Quantum melting of the long-range antiferromagnetic order and spin-wave condensation in $t - J - V$ model

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(June 26, 1994)

Abstract

We consider two-dimensional $t - J - V$ model. The wave function of the ground state is constructed. We demonstrate that the doping by holes results in condensation of the spin-waves, destruction of the long-range antiferromagnetic order and formation of the gap in the spin-wave spectrum.

PACS numbers: 71.27.+a, 74.20.Hi, 75.50.Ee

It is well known that the long-range antiferromagnetic (AF) order in Cooper Oxide superconductors is destroyed under the doping by the holes. In the frameworks of two-dimensional $t - J$ model the origin of this instability was realized. (see e.g. Refs. [1–6]). The instability is due to the strong interaction of spin-waves with mobile holes. However a structure of the ground state as well as a spectrum of excitations was not understood. In the present work we discuss the ways to stabilize the hole-hole pairing, construct the ground state wave function as a condensate of spin-waves and discuss the spectrum of bosonic excitations.

At half-filling (one hole per site) the $t$-$J$ model is equivalent to the Heisenberg AF model which has long-range AF order in the ground state. We consider the doped system starting from this ground state which we denote by $|0\rangle$. In spite of the destruction of the long-range AF order it is convenient to use $|0\rangle$ and corresponding quasiparticle excitations as a basis set in the problem with doping.

The effective Hamiltonian for $t - J$ model was derived in works [7–9]

$$H_{\text{eff}} = \sum_{k\sigma} \epsilon_k h_{k\sigma}^\dagger h_{k\sigma} + \sum_{q} \omega_q (\alpha_q^\dagger \alpha_q + \beta_q^\dagger \beta_q) + H_{h,sw} + H_{hh}.$$  

It is expressed in terms of usual spin-waves on AF background $\alpha_q, \beta_q$ (see e.g. Ref. [10]), and composite hole operators $h_{k\sigma}$ ($\sigma = \pm 1/2$). The summations over $k$ and $q$ are restricted.
inside the Brillouin zone of one sublattice where \( \gamma_q = \frac{1}{2} (\cos q_x + \cos q_y) \geq 0 \). The spin-wave dispersion is \( \omega_q = 2 \sqrt{1 - \gamma^2_q} \approx \sqrt{2} |q| \), at \( q \ll 1 \). Let us recall that the parameters of \( t - J \) model are \( t \) and \( J \). We set hereafter \( J = 1 \), so all energies are measured in units of \( J \). Single hole dispersion has minima at the face of magnetic Brillouin zone \( k_0 = (\pm \pi/2, \pm \pi/2) \). Near these points the dispersion can be presented in a usual quadratic form \( \epsilon_p \approx \frac{1}{2} \gamma_1 p_1^2 + \frac{1}{2} \gamma_2 p_2^2 \) \( (\beta_2 \ll \beta_1) \), where \( p = k - k_0 \), and \( p_2 \) is projection along the face of Brillouin zone, \( p_1 \) is orthogonal projection of the momentum. For \( 5 \geq t \geq 1 \) \( \beta_1 \approx 0.65 t \) (see e.g. Refs. [11,13]). Following Refs. [11,13] we will set \( a = \beta_1/\beta_2 \approx 5 - 7 \). For the small concentrations \( \delta \ll 1 \) under consideration, holes are localized in momentum space in the vicinity of the minima of the band and the Fermi surface consists of ellipses. The Fermi energy and Fermi momentum of non-interacting holes are: \( \epsilon_F = \frac{1}{2} \pi (\beta_1/\beta_2)^{1/2} \delta, \ p_F \sim (\pi \delta)^{1/2} \). The Fermi momentum \( p_F \) is measured from the center of the corresponding ellipse. Let us stress that the numerical value of \( \epsilon_F \) is very small. For realistic superconductors \( t/J \approx 3 \) (see, e.g., Refs. [14,15]). Therefore at \( \delta = 0.1 \) and \( J = 0.15 \text{ eV} \) one gets \( \epsilon_F \approx 15 \text{ meV} \approx 175 \text{ K} \).

The effective interaction of a composite hole with a spin-wave is of the form (see, e.g. Refs. [1,7])

\[
H_{h,sw} = \sum_{k,q} g(k, q) \left( h_{k+q \uparrow}^\dagger h_{k \uparrow} \alpha_q + h_{k+q \downarrow}^\dagger h_{k \downarrow} \beta_q + H.c. \right). \tag{2}
\]

For \( k \approx k_0 \) and \( q \ll 1 \) the vertex is \( g(k, q) \approx 2^{3/4} f q_1/\sqrt{q} \). The component \( q_1 \) is perpendicular to the face of Brillouin zone. The coupling constant \( f \) was calculated in the Ref. [7]. For \( t = 3 \) it is equal \( f \approx 1.8 \), for large \( t \) the coupling constant \( f \) approaches to 2.

The interaction between the two holes can be caused by the exchange of single spin-wave. Alongside with that there is a contact hole-hole interaction which is denoted in [1] by \( H_{hh} \). It is of the form

\[
H_{hh} \approx 8 \sum_{1,2,3,4} \left[ A \gamma_{k_1 - k_2} + \frac{C}{2} (\gamma_{k_1 + k_3} + \gamma_{k_2 + k_4}) \right] h_{3\downarrow}^\dagger h_{4\downarrow}^\dagger h_{2\uparrow} h_{1\uparrow} \delta_{12,34}. \tag{3}
\]

An expressions for the coefficients \( A \) and \( C \) as a functions of \( t \) are presented in the works [8,9].

It was demonstrated in the works [10,17] that the spin-wave exchange results in very strong pairing between the holes. The pairing is strongest in d- and g-waves where the superconducting gap \( \Delta \) is of the order of Fermi energy \( \epsilon_F \). The approach works [10,17] is based on the observation that at the typical momentum \( q \approx p_F \) the spin-wave frequency is much larger then Fermi energy: \( \omega_q \approx p_F \sim (\pi \delta)^{1/2} \Rightarrow \epsilon_F \approx \frac{1}{2} (\beta_1/\beta_2)^{1/2} \delta \). This is why we
can calculate pairing using unrenormalized spin-waves. Now we are going to discuss what happens with spin-waves at \( q < p_F \). Let us consider renormalized spin-wave Green function.

\[
G(\omega, q) = \frac{1}{\omega^2 - \omega_q^2 + P(\omega, q)}. \tag{4}
\]

For stability of the system the condition

\[
\omega_q^2 > P(0, q) \tag{5}
\]

should be fulfilled. Otherwise the Green function (4) would possess a pole with imaginary \( \omega \). The diagrams for polarization operator are presented in Fig.1. Chaining is due to the contact interaction (3). In \( t - J \) model the constant \( C \) in contact interaction is small at any \( t \), and the constant \( A \) vanishes exactly near the point which we are interested in: \( t \approx 3 \). Therefore the contact interaction is small and polarization operator is given by first diagram only. If we assume the holes be a normal Fermi liquid the calculation \( P(\omega, q) \) is very simple. For \( q \ll p_F \) one gets

\[
P(0, q) \approx \frac{4f^2}{\pi \sqrt{\beta_1 \beta_2}} q^2. \tag{6}
\]

After the substitution of the values of \( f \) and \( \beta_1, \beta_2 \) presented above, we see that condition (5) is violated, and \( P \) is about 2.5 times larger than \( \omega_q^2 \). This indicates the instability of normal Fermi liquid ground state [1–6]. What happens if we take into account the hole-hole pairing? In this case there is no simple analytical expression for the polarization operator. Our numerical computations show that pairing practically does not influence \( P(0, q) \). With pairing calculated in the works [16,17] \( P(0, q) \) is only by 8% smaller than the value given by (5). Let us note that it is quite strong pairing: the maximal value of superconducting gap on the Fermi surface is \( \Delta \sim 0.7\epsilon_F \), and this gives reasonable values of critical temperature. Even if we enhance pairing by hands up to the value \( \Delta \sim 1.3\epsilon_F \), \( P(0, q) \) is only by 14% smaller then the value given by (6). Thus even with pairing we have instability of ground state. Let us stress that this conclusion is practically independent of the mechanism of pairing.

One can believe that nonlinear interaction of spin-waves which is not included into effective Hamiltonian (1) could stabilize the system. However the maximal magnitude of imaginary \( \omega \) is at \( q \sim p_F \). Here the spin-wave residue of unstable mode in Green function (5) is very small. It means that actually the system is unstable with respect to spin-sound in hole Fermi liquid. The picture is as follows: The Green function (5) has two collective poles: 1) the upper pole which originates from initial spin-wave, 2) the lower pole which originates from spin-sound. Due to the interaction the spin sound is repulsed down from initial
spin-wave. The repulsion is so strong that it acquires imaginary frequency. The nonlinear interaction of spin-waves practically does not influence the spin sound and therefore can not eliminate the instability. We do not see any possibility to stabilize $t - J$ model without contact interaction. The true ground state in this case is probably some spiral phase.

Let us introduce now the hole-hole repulsion $V$ at nearest sites and consider $t - J - V$ model. In the effective Hamiltonian (1) only contact interaction (3) is changed: we should consider the constant $A$ as independent parameter of the model ($A \approx V$). Now the chain in Fig.1 becomes essential, and simple estimations show that value $A \sim 1.0 - 1.3$ is enough to eliminate the instability. If $J = 0.15eV$ it means that $A \sim 0.2eV$. It is hardly believed that in realistic systems there is no such a small Coulomb repulsion between the holes at nearest sites. The repulsion is probably even larger, but in this case, for the chain Fig.1 one has to use hole-hole scattering amplitude instead of simple matrix element $H_{hh}$. Calculation of this amplitude is in the progress.

Consider now the problem of long-range AF order in $t - J - V$ model with $V$ big enough, so that the paired hole Fermi liquid is stable. For this question it is convenient to use Hamiltonian technique instead of Feynman one because we need explicit construction of ground state wave function. The polarization operator $P(\omega, q)$ in (4) corresponds to normalization $2\omega_q$ spin-waves in the volume. For Hamiltonian approach let us introduce the polarization operator $\Pi(\omega, q)$ corresponding to normalization one spin-wave in the volume: $P(\omega, q) = 2\omega_q \Pi(\omega, q)$. The wave function of renormalized spin-wave corresponding to Green function (4) is a combination of $\alpha_q^\dagger$ and $\beta_{-q}$. To find this wave function write down the effective spin-wave Hamiltonian.

$$H_{sw} = \sum_q \left( (\omega_q - \Pi(\omega, q))(\alpha_q^\dagger \alpha_q + \beta_{-q}^\dagger \beta_{-q}) + \Pi(\omega, q)(\alpha_q \beta_{-q} + \alpha_{-q}^\dagger \beta_{-q}^\dagger) \right).$$ (7)

The term proportional to $\omega_q$ comes from “bare” Hamiltonian (1). First “$\Pi$ term” comes from diagram Fig.2a where one spin-wave is annihilated and the other is created. (For simplicity we do not present the chain with hole-hole contact rescattering) Second “$\Pi$ term” comes from diagrams Fig.2bc where two spin-waves are annihilated or created. Let us note that spin-waves have definite values of $S_z$: $\alpha_q^\dagger$ has $S_z = -1$ and $\beta_{-q}$ has $S_z = +1$. Therefore they can appear only in combinations presented in (4). One can certainly prove this explicitly using the vertex (2) and calculating the polarization operator. In the second “$\Pi$ term” the spin-waves have the opposite momenta. The vertex (4) is proportional to the momentum. Just due to this reason the second “$\Pi$ term” has different sign in comparison with first one.
Diagonalization of Hamiltonian \([7]\) by Bogoliubov transformation gives the spectrum of Bose excitations in the system

\[
\Omega_q^2 = (\omega_q - \Pi)^2 - \Pi^2 = \omega_q^2 - \omega_q \Pi (\Omega_q, q). \tag{8}
\]

This is exactly the equation for the poles of Green function \([4]\). To find new ground state we have diagonalize \([7]\) at \(\omega = 0\). As usually for Bogoliubov transformation this ground state is of the form

\[
|gs\rangle \propto \exp \left( \sum_q c_q \alpha_q^\dagger \beta_{-q}^\dagger \right) |0\rangle. \tag{9}
\]

This is exactly the condensate of spin-waves.

We started from Neel ground state \(|0\rangle\) with two sublattices \(A\)-up and \(B\)-down. The difference in magnetization of two sublattices is of the form (see e.g. Ref. \([18]\))

\[
\frac{1}{2}(S_A^z - S_B^z) = 1 - f_0 - 2 \sum_q \frac{1}{\omega_q} \left( \alpha_q^\dagger \alpha_q + \beta_q^\dagger \beta_q - \gamma_q (\alpha_q \beta_{-q} + \alpha_q^\dagger \beta_{-q}^\dagger) \right), \tag{10}
\]

where \(1 - f_0 \approx 0.303\). Using parameters of transformation diagonalizing \([7]\) one can easily calculate renormalized magnetization

\[
\langle gs | \frac{1}{2}(S_A^z - S_B^z) | gs \rangle = 1 - f_0 - 2 \int \left( \frac{1}{\Omega_{0q}} - \frac{1}{\omega_q} \right) \frac{d^2q}{(2\pi)^2}, \tag{11}
\]

where \(\Omega_{0q} = \sqrt{\omega_q^2 - P(0, q)}\) At small \(q\) due to the superconducting gap \(\Omega_{0q} \approx \Omega_q\). At \(q \gg p_F\) the polarization operator vanishes and \(\Omega_{0q} \to \omega_q\). Therefore the integral in Eq.(11) converges at \(q \sim p_F\), and we get the estimation for \(\delta S_z\) caused by spin-wave condensation

\[
\delta S_z \sim -\sqrt{\frac{\delta}{2\pi \tilde{v}}}. \tag{12}
\]

Here \(v = \sqrt{2}\) is unrenormalized spin-wave velocity and \(\tilde{v}\) is renormalize that which follows from Eq.(8). If \(|\delta S_z| = 0.303\) the magnetization vanishes and one should conclude that the long range AF order is destroyed. Due to estimation (12) for \(v/\tilde{v} \approx 4\) it happens at \(\delta = \delta_c \approx 0.04\). Note that the considered effect of enhancement of spin quantum fluctuations due to the polarization of fermionic subsystem is similar to the well known Casimir effect in Quantum Electrodynamics.

What happens if \(\delta > \delta_c\) and magnetization calculated using formula (11) becomes negative? It means that there are a lot of spin-waves in condensate and we have to take into account their nonlinear interaction. We can not do it exactly. Fortunately there is a simple
approximate way suggested by Takahashi in the work on Heisenberg model at nonzero temperature \[18\]. Following Takahashi let us impose the condition that sublattice magnetization vanishes.

\[
\langle gs| \frac{1}{2}(S_A^z - S_B^z)|gs \rangle = 0. \tag{13}
\]

To find the ground state with this condition we have to diagonalize

\[
H_\nu = H_{sw} - \frac{1}{8} \nu^2 (S_A^z - S_B^z), \tag{14}
\]

where \(H_{sw}\) is given by (7) and \((S_A^z - S_B^z)\) by (10). Simple calculation shows that instead of (8) we get a spectrum of excitations with a gap

\[
\Omega_\nu^\nu = \sqrt{\Omega_0^2 + \nu^2}. \tag{15}
\]

The average value of magnetization is given by the formula (11) with \(\Omega_{0q}^\nu = \sqrt{\Omega_0^2 + \nu^2}\) instead of \(\Omega_{0q}\). We have to find the gap \(\nu\) substituting this formula into condition (13). Let us stress that this condition reflects strong nonlinearity of theory. In essence it is effective cutoff of unphysical states in Dyson-Maleev approach (see discussion in the work \[19\]).

Certainly the suggested solution is not exact. It is kind of variational approach.

From the Eqs. (11), (13), (15) we conclude

\[
\nu \propto (\sqrt{\delta} - \sqrt{\delta_c}). \tag{16}
\]

However for detailed calculations of the spin-wave gap we have to take into account not only the “Casimir” contribution (11), (12) into spin quantum fluctuation, but also the contribution which is due to the spin-wave exchange in hole-hole pairing. Such detailed calculation will be presented elsewhere.

In this work we have introduced the short range hole-hole repulsion \(V\). One can prove that very small value of \(V\) practically destroys the d-wave hole-hole pairing. However it does not influence the g-wave pairing which has the same long-range behaviour as d-wave, but quite different short-range one \[16,17\]. Therefore the presented scenario favours the g-wave pairing.

**ACKNOWLEDGMENTS**

We are very grateful to V. V. Flambaum and A. V. Dotsenko for valuable discussions. This work was supported in part by a grant of the Australian Research Council.
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FIGURE CAPTIONS

FIG. 1. Spin-wave polarization operator.

Fig. 2. Spin-wave polarization operator in Schrodinger representation:
a) One spin-wave is annihilated and the other is created.
b,c) Two spin-waves are annihilated or created.