SC state in the underdoped high-$T_c$ cuprates as a quantum spin liquid. A microscopic theory.

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We have discovered a new example of quantum spin liquid which is a superconducting (SC) phase in 2D electron system close to electronic topological transition. As a quantum spin liquid in low dimensional localized spin systems it is characterized by a resonance spin mode and a well separated two-particle continuum. Application of the theory to the high-$T_c$ cuprates allows to shed light on many observed in the underdoped regime features such as the so called $40 meV$ resonance peak, incommensurability at lower $\omega$, spin gap etc.

Two most intriguing problems of high-$T_c$ cuprates, normal state anomalies including a pseudogap phenomenon observed by ARPES and by many other experiments and a peculiar SC state spin dynamics observed by neutron scattering (including the so called resonance peak, incommensurability at lower $\omega$, spin gap etc.), are considered today as key problems for understanding the physics of the cuprates. Have these phenomena (both occurring in the underdoped regime) some interrelation or are they completely independent? Is there some interrelation with the third phenomenon, existence of high-$T_c$ itself? There is a number of theories devoted to each of three problems. Most of them are phenomenological, use certain anzatzes which moreover are different to explain the different phenomena.

In the present paper where we concentrate on the problem of spin dynamics in SC state we show that the observed by inelastic neutron scattering (INS) peculiar behaviour can be naturally understood within the same theoretical concept which we used before to explain normal state anomalies and high value of SC gap. This concept is: (i) proximity of the 2D system of fermionic quasiparticles on a square lattice to electronic topological transition (ETT) (while this ETT is quite unusual in the case of electron-hole asymmetry or by other words of hoping beyond nearest neighbors) and (ii) existence of strong exchange AF interaction between these quasiparticles. [For the high-$T_c$ cuprates the latter are the bare electrons but the quasiparticles in the strongly correlated CuO$_2$ plane (described by the $t-t-J$ model) which dispersion law is also determined by the topology of 2D square lattice.] In we have shown that obligatory consequences of (i) and (ii) are developing of d-wave superconductivity around ETT point $\delta = \delta_c$, $T = 0$, with maximum $T_{sc}$ at $\delta = \delta_c$ and the existence in the underdoped regime above $T_{sc}$ of anomalous metallic state with strong spin density wave (SDW) fluctuations of relaxation type. In the present paper we show that this state transforms into SDW quantum liquid of resonance type (quantum spin liquid) when the system passes to the SC state. This means that the state below $T_{sc}(\delta)$ is at the same time an ordered SC state with respect to electronic degrees of freedom and a quantum spin liquid state with respect to spin degrees of freedom. This duality as we show is at the origin of the observed by different neutron scattering groups specific behaviour which includes the so called $40 meV$ resonance peak, incommensurability at lower $\omega$, spin gap and other features.

In the case we consider, the fermionic subsystem is characterized by the spectrum

$$\tilde{c}(k) = -2\omega(k_x + \cos k_y) - 4t' \cos k_x \cos k_y - ...$$

It has a hyperbolic metric in a proximity of ETT:

$$\tilde{c}(k) = -\mu - Z + ak^2 - bk^2$$

In $k_x$, $k_y$ are distances from saddle-point (SP) wavevector $k = k_{SP} = (0, \pi)$, $a = t - 2t'$, $b = t + 2t'$. The important parameter $Z = \mu - \epsilon_s \propto \delta_c - \delta$ ($\epsilon_s = 4t'/t$ is SC energy) measures the energy and doping distance from ETT and determines a new energy scale in the system. In the SC state of the d-wave symmetry which develops around ETT point, the spectrum gets a gap $\Omega_k = \sqrt{\epsilon_k^2 + \Delta_k^2}$. The parameter $Z > 0$, $\Delta = \Delta(\omega, \delta)$ which determines a second low energy scale in the system. SDW fluctuations in this SC state in RPA approximation are described by

$$\chi(q, \omega) = \chi^0(q, \omega)/(1 + V_q \chi^0(q, \omega)),$$

$$\chi^0(q, \omega) = \frac{1}{N} \sum_{k, \pm} M_{qk}^\pm 1 - n_F(\pm \Omega_k - n_F(\pm \Omega_{q+k})) / \Omega_{q+k} \pm \Omega_k - \omega - i\delta$$

where $M_{qk}^\pm = 1 \pm (\epsilon_k \pm \Delta_k) / \Omega_{q+k}$. The interaction entering in $\chi^0(q, \omega)$ comes from the J-term in the $t-t'-J$ model: $V_q = J_q = 2J(\cos k_x + \cos k_y)$.

As known, in the normal state ($\Delta = 0$) $\chi^0(q, \omega)$ diverges as $Z \to 0$, $T \to 0$, $q \to Q = (\pi, \pi)$ so that SDW instability with $q = Q$ obligatory occurs in a vicinity of ETT point. The metallic state above keeps a memory about this instability anomalously far in doping. The parameter $\kappa^2 = 1 - |q| \chi^0(Q, 0)$ which describes a "proximity" to SDW instability increases anomalously slow with increasing a doping distance from the instability. This occurs only in the underdoped regime $Z > 0$. 


The reason is analysed in [13]. In the SC state \( \chi^0(Q,0) \) behaves as in the normal state when \( Z \gg \Delta \) while the behaviour changes strongly when \( Z \leq \Delta \), see Fig.1a. In the latter case instead to diverge \( \chi^0 \) strongly decreases as \( Z \to 0 \). As a result, SDW instability around ETT point, \( Z = 0 \), disappears but a memory about it (a SDW liquid state with small \( \kappa^2 \)) exists at larger \( Z \). So far as for the cuprates \( \Delta(\delta) \approx \text{Const} \) [14] while \( Z(\delta) \sim \delta_c - \delta \) by the definition, this means the existence of two doping regimes within the underdoped regime, the first close to optimal doping, \( \delta^* < \delta < \delta_c \), for which \( \kappa^2 \) (i.e. a disorder) increases with increasing doping and the second \( \delta < \delta^* \) where it behaves in the opposite way, see Fig.1b. The point \( \delta = \delta^* \) turns out to be a point of a minimum disorder in this SDW liquid [15]. A value of \( \delta^* \) depends on \( \Delta/t \) for fixed \( t'/t \).

**FIG. 1.** Doping dependences of \( 4J\chi^0(Q,0) \) and \( \kappa^2 \) in the underdoped regime \( Z > 0 \) (\( \delta < \delta_c \)). \( \chi^0 \) is presented as a function of \( Z \), \( \kappa^2 \) as a function of \( \delta_c - \delta \) (\( T = 0 \)). Here and later on \( t'/t \approx -0.3 \), \( t/J = 2 \) [16]. \( \delta_c = 0.27 \) for \( t'/t = -0.3 \).

Let’s study now a spin dynamics in the SC state. For this let’s firstly analyse \( \chi^0 \) as a function of \( \omega \) and \( q \). Most important features are summarized in Fig.2. In Fig.2 we show \( \chi^0 \) calculated numerically as a function of energy for different wavevectors in a vicinity of \( q = Q \).

**FIG. 2.** \( J_q \Re\chi^0(q, \omega) \) and \( J_q \Im\chi^0(q, \omega) \) for different \( q \) in the direction \((q_x, 1)\pi \). \( Z/t = 0.2 \), \( \Delta/J = 0.2 \), \( T = 0 \)

Analytical calculations performed simultaneously show that for \( q = Q \), \( \Re\chi^0 \) diverges logarithmically while \( \Im\chi^0 \) has a jump at the energy [17]

\[
\omega = \omega_1^* = 2\Delta \sqrt{1 - Z/[4t'] - (\Delta/8t')^2}
\]

corresponding to opening of the gap in \( \Im\chi^0(Q, \omega) \) while for \( q \neq Q \) the logarithmic singularity splits into two logarithmic singularities. The first one occurs at the energy corresponding to the low energy border in \( \Im\chi^0(q, \omega) \), \( \omega = \omega^\text{cont}(q) \), the second, \( \omega = \omega^\text{cont}(q) \), lies in the continuum of electron-hole excitations. [At both energies \( \Im\chi^0(q, \omega) \) jumps.] These two energies are important characteristics of the continuum, we plot them as functions of wavevector in Fig.3. One can see that the low energy border of the continuum behaves in a very nontrivial way. It is highly nonmonotonal so that for \( \omega < \omega^\text{cont}(Q) = \omega_1^* \), spin-flip electron-hole excitations exist in an extremely narrow \( q \) range. The important wavevector is \( q_m \) [20], see Fig.3. Its absolute value in the direction \((q_x, 1)\pi \) (which as we will see later on corresponds to maximum \( \Im\chi^0 \) for given \( \omega \)) and the corresponding energy of the continuum are given by

\[
\pi q_m = 2\arccos(|4t'| - Z)/2t,
\]
\[
\omega_2^* = \omega^\text{cont}(q_m) = \Delta(|4t'| - Z)/2t.
\]

As \( Z \sim \delta_c - \delta \), both \( \omega_2^* \) and the deviation of \( |q_m| \) from \((\pi, \pi)\) increase with increasing doping. \( \omega_2^* \) determines a minimum gap in the spin excitations for given direction [21]. Another outstanding point is \( q = Q \), \( \omega = \omega_1^* \); for \( \omega > \omega_1^* \), the continuum occupies the whole \( q \) space. \( \omega_1^* \) also increases with increasing doping, see eq. [4]. For fixed \( Z \) (doping) both \( \omega_1^*, \omega_2^* \) are proportional to the SC gap \( \Delta \) (when \( |4t'| \ll 1 \)).

**FIG. 3.** Energies of the electron-hole continuum \( \omega^\text{cont}(q) \) and of the spin-exciton mode \( \Omega_q \) as functions of wavevector for the direction \((1 - Q_x, 1)\pi \). \( Z/t = 0.2 \), \( \Delta/J = 0.2 \).

Let’s consider now features of total \( \chi(q, \omega) \), i.e. a collective spin dynamics. The divergence of \( \Re\chi^0 \) for \( q \) in the vicinity of \((\pi, \pi)\) means that there are poles in \( \chi(q, \omega) \) at energies for which

\[
1 - |J_q \Re\chi^0(q, \omega)| = 0.
\]

One of them obligatory lies below the electron-hole continuum (at some \( \omega = \Omega_q \)) and therefore \( \Im\chi^0(q, \Omega_q) = 0 \). Spin susceptibility near this pole is given by
This expression describes a collective mode of resonance type - spin exciton. Details about it depend on details of \( \chi^0(q, \omega) \). One has to distinguish two different situations: (i) \( Z \gg \Delta \) (highly underdoped regime) and (ii) \( Z \sim \Delta \) or \( Z < \Delta \) (moderate and close to optimal doping).

In the case (i) the energy dependences of \( Re\chi^0 \) and \( Im\chi^0 \) are close to those in the normal state (compare Fig.3a,b). The logarithmic singularity appearing in \( Re\chi^0 \) is quite weak so that any extra factor leading to a finite damping such as small amount of impurities, a temperature effect etc. easily eliminates the singularity and the condition (6) is not fulfilled. On the other hand, the jump in \( Im\chi^0 \) is small, therefore due to the same damping the gap in \( Im\chi^0 \) is easily filled up. As a result the spin dynamics in the highly underdoped regime is close to that in the normal state. This is exactly what is observed in \( YBCO_{6.5} \) [22].

\[
Im\chi(q, \omega) = (1/J^2_q) \partial Re\chi^0(q, \omega)/\partial\omega |^{-1} \delta(\omega - \Omega_q). \quad (7)
\]

A picture of \( q \) dependence of the total susceptibility in this regime is qualitatively different for different \( \omega \) ranges.

1. For \( \omega < \omega^* \) there is no magnetic fluctuations neither of two-particle nor of collective nature. This is a "spin gap" regime [21]. As we discussed above, \( \omega^* \) i.e. the "spin gap" increases with increasing doping that explains well the observed by INS general tendency.

2. For \( \omega > \omega^* \), rather strong incommensurate spin fluctuations appear with a very narrow \( q \)-width. Their nature changes progressively (with increasing \( \omega \) from two-particle excitations to the collective resonance excitations; respectively the intensity increases with increasing \( \omega \). The \( q \) dependence of \( Im\chi(q, \omega) \) for this \( \omega \) range is shown in Fig.3a. It is strikingly similar to that observed recently experimentally for \( YBCO_{6.6} \) [7], see Fig.3b.

3. A maximum intensity of spin fluctuations occurs at \( E_r = \Omega_q \). Due to flatness of the dispersion \( \Omega_q \), the \( q \)-width of \( Im\chi(q, \omega) \) is much larger for \( \omega \approx E_r \) than for energies corresponding to the incommensurate fluctuations that is in a good agreement with experiment [7].

4. For \( \omega > \omega^* \), the spin fluctuations has a two-particle nature, the \( q \) dependence is very broad. There is still a maximum of intensity at the incommensurate position corresponding to another pole determined by eq.(6) which lies inside the continuum. This is also in a good agreement with experiment [7].

The obtained picture of the spin dynamics combining a resonance mode plus two-particle continuum features is typical for quantum spin liquid (QSL). Until now the latter was known as an attribute of low dimensional localized spin systems [23]. We have shown that SC state in 2D electron system close to ETT is another example of QSL state. Is d-wave symmetry of SC gap necessary for this? The answer is no. For the isotropic s-wave and for all other symmetries except the extended s-wave (this exception was already emphasized in [15]) there is always a gap in \( Im\chi^0(Q, \omega) \), i.e. the necessary condition for the existence of the resonance mode with \( q \) close to \( Q \) is fulfilled. The difference with the d-wave symmetry (or with any other symmetries for which the SC gap changes sign between different sectors of BZ, d+s ...) is that due...
to the absence of singularity in $Re\chi^0$ [24] the resonance mode exists only when $J/t$ exceeds some threshold value. Another more significant difference is that in the case of the isotropic s-wave symmetry the low energy border of the continuum does not depend on wavevector, as a result the effect of incommensurability at low $\omega$ disappears. On the other hand, two conditions, d-wave symmetry of SC gap and a proximity to ETT quantum critical point (small $Z$ or a proximity of Fermi level to SP) are sufficient for the SC state to be a QSL. Both conditions are known to be fulfilled for the hole-doped high-$T_c$ cuprates.

Coming back to the cuprates let’s analyse a doping dependence of the spin exciton energy. The latter is given by the condition (6). If it were fulfilled for low $\omega$, the dispersion law would be written as $\Omega_q = \sqrt{\Delta^2 + a(q - Q)^2}$ with $\Delta^2 \propto \kappa^2$ (since $Re\chi^0(q, \omega) \propto \omega^2$ for low $\omega$) that is a typical dispersion law for a quantum spin liquid. For realistic for the cuprates values of parameters, $t/J \approx 2$, $\Delta/J \approx 0.2$, the condition (6) is fulfilled for relatively high $\omega$ for which roughly $\Delta_\tau \propto \kappa^2$. These simple arguments explain the calculated doping dependence $E_r(\delta) \equiv 1\Omega_q(\delta)$ which follows qualitatively the doping dependence of $\kappa^2$, compare Fig.6 with Fig.1. The experimental dependence for the underdoped $YBCO_{6+x}$ is shown in Fig.6b where we summarized all reported by different INS groups data for moderate and close to optimal doping. The theoretical and experimental curves are strikingly similar. [Note when comparing that for the cuprates $J \approx 120 \text{meV}$.]

![Diagram](image)

FIG. 6. Doping dependence of the resonance peak in the underdoped regime: theoretical calculated with $\Delta/J = 0.2$, $t/J = 2$ and experimental for YBCO$_{6+x}$ [2-7].

Summarising, the study performed in the present paper has a significance in two points.

1. We discover a new example of a quantum spin liquid which is a 2D itinerant spin system in the SC state. As a quantum spin liquid in low dimensional localized spin systems it is characterized by the resonance spin mode and by well separated two-particle continuum.

2. The picture obtained with using parameters characteristic for the high-$T_c$ cuprates allows to shed light on many observed in the underdoped regime features such as the very fact of incommensurability at low $\omega$, the absolute value of the incommensurability wavevector and the details of $q$ dependence of $Im\chi$ in different directions in BZ, the absolute value of the resonance energy $E_r$ for optimal doping and its doping dependence, the interrelation between the $q$-width of $Im\chi$ in the case of commensurate and incommensurate fluctuations etc. The agreement with experiment is quite impressive regarding that we did not use any external hypothesis or adjustable parameters [16].

Note that we did not consider the case of $|t'/t| \rightarrow 0$ which corresponds to another class of universality as we emphasized in [10]. This case (presumably corresponding to LSCO) for which an incommensurability exists both below and above $T_{sc}$ will be analysed elsewhere.

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