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ON THE GROUND STATE STRUCTURE OF TWO-DIMENSIONAL HUBBARD MODEL ON SQUARE LATTICE. QUANTUM MELTING OF THE NEEL ORDERING

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НОВОСИБИРСК

On the Ground State Structure of Two-Dimensional Hubbard Model on Square Lattice. Quantum Melting of the Neel Ordering

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ABSTRACT

Two dimensional t-J model equivalent at t » J to the Hubbard model is considered by the variational method. We suggest the compact anzats for the mobile hole wave function. The dispersion of this hole on the Neel and RVB background is calculated. It is shown that the doping induce transition from the Neel state to the spin-liquid RVB state. At 1≤t/J≤4 the transition point is at hole concentration x ~ 0.1.

The investigation of strongly correlated two dimensional Hubbard model is of interest in connection with the problem of high temperature superconductivity. In the Ref.[1] Anderson has suggested to use the Hubbard model as well as the picture of resonating-valence-bond (RVB) spin-liquid for the description of this phenomena. It is well known that at half-filling and at strong repulsion the Hubbard model is equivalent to the Heisenberg model (see e.g. Refs.[2,3]). There is Neel ordering in the ground state of two dimensional Heisenberg model[4,5,6]. This picture is in accordance with the experimental data. Magnetic phase diagram for the compound $La_{2-x}Sr_xCuO_4$ is presented in the Ref[7]. The value x=0 corresponds to half-filling and actually there is the Neel order at x=0. However at doping by the holes the order disappears at $x \sim 2\text{-}4\ 10^{-2}$. The peculiarity of two dimensional Heisenberg model on square lattice is the closeness of the RVB spin liquid state to the ground Neel state. The difference in energy is about 2-3% [4-6,8-11]. It is evident that the melting of long range Neel ordering at doping is due to this small difference. Nevertheless the problem is still unresolved. One should calculate the hole energy at doping away from half-filling.

Just this calculation is the subject of the present work. To study the dynamics of holes in doped antiferromagnet (AF) numerous approximations have been proposed [12-21] Calculations based on the moment method of Brinkman and Rice [12] are carried out in the limit $U/t\to\infty$ [13-15]. Calculation of Trugman[16] is an exact diagonalization of Hamiltonian within a retained portion of the Hilbert space. Approach of Dagotto et. al. [17] is an exact diagonalization on small lattices. We use variational method which is somewhat similar to the approach of Ref.[16], but our calculations are not restricted by the Neel background. The trial wave function (WF) is generated by the powers of hopping Hamiltonian. This way of WF generation is analogous to that used in Ref.[17] for the perturbation theory in large J/t limit.

In the large U-limit, the Hubbard model can be transformed into t-J model with Hamiltonian[3]

$$H = H_t + H_J = t\sum_{<ij>\sigma}\left(\hat{n}_{i-\sigma}a^{+}_{i\sigma}a_{j\sigma}\hat{n}_{j-\sigma} + H.c.\right) + J\sum_{<ij>}\vec{S_i}\vec{S_j} \qquad (1)$$

where $\hat{n}_{i\sigma} = a^{+}_{i\sigma}a_{i\sigma}$. The $a^{+}_{i\sigma}$ is the hole creation operator. The other notations are standard. We will set below J=1. Appearance of factors $\hat{n}_{-\sigma}$ in H_t is obvious. They forbid the hopping at half-filling. It is useful to rewrite H_t in the following form [21]

$$H_t = t\sum_{<ij>}\left(a^{+}_{i\uparrow}S^{-}_{i}S^{+}_{j}a_{j\uparrow} + a^{+}_{i\downarrow}S^{+}_{i}S^{-}_{j}a_{j\downarrow} + H.c.\right) \qquad (2)$$

where $S^{+}_{i} = a^{+}_{i\uparrow}a_{i\downarrow}$, $S^{-}_{i} = a^{+}_{i\downarrow}a_{i\uparrow}$, $S^{z}_{i} = \frac{1}{2}(a^{+}_{i\uparrow}a_{i\uparrow} - a^{+}_{i\downarrow}a_{i\downarrow})$. Due to Eqs.(1),(2) the holes in an AF background cannot move freely but couple strongly with spin excitations.

Let us forget that (1) is originated from the Hubbard

model. Then we can consider it for any t. At $t \ll 1$ it is quite natural to suppose the WF of the hole above half-filling be of the form

$$\psi_{k\uparrow} = \sum_{n} e^{i\vec{k}\vec{r}_n} a^{+}_{n\uparrow}|0> \qquad (3)$$

Here $|0>$ is the WF of Neel AF background with the half-filling. In further calculation we wish to consider the dependence of background spin-state on the doping. Therefore below we do not fix the spin structure of $|0>$. It can be Neel or RVB state. Real ground state corresponds to minimum of the total energy. It should be noted that for any $|0>$ the condition $H_t|0>=0$ is fulfilled.

Due to the spin quantum fluctuations there is admixture of other components to the WF (3) even for t=0. Nevertheless (3) is good zero approximation. Treating H_t as perturbation one can find the hole dispersion.

$$\varepsilon_k = <\psi_{k\uparrow}|H_t|\psi_{k\uparrow}> = \frac{t}{2}(1+4\rho_1)(\cos k_x + \cos k_y), \qquad (4)$$

where $\rho_1 = <0|\vec{S}_i\vec{S}_j|0> \approx -0.33$ is the neighbor spin correlator. In agreement with Ref.[17] further calculation shows that simple formula (4) is valid only for very small t: $t \le 0.05$. Here it has accuracy about 30%. We remind that it is not regular perturbation theory. Even at t=0 WF (3) is not exact due to the spin quantum fluctuations. It is evident that (4) is violated at so small t due to the smallness of coefficient $\frac{1}{2}(1+4\rho_1)\approx -0.16$

Acting on the WF (3) by H_t one can find the components of ψ which are generated by one step hopping. After the simple commutations we get

$$H_t|1\rangle = t\Big[(\cos k_x + \cos k_y)|1\rangle - e^{-ikx}(|2\rangle+|6\rangle) - e^{ikx}(|3\rangle+|7\rangle) - e^{-iky}(|4\rangle+|8\rangle) - e^{iky}(|5\rangle+|9\rangle)\Big] \qquad (5)$$

where

$$|i\rangle = \sum_n e^{i\vec{k}\vec{r}_n} A_n^{(i)}|0\rangle$$

$$A_n^{(1)} = a^+_{n\uparrow} \qquad (6)$$

$$A_n^{(2)} = a^+_{n\uparrow} S^z_{n-x}, \quad A_n^{(3)} = a^+_{n\uparrow} S^z_{n+x}, \quad A_n^{(4)} = a^+_{n\uparrow} S^z_{n-y}, \quad A_n^{(5)} = a^+_{n\uparrow} S^z_{n+y}$$

$$A_n^{(6)} = a^+_{n\downarrow} S^+_{n-x}, \quad A_n^{(7)} = a^+_{n\downarrow} S^+_{n+x}, \quad A_n^{(8)} = a^+_{n\downarrow} S^+_{n-y}, \quad A_n^{(9)} = a^+_{n\downarrow} S^+_{n+y}$$

The notations $\pm x$, $\pm y$ correspond to one step on square lattice. The states $|1\rangle - |5\rangle$ are linearly independent only due to the spin quantum fluctuations in the background state $|0\rangle$. Without quantum fluctuations ($S^z_n = \pm 1/2$) $|i\rangle \sim |1\rangle$ for $2 \le i \le 5$. Now the set (6) defines variational Hilbert space of the dimension N=9 and we can calculate the energy by variational method. The only complication is that the set (6) is not ortonormalized. For the background we suppose

$$\langle\langle 0|\vec{S}_n|0\rangle\rangle = 0 \qquad (7)$$

Double brackets mean averaging both over quantum state and over the lattice sites n. Then the calculation of normalization matrix is straightforward. By commutations the matrix elements can be reduced to the combinations of background spin correlators.

$$\langle i|k\rangle = \begin{pmatrix}
\frac{1}{2} & -p_1 & -p_1 & -p_1 & -p_1 & -2q_1 & -2q_1 & -2q_1 & -2q_1 \\
 & \frac{1}{8} & \frac{1}{2}p_2 & \frac{1}{2}p_2 & \frac{1}{2}p_2 & -q_1 & 0 & 0 & 0 \\
 & & \frac{1}{8} & \frac{1}{2}p_2 & \frac{1}{2}p_2 & 0 & -q_1 & 0 & 0 \\
 & & & \frac{1}{8} & \frac{1}{2}p_2 & 0 & 0 & -q_1 & 0 \\
 & & & & \frac{1}{8} & 0 & 0 & 0 & -q_1 \\
 & & & & & \frac{1}{4} & -p_1 & q_2 & q_2 & q_2 \\
 & & & & & & \frac{1}{4} & -p_1 & q_2 & q_2 \\
 & & & & & & & \frac{1}{4} & -p_1 & q_2 \\
 & & & & & & & & \frac{1}{4} & -p_1
\end{pmatrix} \qquad (8)$$

Only the upper right part of the symmetric matrix is presented. Parameters p_i, q_i are the following correlators.

$$p = \langle 0|S^z_i S^z_j|0\rangle, \quad 2q = \langle 0|S^+_i S^-_j|0\rangle, \quad \rho = p + 2q = \langle 0|\vec{S}_i\vec{S}_j|0\rangle \qquad (9)$$

p_1, q_1, and ρ_1 correspond to neighbor sites i, j; p_2, q_2, and ρ_2 correspond to next neighbor sites; and p_3, q_3, and ρ_3 correspond to next next neighbor sites. We suppose that the next and next next neighbor correlators are independent on the path between points i and j. It had been proofed that the hole energy is not sensitive to this supposition.

Instead of Heisenberg Hamiltonian H_J let us introduce $\tilde{H}_J$ with subtracted background energy:

$$\langle i|H_J|k\rangle \to \langle i|\tilde{H}_J|k\rangle = \langle i|H_J|k\rangle - (\langle 0|H_J|0\rangle - 4\rho_1)\langle i|k\rangle \qquad (10)$$

The calculation of $\langle i|\tilde{H}_J|k\rangle$ and $\langle i|H_t|k\rangle$ is similar to the calculation of normalization matrix. Similar to Eq.(7) we suppose vanishing of the three and five-fold correlators.

$$\langle\langle 0|\vec{S}_n\vec{S}_{n+i}\vec{S}_{n+i+j}|0\rangle\rangle = 0 \qquad (11)$$

It means that $|0\rangle$ is T and P-even. For the four and six-fold correlators the ground state factorization is supposed. For example

$$\langle 0|S^+_{n-y}S^-_nS^z_{n-x}S^z_{n-2x}|0\rangle\approx\langle 0|S^+_{n-y}S^-_n|0\rangle\langle 0|S^z_{n-x}S^z_{n-2x}|0\rangle=2q_1p_1 \qquad (12)$$

Similar procedure had been used in Refs.[13-15]. This is rather crude estimation, but the hole energy is not very sensitive to these high correlators. Thus the calculation of $\langle i|\tilde{H}_J|k\rangle$ and $\langle i|H_t|k\rangle$ is straightforward, but the final matrices are rather cumbersome. Therefore we present here only a few typical matrix elements as an example (H_t in the units t).

$$\langle 1|\tilde{H}_J|2\rangle = -3/4p_2+3p_1\rho_1 \qquad \langle 1|\tilde{H}_J|6\rangle = -3/2q_2+6q_1\rho_1$$

$$\langle 2|\tilde{H}_J|2\rangle = -3/4q_1 \qquad \langle 2|\tilde{H}_J|6\rangle = 3/4q_2+3q_1\rho_1$$

$$\langle 1|H_t|2\rangle=-p_1(\cos k_x+\cos k_y)+(q_1-1/8)e^{+ikx}-$$

$$-p_2(\cos k_y+1/2e^{-ikx}) \qquad (13)$$

$$\langle 1|H_t|6\rangle=-2q_1(\cos k_x+\cos k_y)+(q_1+p_1-i/4)e^{+ikx}-$$

$$-q_2(2\cos k_y+e^{-ikx})$$

$$\langle 2|H_t|2\rangle=1/2p_1(\cos k_x+\cos k_y)+1/2p_2\cos k_x+2p_1\rho_1\cos k_y$$

$$\langle 2|H_t|6\rangle=1/2(q_1-q_2)e^{-ikx}+1/2(p_1-p_2)e^{ikx}+4(p_1q_1+p_2q_2)\cos k_y$$

The further calculation is direct diagonalization of the Hamiltonian matrix $\langle i|H_t+\tilde{H}_J|k\rangle$ with the normalization condition (8). The only input is the background spin correlators. We consider the three types of background. The first is AF state without quantum fluctuations ($S^z_n=\pm 1/2$). It is the ground state of the Ising model and we denote it as Ising state: $|0\rangle=|I\rangle$. The second is real Neel state $|N\rangle$, and the third is RVB spin liquid state $|SL\rangle$. Spin correlators for the Ising state are trivial. For the SL we use the result of the numerical simulations [8-11,22]. For the Neel state following to the standard approach (see e.g. Ref.[6]) we split H_J into the two parts: $\vec{S}_i\vec{S}_j=S^z_iS^z_j+\alpha S^\perp_iS^\perp_j$, $\alpha=1$; and treat the α term perturbatevely in the leading order in α for each correlator. Thus we get

$$\text{I:} \qquad p_1=p_3=-p_2=-\tfrac{1}{4}, \quad q_i=0$$

$$\text{N:} \qquad \alpha=1, \quad p_1=-\tfrac{1}{4}(1-\tfrac{1}{3}\alpha^2), \quad q_1=-\alpha/12;$$

$$s_z=\tfrac{1}{2}(1-\tfrac{2}{9}\alpha^2), \quad p_2=-p_3=s_z^2, \quad q_2=q_3=0. \qquad (14)$$

$$\text{SL:} \qquad p_1=q_1=-0.1056, \quad p_2=q_2=0.0469, \quad p_3=q_3=-0.0296.$$

The eigenvalues of the normalization matrix (8) are as follow

I: 1 0.5 0.5 0.5 0.5 0 0 0 0

N: 0.96 0.43 0.43 0.43 0.30 0.032 0.032 0.032 0.010 (15)

SL: 0.98 0.35 0.35 0.35 0.18 0.057 0.057 0.057 0.027

In accordance with the remark below Eq.(6) the rank of normalization matrix for Ising state is equal to 5. For N- and for SL-state the rank is equal to 9. Nevertheless there

are very small eigenvalues, especially for the Neel state. Moreover by a small variation of parameters in (14) the smallest eigenvalue can be made negative. Surely the norma is positive and appearance of a ghost state is due to the approximate calculation of correlators. Anywhere, very small eigenvalues of the normalization matrix indicate that the Hilbert space is almost degenerate. To do the calculation reliable and stable with respect to small variations of parameters in Eqs.(14) the combinations of the basis states (6) corresponding to these small eigenvalues should be excluded from the trial wave function. Practically we do the calculation in the following way. First of all we diagonalize the normalization matrix (8). Then we take M eigenstates corresponding to the largest eigenvalues and cut the rest of a Hilbert space. Selected in such a way M states define a new variational Hilbert space. For M=9, i.e. without any cutoff, the calculation is unstable just due to the degeneracy of the Hilbert space. For $5 \le M \le 8$ results of the hole dispersion calculation are practically independent of M. (Surely for the Ising state only M=5 is possible.) They are presented in the table 1. In accordance with the Refs.[16,17] the band minimum is located at the point $\vec{k}_0=(\lambda,\lambda)$ $\lambda \approx \pi/2$, and hole dispersion near the bottom is of the form.

$$\varepsilon(\vec{k})=\varepsilon_0+\frac{1}{2}(\beta_{\parallel}\delta k_{\parallel}^2+\beta_{\perp}\delta k_{\perp}^2) \qquad (16)$$

Directions are parallel and orthogonal with respect to $\vec{k}_0$. The values of ε_0, $\beta_{\parallel}$, and quasiparticle pole residue Z (the weight of the state $|1\rangle$ in total wave function) are listed at the table 1. The value of $\beta_{\perp}$ is zero for Ising state. For Neel and spin liquid state $\beta_{\perp} \approx 0.1$ at $1 \le t \le 4$.

From the table 1 one see that for N- and SL-state $\varepsilon_0>0$ at t=0. Surely ε_0 can not be positive. The wrong value is

due to the inaccuracy of Heisenberg energy calculation using factorization estimation (12) for high correlators. However this error is relatively small (it should be compared with the total Heisenberg energy of the cluster corresponding to trial WF (6): $E_H=12\rho_1 \approx -4$). Moreover this error is completely negligible in the difference in energy between N- and SL-state which is crucial for the problem of Neel ordering melting,

According to the table 1 there is no dispersion for the Ising state. This result is obvious. Actually anzats (6) includes only the hole hopping to closest neighbor, but this mean the hole localization for the Ising state. The energy corresponding to this case can be easily derived analytically

$$\varepsilon_0 = 3/4 - \sqrt{9/16+4t^2} \qquad (17)$$

Thus with the trial function (6) practically there is no difference in the hole energy between N- and SL-state. We should go further and extend variational Hilbert space by considering the two step hopping. To do it similar to Eq.(5) one should act by H_t onto states $|i\rangle$ defined by the Eq.(6). In this way the new types of operators appear in addition to $A^{(1-9)}$. These are the sixteen next neighbor spin operators (for example $a^+_{n\uparrow} S^z_{n+x+y}$, $a^+_{n\downarrow} S^+_{n-2x}$ ...) and 48 double spin operators (for example $a^+_{n\uparrow} S^z_{n+x} S^z_{n+x+y}$, $a^+_{n\uparrow} S^-_{n+x} S^+_{n+x+y}$, $a^+_{n\downarrow} S^+_{n+x} S^z_{n+x+y}$, $a^+_{n\downarrow} S^z_{n+x} S^+_{n+x+y}$ ...). The dimension of Hilbert space is N=73. The further calculation is similar to the previous one for N=9. The only difference is that for N=73 algebraic work on the calculation of normalization matrix and especially of the Hamiltonian matrix is very large. Therefore the special algebraic code was created to calculate all commutations and spin pairings.

The results of numerical diagonalization of Hamiltonian

matrix for Hilbert space cutoff parameter M=17,52 are presented at the table 2. We remind the reader that the cutoff excludes the combinations of the basis states corresponding to very small positive and negative eigenvalues of normalization matrix. (Negative eigenvalues are due to the approximate calculation of high spin correlators.) For the Ising state the rank of normalization matrix is equal to 17. Therefore only M=17 is possible. We would like to point out on the sizable gain in energy for the I-state at t=0 in comparison with N=9 case. This is due to the double spin-flip components of WF. The I-state is not eigenstate of Heisenberg Hamiltonian and these components correct the WF of background without any hopping. The second new point for the I-state is appearance of longitudinal dispersion ($\beta_{\|}\neq 0$), which also is due to the double spin-flip components of WF. The minimum of the band is located exactly at $\vec{k}_0=(\pi/2,\pi/2)$, and still there is no transversal dispersion: $\beta_{\perp}=0$.

For the Neel and SL-state calculation becomes unstable at M>52. However at 40<M≤52 results are practically independent of M. The minimum of the band is at $\vec{k}_0=(\lambda,\lambda)$ $\lambda\approx\pi/2$. The transversal inverse mass $\beta_{\perp}\sim$ 0.1 We think that our calculation is valid at t≤3 - 4. At higher t the overlapping between wave functions obtained at N=9 and N=73 becomes small and it means that the variational Hilbert space should be extended. All our results for N-state are very close to that obtained in Refs[16,17].

From the table 2 one see that at 1≤t≤4 and M=17 the band bottom for the Neel state is lower than that for the spin liquid state. However at M=52 situation is opposite. One can easily understand it qualitatively. At M=17 the part of the Hilbert space which is due to the background spin quantum fluctuations is cut out. In this situation the double spin-flip components of WF like $a^{+}_{n\uparrow}\,S^{-}_{n+x}\,S^{+}_{n+x+y}$ are more effective for Neel state and even for the Ising state.

At M=52 all sizable effects of background quantum fluctuations are included into the variational Hilbert space. For the spin liquid the fluctuations are larger and therefore the variational volume of Hilbert space is larger (cf. the eigenvalues of normalization matrix (15) for N- and SL-state at N=9). Just this give a gain in hole energy for the spin liquid. According to the table 2 the gain in hole energy for spin liquid state with respect to Neel state at 1≤t≤4 is roughly independent of t, and it is not very large: $\Delta\varepsilon_0\approx 0.3\text{-}0.4$. However if we take it seriously as well as difference in background energy [4-6,8-11] $\rho_1^{SL}-\rho_1^{N}\approx 0.016$, we can estimate the critical concentration of holes at Neel ordering melting point

$$x=\frac{1}{2}\Delta\varepsilon_0/(\rho_1^{SL}-\rho_1^{N})\approx 0.1 \qquad (18)$$

Our results for Neel background are very close to that obtained earlier in Refs.[16,17]. However our conclusion concerning the Neel ordering melting is in disagreement with the works [13-15] based on moment method of Brinkman and Rice in the limit $t/J\to\infty$. The relation of those works with the present approach is at present not clear.

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Table 1

t	state	ε_0	$\beta_\parallel$	Z
0	I	0	0	1
	N	0.33	0	0.87
	SL	0.46	0	0.87
1	I	-1.39	0	0.68
	N	-1.31	0.8	0.60
	SL	-1.27	0.9	0.60
2	I	-3.32	0	0.59
	N	-3.44	1.6	0.54
	SL	-3.36	1.8	0.55
3	I	-5.30	0	0.56
	N	-5.59	2.5	0.52
	SL	-5.46	2.8	0.54
4	I	-7.29	0	0.55
	N	-7.75	3.3	0.51
	SL	-7.58	3.7	0.53

Parameters of quasihole dispersion calculated for Ising, Neel, and spin liquid states at the dimension of variational Hilbert space N=9, and cutoff $5 \le M \le 8$. The ε_0 is minimal energy of the band, $\beta_\parallel$ is inverse longitudinal mass, and Z is the quasiparticle pole residue.

Table 2

		m=17			m=52		
t	state	ε_0	$\beta_\parallel$	Z	ε_0	$\beta_\parallel$	Z
0	I	-0.89	0	0.79	–	–	–
	N	0.36	0	0.97	0.05	0	0.51
	SL	0.12	0	0.90	0.04	0	0.94
1	I	-2.22	0.54	0.56	–	–	–
	N	-1.33	0.75	0.60	-1.85	0.67	0.40
	SL	-1.35	0.68	0.63	-2.14	0.97	0.42
2	I	-4.59	0.81	0.43	–	–	–
	N	-3.76	1.40	0.49	-4.40	1.21	0.38
	SL	-3.49	1.25	0.56	-4.72	1.83	0.39
3	I	-7.14	0.91	0.38	–	–	–
	N	-6.25	2.01	0.45	-7.02	1.67	0.37
	SL	-5.70	1.43	0.53	-7.36	2.59	0.37
4	I	-9.73	0.96	0.36	–	–	–
	N	-8.77	2.60	0.43	-9.70	2.09	0.37
	SL	-7.94	1.80	0.51	-10.05	3.29	0.36

Parameters of quasihole dispersion calculated for Ising, Neel, and spin liquid states at the dimension of variational Hilbert space N=73, and cutoff M=17,52. The ε_0 is minimal energy of band, $\beta_\parallel$ is inverse longitudinal mass, and Z is the c a rticle pole residue.

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