matrix is streightforward.

$$\begin{aligned} <1|1> \ &= \ (1/2+\sigma), \quad <1|i>=0, \quad i,j = 2,3,4,5 \ , \\ <i|j> \ &= \ (1/4+\sigma-p_1)\delta_{ij} + 2q_2(1/2+\sigma)(1-\delta_{ij}) \ . \qquad (6) \end{aligned}$$

Here $\sigma = |<0|S^z_n|0>|$. Parameters p_i, q_i are the following correlators

$$p =<0|S^z_n S^z_m|0>, \quad 2q =<0|S^+_n S^-_m|0>, \quad \rho = p + 2q =<0|\vec{S}_n \vec{S}_m|0> . \qquad (7)$$

p_1, q_1 and ρ_1 correspond to the neighbour sites n,m; p_2, q_2, ρ_2 correspond to the next neighbour sites; and p_3, q_3, ρ_3 correspond to the next next neighbour

In the spin-wave theory for the Heisenberg model (see Ref.[20] for a review) one magnon state is $c^+_q|0>$, where c^+_q is a magnon creation operator

$$c^+_q = \alpha_q b^+_q - \beta_q b_{-q}, \qquad b^+_q = \frac{1}{\sqrt{N}}\sum_n a^+_n e^{i\vec{q}\vec{r}_n}. \tag{10}$$

α_q and β_q are the parameters of Bogoliubov transformation. The frequency of a magnon and the transformation parameters are as follow

$$\begin{aligned} \omega_q &= 2\sqrt{1-(cosq_x+cosq_y)^2/4} \quad \rightarrow \quad \sqrt{2}q, \ at\ q \ll 1\,, \qquad (11)\\ \alpha_q &= \sqrt{\frac{1}{\omega_q}+\frac{1}{2}}, \quad \beta_q = -\frac{cosq_x+cosq_y}{|cosq_x+cosq_y|}\sqrt{\frac{1}{\omega_q}-\frac{1}{2}}\,. \end{aligned}$$

In a simple perturbation theory the hole-magnon vertex is the matrix element of the Hamiltonian (1): $<0|h_{k+q\downarrow}Hh^+_{k\uparrow}c^+_q|0>$. In the present case the situation is slightly more complicated because the states $h^+_{k+q\downarrow}|0>$ and $h^+_{k\uparrow}c^+_q|0>$ are not orthogonal. Actually, the wave function (6) corresponds to the hole dressed by the cloud of magnons. Short wave length magnons give the main contribution to the cloud. However there is a long wave length tail as well. This tail has no physical sense, but due to it the states we mention above are not orthogonal. It is obvious that one should subtract these unphysical components from the wave function (6). Therefore the hole-magnon vertex is equal to

$$\Gamma_0 = <0|h_{k+q\downarrow}Hh^+_{k\uparrow}c^+_q|0> - <0|h_{k+q\downarrow}h^+_{k\uparrow}c^+_q|0><0|c_q h_{k\uparrow}Hh^+_{k\uparrow}c^+_q|0>\,. \tag{12}$$

This is well known subtraction procedure which is usually used in many-body theory for nonorthogonal states. However we would like to stress once more that in our case it is justified only for $q \ll 1$.

First of all let us calculate the overlapping $<0|h_{k+q\downarrow}h^+_{k\uparrow}c^+_q|0>$. In calculation we will use the ground state factorization. For example

$$\begin{aligned} &<0|\lambda_n S^z_n S^+_{n+\vec\delta} c^+_q|0> \approx\\ &\approx <0|\lambda_n S^z_n|0><0|S^+_{n+\vec\delta}c^+_q|0> = \sigma <0|S^+_{n+\vec\delta}c^+_q|0>, \qquad (13)\\ &<0|\lambda_n S^z_n S^-_{n+\vec\delta} S^+_{n+\vec\delta+\vec\delta'}|0> \approx\\ &\approx <0|\lambda_n S^z_n|0><0|S^-_{n+\vec\delta}S^+_{n+\vec\delta+\vec\delta'}|0> = 2q_1\sigma\,. \end{aligned}$$

The estimations show that the factorization procedure hase a good accuracy for the correlators which we need. Using the Eq.(6) one can easily get

$$\begin{aligned} &<0|h_{k+q\downarrow}h^+_{k\uparrow}c^+_q|0> =\\ &= (1/2+\sigma)\Big\{X\sum_{\vec\delta} e^{i\vec{q}\vec{\delta}}\Big(\nu^*(k+q)\xi_{\vec\delta}(k)+\nu(k)\xi^*_{\vec\delta}(k+q)\Big) -\\ &-Y\sum_{\vec\delta} e^{i\vec{q}\vec{\delta}}\Big(\nu^*(k+q)\xi_{\vec\delta}(k)-\nu(k)\xi^*_{\vec\delta}(k+q)\Big)\Big\}\,, \end{aligned} \tag{14}$$

where

$$X = \frac{1}{N}<0|\sum_n e^{-i\vec{q}\vec{r}_n}S^+_n c^+_q|0>, \quad Y = \frac{1}{N}<0|\sum_n e^{-i\vec{q}\vec{r}_n}\lambda_n S^+_n c^+_q|0>\,. \tag{15}$$

Due to the Eqs. (9), (10), (11)

$$\begin{aligned} X &= \frac{1}{2\sqrt{N}}(\alpha_q+\beta_q) \approx \frac{1}{\sqrt{N}}\times\frac{1}{2^{7/4}}\times\sqrt{q}, \ at\ q \ll 1\,,\\ Y &= \frac{1}{2\sqrt{N}}(\alpha_q-\beta_q) \approx \frac{1}{\sqrt{N}}\times\frac{1}{2^{1/4}}\times\frac{1}{\sqrt{q}}, \ at\ q \ll 1\,. \end{aligned} \tag{16}$$

Thus we can set q=0 in the coefficient before X, and we should keep linear in q terms in the coefficient before Y. After this transformation the overlapping (14) is of the form

$$\begin{aligned} <0|h_{k+q\downarrow}h^+_{k\uparrow}c^+_q|0> &= \frac{t}{gS}\Big\{2X(1-u)(cosk_x+cosk_y)+\\ &+ Y(1+u+2v)(q_x sink_x+q_y sink_y)\Big\}\,. \end{aligned} \tag{17}$$

The bottom of the band (4) lies at the line $cosk_x+cosk_y=0$. To simplify the formulae we will consider the holes only near the band bottom. Therefore we set $cosk_x+cosk_y=0$, and

$$<0|h_{k+q\downarrow}h^+_{k\uparrow}c^+_q|0> = \frac{t}{gS}(1+u+2v)Z, \qquad Z = Y(q_x sink_x+q_y sink_y)\,. \tag{18}$$

Thus the overlapping is proportional to $\sim\sqrt{q}$.

Calculation of the $<0|c_q h_{k\uparrow}Hh^+_{k\uparrow}c^+_q|0>$ in long wave limit ($q \rightarrow 0$) is very simple.

$$<0|c_q h_{k\uparrow}Hh^+_{k\uparrow}c^+_q|0> = E(k)+E_0\,. \tag{19}$$

Using the Eqs. (6), (11) one can verify that after subtraction the off-diagonal matrix elements $<i|\tilde{H}_J|j>$ become very small and can be neglected. Non-vanishing matrix elements are

$$i = 2,3,4,5: \ <i|\tilde{H}_J|i> = <i|H_J|i> - \epsilon_0 <i|i> = \Delta <i|i>,$$

$$\Delta = \begin{cases} 1.5 & \text{for I-state} \\ 1.33 & \text{for N-state} \end{cases} . \qquad (19)$$

Calculation of the H_t matrix is even more simple. Non-vanishing matrix elements are as follow

$$<1|H_t|i> = -t\left\{(1/4+\sigma-p_1)e^{-i\vec{k}\vec{\delta}_i} + 2(q_1+q_2)(1/2+\sigma)\sum_{\vec{\delta}'\neq\vec{\delta}_i} e^{-i\vec{k}\vec{\delta}'}\right\}. \qquad (20)$$

Here $\vec{\delta}_i$ is the unit vector corresponding to the state $|i>$. For example for i=2 it is $\vec{\delta}_x$. Diagonalization of the Hamiltonian matrix $H = H_t + H_J$ (Eqs.(19),(20)) with normalization conditions (6) gives the hole energy

$$\epsilon(k) = \frac{\Delta}{2} - S(k), \qquad (21)$$

$$S(k) = \sqrt{\Delta^2/4 + 4t^2(1+y) - t^2(x+y)(cosk_x + cosk_y)^2}.$$

Here

$$x = 1 - \frac{(g + 6(q_1+q_2)/g)^2}{1+6q_2} \approx 0.557,$$

$$y = \frac{(g - 2(q_1+q_2)/g)^2}{1-2q_2} - 1 \approx 0.138, \qquad (22)$$

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

For the Ising state $x = y = 0$, $g = 1$. Expansion coefficients in the wave function (4) are as follow

$$\nu(k) = \frac{1}{2}\sqrt{\frac{\Delta+2S}{(1/2+\sigma)S}},$$

$$\xi_{\vec{\delta}}(k) = \frac{t}{\sqrt{(1/4+\sigma-p_1)S(\Delta+2S)}} \times \qquad (23)$$

$$\times \left((1+v)e^{i\vec{k}\vec{\delta}} - \frac{1}{2}(u+v)(cosk_x + cosk_y)\right),$$

where

$$u = 1 - \frac{g + 6(q_1+q_2)/g}{1+6q_2} \approx 0.416, \quad v = \frac{g - 2(q_1+q_2)/g}{1-2q_2} - 1 \approx 0.124. \quad (24)$$

The Brillouin zone for the wave function (4) is the square $cosk_x + cosk_y = 0$. Number of states is $N/2$ because one can create spin up hole only on the spin down sites. Due to Eq. (21) the hole energy is minimal at the edge of Brillouin zone. The values of minimal energy for different t are presented at the Table 1. At the same Table we present the results of numerical calculations [20, 23]. We see that present calculation at $1 \leq t \leq 4$ has the accuracy about 15−19%. Thus the correction is relatively small. It is due to the interaction of a hole with long wave length magnons because short wave length magnons are included into the trial function (4). The Neel state instability is due to the interaction with long wave length magnons as well. This question will be considered elsewhere [25].

Table 1. Minimal energy of a hole for different values of t

t	a	b	c	d
0.2	-0.125	-0.096		
0.5	-0.592	-0.580		
0.667	-0.905	-0.923		
1	-1.57	-1.69	-1.85	0.85
2	-3.65	-4.32	-4.40	0.83
3	-5.77	-7.06	-7.02	0.82
4	-7.89	-9.94	-9.70	0.81

a) Analytical calculation of the present work.
b) Numerical calculation [20]. Results of the Ref.[20] are recalculated to J=1 and zero energy level excepted in the present work.
c) Numerical calculation [23].
d) The ratio of analytical result to numerical one of Ref.[23].

Acknowledgments. I am grateful for the helpful discussions to V.I.Belinicher V.F.Dmitriev, V.V.Flambaum, P.N.Isaev, I.V.Kolokolov, V.V.Sokolov and V.B.Telitsin.

REFERENCES

[1] M.A.Kaster et al., in High-T_c Superconductors, eds. by A.Biancony and A.Marcelli (Pergamon Press, Oxford, 1989) p. 126.

[2] J.Oitmaa and D.D.Betts, Can. J. Phys. 56, 897 (1971)

[3] J.E.Hirch, Phys. Rev. B 31, 4403 (1985).

[4] D.A.Huse, Phys. Rev. B 37, 2380 (1988).

[5] B.Shraiman and E.Siggia, Phys. Rev. Lett. 61, 467 (1988).

[6] S.Schmitt-Rink, C.M.Varma, and A.E.Ruchenstein, Phys. Rev. Lett. 60, 2793 (1988).

[7] C.L.Kane, P.A.Lee, and N.Read, Phys. Rev. B 39, 6880 (1989)

[8] S.Sachdev, Phys. Rev. B 39, 1232 (1989)

[9] C.Gross and M.D.Johnson, Phys. Rev. B 40, 9423 (1989)

[10] J.H.Xu, C.S.Ting, and T.K.Lee, Phys. Rev. B 43, 8733 (1990)

[11] O.P.Sushkov, Preprint INP 92-13, Novosibirsk 1992.

[12] S.A.Trugman, Phys. Rev. B 37, 1597 (1988)

[13] S.A.Trugman, Phys. Rev. B 41, 9049 (1990)

[14] E.Kaxiras and E.Manousakis, Phys. Rev. B 38, 866 (1988)

[15] J.Bonca, P.Prelovsek and I.Sega, Phys. Rev. B 39, 7074 (1989)

[16] E.Dagotto, A.Moreo and T.Barnes, Phys. Rev. B 40, 6721 (1989)

[17] E.Dagotto, R.Joynt, S.Bacci and E.Cagliano, Phys. Rev. B 41, 9049 (1990)

[18] O.P.Sushkov, Preprint INP 91-101, Novosibirsk 1991; Phys. Lett. A, to be published.

[19] E.Dagotto, A.Moreo, F.Ortolani, D.Poilblanc, J.Riera and D.Scalapino, Preprint NSF-ITP-91-54, Santa Barbara, 1991.

[20] C.Kittel, Quantum Theory of Solids (Wiley, New York, 1963).

[21] E.Dagotto, International Journal of Modern Physics B 5, 907 (1991).

[22] A.Aharony et al, Phys. Rev. Lett. 60, 1330 (1988).

[23] O.P.Sushkov, Preprint INP 91-101, Novosibirsk 1991; Phys. Lett. A, to be published.

[24] V.V.Flambaum and O.P.Sushkov, Physica C, to be published.

[25] O.P.Sushkov, Preprint INP 92-14, Novosibirsk 1992.

[26] C.Gross, R.Joynt and T.M.Rice, Phys. Rev. B 36, 381 (1987).