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The effect of spin correlations on a superconducting phase of the spin polarons in 2D Kondo lattice

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Abstract. The effect of the magnetic correlators on the spin polaron superconducting phase is studied in terms of 2D Kondo lattice model. It is shown that hopping integrals are renormalized by the magnetic correlators and as a result the $T_c$ phase diagram is changing significantly. By computation the effect of magnetic correlation functions on the concentration dependence of $T_c$ was analysed and their substantial role in description of doped antiferromagnets is demonstrated. The obtained phase diagram is in qualitative agreement with experimental data for temperature dependence of the superconducting phase transition with d-type symmetry in cuprates.

It is well known that the electron energy structure of the high temperature superconductor's CuO$_2$ plane is well represented by Emery model [1]. In the case when the mixing parameter between p- and d- orbitals is much less than the difference in the energy ($t_{pd} \ll \Delta_{pd} = \varepsilon_p - \varepsilon_d$) this model is reduced to the effective Hamiltonian $H_{\text{eff}}$ describes the exchange interaction between spin moments of the Cu ions and kinetic energy of the holes. Therefore the 2D Kondo lattice model may be used for analysing the magnetic mechanism of the Cooper instability in the cuprate superconductors.

If the $s - d$ exchange coupling is much greater than the hopping integral the Fermi-type elementary excitation spectrum of the Kondo lattice is well described in a spin polaron approach [2, 3]. In such way the energy spectrum is formed by a hole-type carriers moving on a spin fluctuation background. The superconducting phase of spin polarons in the Kondo lattice model was discussed in [4]. It was shown that two- and three-site interactions are induced between spin polarons in 2D Kondo lattice.

It is common knowledge that the spin-liquid correlations significantly affect on the existence conditions of the superconducting phase. Meanwhile, in [4] the superconducting phase has been analysed without considering this correlations. That is way the development of the superconducting phase theory of an ensemble of the spin polarons when magnetic fluctuations are taken into is of great interest here.

Kondo lattice model takes into account the interaction between spins of bare ions described by Heisenberg antiferromagnetic coupling $I$. The holes moving on this background are bounded with local sites by the means of $s - d$ exchange coupling $J$. In case of two carriers sitting on the site the Hubbard repulsion is taken into account. Thus the Hamiltonian of the Kondo lattice

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model can be written as

\[ \hat{H} = J \sum_f S_f S_f + U \sum_f \hat{n}_{f \uparrow} \hat{n}_{f \downarrow} + \sum_{f,g,\alpha} t_{fg} c_{f\alpha}^+ c_{g\alpha} + \frac{1}{2} \sum_{fg} I_{fg} S_f S_g. \]  

(1)

Here \( c_{f\alpha}^+ \) and \( c_{f\alpha}^+ \) stand for the fermion creation operators of a hole with spin up and spin down respectively. The \( S_f \) and \( S_g \) correspond to spin operator of a hole and spin operator of a bare ion. To reproduce the particular features of the hole spectrum in real high-\( T_c \) superconducting compounds we account for hops to first \( t_1 \), second \( t_2 \) and third \( t_3 \) neighbours.

If a constant of the \( s - d \) exchange interaction exceeds the hopping integral, then the spin polaron is realized. The spin polaron approach allows to account for all possible one-site quasiparticle states which occurs in the ion-hole system. In the absence of a hole on the site the bare ion can be found in two possible states with different magnetic momentum projections: spin up \( |\uparrow\rangle \) and spin down \( |\downarrow\rangle \). If there is a single hole on the site the magnetic interaction can lead to a singlet state \( |S\rangle = \frac{1}{\sqrt{2}} \left( c_{f\uparrow}^+ |\uparrow\rangle - c_{f\downarrow}^+ |\downarrow\rangle \right) \) with null total spin projection or to one of triplets \( |{-1}\rangle = c_{f\uparrow}^+ |\downarrow\rangle \), \( |0\rangle = \frac{1}{\sqrt{2}} \left( c_{f\uparrow}^+ |\uparrow\rangle + c_{f\downarrow}^+ |\downarrow\rangle \right) \), \( |1\rangle = c_{f\uparrow}^+ |\downarrow\rangle \). The one-site system containing two holes and one ion can exist in one of two states \( (|+\rangle = c_{f\uparrow}^+ c_{f\downarrow}^+ |\downarrow\rangle) \) or \(|-\rangle = c_{f\uparrow} c_{f\uparrow}^+ |\downarrow\rangle \), depending on the total magnetic moment projection.

In the present paper the model is studied under the assumption that the concentration of the carriers is rather low. In addition, the Hubbard repulsion of holes is supposed to be much greater than other parameters of the theory so the contribution of two-hole states becomes small. Since the triplet states are separated from singlet ground state with the gap of the magnitude equal to \( s - d \) exchange interaction \( J \), the contribution of triplet states is also small when \( J \gg |t_1| \).

For marking out the most substantial interactions the Hubbard operators representation [5] is used. As stated above the major contribution belongs to the terms including hole-free and single-hole singlet states. We use the operator form of the perturbation theory to account for the upper states of the system. The quantities \( t/J, t/U \) and \( I/J \) are treated as series expansion parameters. Up to the terms of the second order in the mentioned parameters the projected effective Hamiltonian can be written as

\[ \hat{H}_{\text{eff}} = \sum_f (\varepsilon_{sp} - \mu) X_f^{SS} + \frac{1}{2} \sum_{fm\sigma} t_{fm} X_f^{S\sigma} X_f^{S\sigma} + \frac{1}{2} \sum_{fm} I_{fm} S_f S_m + \frac{1}{2} \sum_{fm} V_{fm} X_f^{SS} X_m^{SS} + \hat{H}(3), \]  

(2)

where \( \sigma = \uparrow, \downarrow \) indicates hole-free states with spin up and spin down respectively. The first term in (2) describes the set of non-interacting spin polarons with the energy

\[ \varepsilon_{sp} = -\frac{3}{4} J - \frac{3}{4} \sum_m \left( \frac{t_{fm} t_{mf}}{J} + \frac{I_{fm} I_{mf}}{4J} \right). \]  

(3)

The kinetic energy of the spin polaron quasiparticles is represented by the second term of the effective Hamiltonian (2). The third term corresponds to Heisenberg interaction between ions and is based on the reduced spin operators \( \hat{S}_f^+ = X_f^{\uparrow\downarrow} \) and \( \hat{S}_f^z = \frac{1}{2} \left( X_f^{\uparrow\uparrow} - X_f^{\downarrow\downarrow} \right) \). The term including the coefficient

\[ V_{fm} = \frac{3}{2} \frac{t_{fm} t_{mf}}{J} - \frac{t_{fm} t_{mf}}{U + 3/2J} + \frac{9}{32} \frac{I_{fm} I_{mf}}{J}. \]  

(4)
appears due to virtual quantum transitions to the triplet and two-hole upper states. The last term in (2) describes three-center interactions

\[
\hat{H}_3(3) = \sum_{fmg\eta \neq \eta} t_{fm\eta} X_f^{S\eta} X_m^{\eta} X_g^{\eta S} - \sum_{fmg\eta \neq \eta} \frac{t_{fm\eta}}{2J} X_f^{S\eta} \left( X_m^{\eta} + \frac{1}{2} X_m^{\eta S} \right) X_g^{\eta S} - \sum_{fmg\eta \neq \eta} \frac{t_{fm\eta}}{4J} X_f^{S\eta} X_m^{SS} X_g^{\eta S} - \sum_{fmg\eta \neq \eta} \frac{t_{fm\eta}}{4J} \bar{S}_f \bar{S}_m X_m^{SS}. \tag{5}
\]

The transitions between lower two states are described by operators \(X_i^{S}, X_i^{S} \) and Hermitian conjugated operators. The superconducting phase of spin polarons is investigated by using normal \( \langle X_f^{S} | X_g^{S} \rangle \) and anomalous \( \langle X_f^{S} | X_g^{S} \rangle \) Green functions. We use Zwanzig-Mori projection technique to derive equations for superconducting phase transition. Averages including magnetic correlators, density-density correlators and kinetic correlators are arising in the course of projection procedure. The most significant correlators with respect to others are magnetic correlators. Therefore, only spin-spin correlators are accounted further. Thus the set of equations for Fourier transform of Green functions is derived

\[
(\omega - \omega(k)) \left( \langle a_{k\uparrow}^+ | a_{k\uparrow}^+ \rangle \right) - \Delta_k \left( \langle a_{-k\downarrow}^+ | a_{k\uparrow}^+ \rangle \right) = \frac{1 + n}{2}, \tag{6}
\]

\[
- \Delta_k^+ \left( \langle a_{k\uparrow}^+ | a_{k\downarrow}^+ \rangle \right) + (\omega + \omega(k)) \left( \langle a_{-k\downarrow}^+ | a_{k\downarrow}^+ \rangle \right) = 0. \tag{7}
\]

With the magnetic correlators taken into account the seed spectrum can be written as

\[
\omega(k) = \varepsilon_{sp} + \sum_q \left( -\frac{1}{1+n} I_q C_q + V_q n \right) + \frac{1 + n}{4} t_k + \sum_q \frac{1}{1+n} t_{k-q} C_q. \tag{8}
\]

The equation derived describes spectrum of spin polarons in normal phase (figure 1). The superconducting parameter can be defined from self-consistent equation including anomalous average \( \langle a_{-q}^+ | a_q^+ \rangle \), which can be determined by means of the spectral theorem. As a result, the integral equation for the superconducting order parameter can be written as

\[
\Delta_k = \frac{1}{N} \sum_q \left( \frac{3}{2} I_{k-q} - 2V_{k-q} - 2t_q \right) \frac{\Delta_q}{4E_q} \tanh \left( \frac{E_q}{2T} \right). \tag{9}
\]

It is well known that such equations have several solutions, which are differed from each other by symmetry type. It should be noted that the parameter \( V_{fm} \) depends on the difference \( f - m \), and as it can be seen in (4), has non-zero value for up to third neighbours. Therefore the solution for \( \Delta_k \) should account for hops to distant coordination spheres. It is shown in [6] that the solution for the \( d_{x^2-y^2} \) symmetry type is given by

\[
\Delta_k = \Delta_1 \varphi_1(k) + \Delta_2 \varphi_2(k), \text{ where } \varphi_i(k) = \cos(lk_x) - \cos(lk_y).
\]

Substituting this order parameter in (8) we obtain system of equations for \( \Delta_1 \) and \( \Delta_2 \). The consistency of equations condition with the assumption that \( \Delta_1 = \Delta_2 = 0 \) give us the expression
Spin polaron spectrum for $J = 3\text{eV}$, $U = 7\text{eV}$, $I = 0.2\text{eV}$, $|t_1| = -0.6\text{eV}$, $|t_2| = 0.7\text{eV}$. $|t_3| = 0.48\text{eV}$, $C_1 = -0.3$, $C_2 = 0.15$, $C_3 = 0.1$. Horizontal dashed line indicates Fermi level at optimal doping.

Figure 1. Spin polaron spectrum for $J = 3\text{eV}$, $U = 7\text{eV}$, $I = 0.2\text{eV}$, $|t_1| = -0.6\text{eV}$, $|t_2| = 0.7\text{eV}$. $|t_3| = 0.48\text{eV}$, $C_1 = -0.3$, $C_2 = 0.15$, $C_3 = 0.1$. Horizontal dashed line indicates Fermi level at optimal doping.

Figure 2. Phase diagram with magnetic correlators (solid line) and without accounting for correlators (dashed line).

for critical temperature

$$
\left(1 - \left(\frac{3}{2}I - 2V_1\right)\right) \frac{1}{N} \sum_q \frac{\varphi_1(q)^2}{4(\omega(q) - \mu)} \tanh\left(\frac{\omega(q) - \mu}{2T_c}\right) \cdot \\
\cdot \left(1 + 2V_3 \frac{1}{N} \sum_q \frac{\varphi_2(q)^2}{4(\omega(q) - \mu)} \tanh\left(\frac{\omega(q) - \mu}{2T_c}\right)\right) + \\
+ \left(\frac{3}{2}I - 2V_1\right) 2V_3 \left( \frac{1}{N} \sum_q \frac{\varphi_1(q)\varphi_2(q)}{4(\omega(q) - \mu)} \tanh\left(\frac{\omega(q) - \mu}{2T_c}\right)\right)^2 = 0. \quad (10)
$$

Superconducting transition phase diagrams are shown on figure 2. The solid line corresponds to the model accounting for magnetic correlations, while dashed line reflects $T_c$ dependence without spin-spin correlators. The minimum of the dispersion curve is located near $(\pi/2, \pi/2)$ like it is shown on figure 1. We used typical values for correlators in a square antiferromagnetic Heisenberg lattice. It is seen that spin-liquid correlators significantly affect on realization of a superconducting transition.

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