Spin fluctuation renormalizations of normal and superconducting state properties in $t - J^*$-model

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Abstract. The effect of spin-fluctuation scattering processes on the region of the superconducting phase in the strongly correlated electrons (Hubbard fermions) has been investigated by the diagram technique for Hubbard operators. It is shown that spin fluctuations in the one-loop approximation for the $t - t' - t'' - J^*$-model taking into account long-range hoppings and three-center interactions are reflected by components of the strength operator. In this approximation for the $d$-type symmetry of the order parameter for the superconducting phase a system of infinite integral equations has been derived. Obtained dependencies of critical temperature on the electron concentrations show that joint effect of long-range hoppings, three-center interactions, and dynamical spin-fluctuation processes leads to strong renormalization of the superconducting phase region. It was shown that these processes essentially modify distribution functions of Hubbard fermions in normal phase.

In spite of more than twenty-year investigation history of high-temperature superconductors [1] a problem of the Cooper pairing mechanism in this materials has not solved yet. There are a plenty of works confirming that the pairing mechanism is conditioned by spin-fluctuation scattering processes [2]. Also it is well known that for a correct theoretical description of high-temperature superconductors is necessary to take into account strong electron correlations. In the framework of the atomic representation the diagram technique for Hubbard operators (DTH) is used often [3-6]. In the context of DTH as it was shown in [7] in graphical series of the perturbation theory it is necessary to take into account a combination of ending diagrams which is called the strength operator $\hat{P}$. In describing the superconducting phase $\hat{P}$ has matrix form with non-zero anomalous components $P_{\sigma,\sigma'}$. The next peculiarity is connected with normal components $P_{\sigma,\sigma'}$ of the strength operator. Beyond the framework of the mean-field approximation (MFA) $P_{\sigma,\sigma'}$ contains terms depending on a quasi-momentum and the Matsubara frequency $\omega_n$. Furthermore $P_{\sigma,\sigma'}$ and $P_{\sigma,\sigma'}$ describe scattering processes on spin fluctuations. It will be shown that taking into account of $P_{\sigma,\sigma'}$ and $P_{\sigma,\sigma'}$ essentially changes the superconducting phase region and distribution functions of Hubbard fermions.

The Hamiltonian of $t - t' - t'' - J^*$-model in the atomic representation can be written as

$$H = \sum_{f,\sigma} (\varepsilon - \mu) X_f^{\sigma} + \sum_{f,\sigma} t_f X_f^{\sigma} X_0^{\sigma} + \sum_{f,\sigma} J_f X_f^{+} X_m^{-} - X_f^{+} X_m^{-} + \sum_{f,\sigma} \frac{J_f}{t_m X_{m\sigma}} (X_f^{\sigma} X_m^{\sigma} X_0^{\sigma} - X_f^{\sigma} X_m^{\sigma} X_0^{\sigma}) + \sum_{f,\sigma} \frac{J_f}{t_m X_{m\sigma}} (X_f^{\sigma} X_m^{\sigma} X_0^{\sigma} - X_f^{\sigma} X_m^{\sigma} X_0^{\sigma}),$$

(1)
where \( X_f^{0\sigma} \) are Hubbard operators: \( X_f^{0\sigma} \left( X_f^{0\bar{\sigma}} \right) \) describes a transition of the ion situated in site \( f \) from an one-electron state with the spin projection \( \sigma \) (\( \bar{\sigma} = -\sigma \)) to the state without elections, \( X_{f-}^{0} \) describes inverse process. One-site transitions associated with the spin projection are reflected by operators \( X_f^{-} \) and \( X_f^{+} \). Diagonal operators \( X_f^{0\sigma} \) and \( X_f^{0\bar{\sigma}} \) are projectors for one-electron and zero-electron sectors of the Hilbert space corresponding to the \( f \)-site. The energy of the one-electron one-ionic state is indicated by \( \varepsilon \), \( \mu \) is a chemical potential of the system, \( t_{fm} \) is hopping parameter of an election from \( m \)-site to \( f \)-site, \( J_{fm} \) is parameter of exchange coupling between one-electron states on \( m \)- and \( f \)-sites.

First three terms of Hamiltonian (1) correspond to \( t-J \)-model, last term represents three-site interactions \((H_{(3)})\) which is called correlated hoppings sometimes. The Hamiltonian can be deduced from Hubbard model in a strong correlation regime \(| t_{fm} | \ll U\) if the concentration of current carriers \( n < 1 \). Inclusion of \( H_{(3)} \) depends upon the fact that effects induced by this contribution essentially influence on a concentration dependency of a critical temperature \( T_c(n) \). Since concrete character of the dependency \( T_c(n) \) changes at addition of hoppings between sites from long-range coordination spheres hereinafter it should not be restricted to the nearest neighbor approximation and we shall assume that three hopping parameters \( t \), \( t' \), and \( t'' \) are not equal to zero. In scientific publications such model sometimes is called \( t-t'-t''-J^* \)-model (sign * points to presence of \( H_{(3)} \)-interactions in the Hamiltonian).

Contributions to the anomalous component of the strength operator originated from interactions of \( t-J \) model is determined by four diagrams

\[
\begin{align*}
\text{(2)}
\end{align*}
\]

The next four diagrams define the anomalous component of the strength operator conditioned by three-site interactions.

\[
\begin{align*}
\text{(3)}
\end{align*}
\]

Using analytical form for anomalous components of the self-energy and the strength operator it has been derived the system of self-consistent integral equations for the superconducting phase \( \Sigma_{12}(\vec{k}) = \Sigma_{01;10}(\vec{k}) \) and \( P(\vec{k}, i\omega_n) = P_{01;10}(\vec{k}, i\omega_n) - P_{01;10}(\vec{k}, i\omega_n) \)

\[
\begin{align*}
\Sigma_{12}(\vec{k}) &= -\frac{T}{N} \sum_{\vec{q},\omega_l} \left( t_{\vec{q}} + \frac{n}{2} J_{\vec{k}-\vec{q}} \right) A_{\vec{q}}(i\omega_l), \\
P(\vec{k}, i\omega_n) &= -\frac{T}{N} \sum_{\vec{q},\omega_l} \left[ t_{\vec{q}} + \frac{1}{2} \left( 1 + \frac{n}{2} \right) J_{\vec{k}-\vec{q}} \right] \chi_s(\vec{q} - \vec{k}, i\omega_l - i\omega_m) A_{\vec{q}}(i\omega_l), \quad (4)
\end{align*}
\]

where

\[
\begin{align*}
A_{\vec{q}}(i\omega_l) = \frac{2\Sigma_{12}(\vec{q}) - t_{\vec{q}} \cdot P(\vec{q}, i\omega_l)}{\det(\vec{q}, i\omega_l)}. \quad (5)
\end{align*}
\]

The dynamical spin susceptibility \( \chi_s \) was represented by the model on the analogy of [8]:

\[
\begin{align*}
\chi_s(\vec{q}, i\omega_n) &= \left( \frac{2\pi}{a} \right)^2 \delta(\vec{q} - \vec{Q}) \cdot \frac{3n}{2\Omega} \tanh \left( \frac{\Omega}{2T} \right) \frac{1}{1 - (i\omega_n/\Omega)^2}, \quad (6)
\end{align*}
\]
where $\vec{Q} = (\pi, \pi)$. Such approach lets to simplify calculations essentially and includes known experimental fact that the spin susceptibility has a peak at point $\vec{q} = \vec{Q}$. The parameter $\Omega$ was found from the sum rule:

$$T \sum_{\vec{q}, i\omega_n} \chi_s(\vec{q}, i\omega_n) = \frac{3n}{4}. \quad (7)$$

Expression for $\text{det} (\vec{k}, i\omega_n)$ contains both terms conditioned by normal, and anomalous components of the self-energy and the strength operator.

$$\text{det} (\vec{k}, i\omega_n) = \left\{ i\omega_n + \varepsilon + \mu + t_{\vec{q}} P_{\sigma_0, \sigma_0}(\vec{k}, i\omega_n) - \Sigma_{\sigma_0, \sigma_0}(\vec{k}, i\omega_n) \right\} \times$$

$$\left\{ i\omega_n + \varepsilon + \mu - t_{\vec{q}} P_{0\sigma, 0\sigma}(\vec{k}, i\omega_n) - \Sigma_{0\sigma, 0\sigma}(\vec{k}, i\omega_n) \right\} -$$

$$- \left\{ \Sigma_{0\sigma, 0\sigma}(\vec{k}, i\omega_n) - t_{\vec{q}} P_{0\sigma, 0\sigma}(\vec{k}, i\omega_n) \right\} \left\{ \Sigma_{\sigma_0, \sigma_0}(\vec{k}, i\omega_n) + t_{\vec{q}} P_{\sigma_0, \sigma_0}(\vec{k}, i\omega_n) \right\}. \quad (8)$$

The one-loop correction of normal component of the strength operator for $t - J$ model is determined by four diagrams

\begin{center}
\includegraphics[width=0.5\textwidth]{diagram1.png}
\end{center}

A contribution to the normal component of the strength operator resulted from three-site interactions is conditioned by

\begin{center}
\includegraphics[width=0.5\textwidth]{diagram2.png}
\end{center}

An analytical form corresponding to the sum of (9) and (10) is

$$P_{0\sigma, 0\sigma}(\vec{k}, i\omega_n) = \left( 1 - \frac{n}{2} \right) + \frac{T}{N} \sum_{\vec{q}, \omega_l} \frac{[t_{\vec{q}} + \frac{1}{2} (1 + \frac{4}{3}) J_{\vec{k} - \vec{q}}] \chi_s(\vec{q} - \vec{k}, i\omega_l - i\omega_n)}{i\omega_l - \varepsilon + \mu - t_{\vec{q}} P_{0\sigma, 0\sigma}(\vec{q}, i\omega_l)}. \quad (11)$$

Solving (4) for $d_{x^2-y^2}$ - order parameter symmetry electron concentration dependencies of the superconducting transition temperature $T_c(n)$ has been calculated. These dependencies for different hopping parameters are shown on figures 1 and 2. For both figures constant $J = 0.4|t|$, dotted lines describe dependencies at MFA-approximation, full lines describe dependencies taking into account spin-fluctuation processes by strength operator components. Thus taking into account of spin fluctuations by strength operator components essentially modifies critical temperature dependencies and sometimes can lead to almost full suppression of the superconducting phase region.

To investigate properties of the normal phase we have chosen another phenomenological model of the spin susceptibility proposed by Pines [9]. This approach lets to take into account a quasi-momentum dependency of the susceptibility more accurately then in (6). The figure 3 demonstrates a role of normal components of the strength operator on a quasi-momentum distribution function of the Hubbard fermions at next parameters: $t' = -0.1|t|, t'' = 0.1|t|, J = 0.4|t|, n = 0.8$. The dotted line coresponds to the MFA approximation. In this case the usual Fermi distribution is obtained. Full line is a dependency when $P_{0\sigma, 0\sigma}$ are taken into account. Therefore it is turned out that spin-fluctuation processes essentially change normal state properties and lead to availability of non-zero probability states beyond the Fermi surface.
Figure 1. The dependency of the $T_c(n)$ for $t' = -0.1|t|, t'' = 0.1|t|$.  

Figure 2. The dependency of the $T_c(n)$ for $t' = -0.1|t|, t'' = -0.1|t|$.  

Figure 3. Quasi-momentum distribution functions at different approximations.

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