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ORDER, DISORDER, AND PHASE TRANSITION IN CONDENSED SYSTEMS

Effect of Spin Fluctuations on the Superconducting Phase of Hubbard Fermions in the t–t'–t''–J^* Model

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Abstract—The effect of spin-fluctuation scattering processes on the region of the superconducting phase in strongly correlated electrons (Hubbard fermions) is investigated by the diagram technique for Hubbard operators. Modified Gor'kov equations in the form of an infinitely large system of integral equations are derived taking into account contributions of anomalous components $P_{0\sigma,\bar{\sigma}0}$ of strength operator $\hat{P}$. It is shown that spin-fluctuation scattering processes 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 normal ($P_{0\sigma,0\sigma}$) and anomalous ($P_{0\sigma,\bar{\sigma}0}$) components of the strength operator. Three-center interactions result in different renormalizations of the kernels of the integral equations for the superconducting d phase in the expressions for the self-energy and strength operators. In this approximation for the d-type symmetry of the order parameter for the superconducting phase, the system of integral equations is reduced to a system of nonhomogeneous equations for amplitudes. The resultant dependences of critical temperature on the electron concentrations show that joint effect of long-range hoppings, three-center interactions, and spin-fluctuation processes leads to strong renormalization of the superconducting phase region.

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1. INTRODUCTION

The microscopic theory of high-temperature superconductivity (HTSC) is developed in most cases using model Hamiltonians reflecting the presence of strong electron correlations in the system. This explains the wide recognition of the Hubbard model [1], as well as multiband generalizations of this model [2, 3]. After [4], the so-called t–J model providing a description for the exchange and spin-fluctuation mechanisms of singlet electron pairing with the d-type order parameter symmetry has become an object of intense investigation [5–12]. At the same time, new mechanisms of pairing in cuprate superconductors were proposed proceeding from general properties of strongly correlated systems [13–15].

In microscopic models of strongly correlated systems, self-consistent equations for the superconducting phase can be derived using several methods. One of these methods is based on the irreducible Green's function constructed on Hubbard operators [5, 7]. Another approach is associated with the graphical form of perturbation theory for the Matsubara Green's functions in the atomic representation [6, 10, 16–19]. This method for studying strongly correlated systems is usually referred to as the diagram technique for Hubbard operators. Calculations performed using these approaches show that the structure of equations obtained for the superconducting phase is qualitatively similar to the structure of equations in the BCS theory.

Beyond the mean-field approximation, the structure of equations for the superconducting phase of strongly correlated systems becomes qualitatively different. One of the reasons for this difference is the presence of so-called terminal diagrams in the graphic series for the Matsubara Green's functions [6, 10, 16]. The important role of these diagrams in the quantum theory of magnetism was established long ago (see, for example, [10, 18]). The complete set of such diagrams is referred to as the terminal factor [6, 10, 18] or strength operator. The latter term was proposed in [20], in which the features of the diagram technique for spin operators were analyzed.

The description of the superconducting phase involves the introduction of normal as well as anomalous Green's functions [21]. Accordingly, the self-energy operator acquires the matrix structure and is characterized by normal and anomalous components. Analogously, we can expect that the strength operator can also be presented in matrix form. Its nondiagonal components reflect the anomalous components of the strength operator and must be taken into account in constructing the theory of the superconducting phase of strongly correlated systems. However, this has not been accomplished so far.

We will show that the diagram series for normal and anomalous Green's functions indeed contains the diagrams belonging to the class of anomalous terminal diagrams and making a contribution to the anomalous components of the strength operator. Taking this fact into account, we will present equations for the Matsubara Green's function graphically for the t–t'–t''–J^* model accounting for long-range hoppings and three-center interactions and write these equations in analytic form. We will prove that the anomalous components of the strength operator play a significant role in the calculation of anomalous means. The calculations will be performed in the one-loop approximation, in which, in contrast to the self-energy operator, the anomalous components of the strength operator are functions of the Matsubara frequency. As a result, the superconducting phase in this approximation can be described by an infinitely large system of integral equations. This system will be solved numerically for calculating the superconducting transition temperature with the d-type symmetry of the order parameter. Our calculations enabled us to analyze the joint effect of electron hoppings to the sites from far coordination spheres, three-center interactions, and spin fluctuations on the superconducting phase region with a preset type of the order parameter symmetry. We will show that spin-fluctuation scattering processes are reflected in normal and anomalous components of the strength operator and considerably affect the concentration dependence of the superconducting transition temperature. The effect of spin fluctuations is manifested most strongly in the range of model parameters, in which the phase diagram of the system in the simplest approximations is close to the experimentally observed diagram. This means that in a consistent development of the theory of the superconducting phase of Hubbard fermions, anomalous components of the strength operators must be taken into account along with anomalous components of the self-energy operator.

The article has the following structure. In Section 2, the derivation of the general equations for normal and anomalous Matsubara Green's functions is described taking in to account the contributions from anomalous components of the strength operator. It is shown that these anomalous components basically change the structure of the expression for anomalous averages. Section 3 is devoted to analytic calculation of anomalous components of the self-energy and strength operators in the one-loop approximation for the t–t'–t''–J^* model. In Section 4, an infinite set of self-consistent integral equations for the superconducting phase is derived. A simplification of this set for the d-type symmetry of the order parameter is given in Section 5, in which the computational algorithm for the superconducting transition temperature is derived. Normal components of the strength and self-energy operators are calculated in Section 6. The results of numerical calculations demonstrating the significant role of spin-fluctuation scattering processes reflected in the strength operator components are also given in this section. The main results of this study are discussed in concluding Section 7.

2. GOR'KOV EQUATIONS TAKING INTO ACCOUNT ANOMALOUS COMPONENTS OF THE STRENGTH OPERATOR

Let us analyze a modification of self-consistent equations for the superconducting phase, induced by taking into account the anomalous components of the strength operator in explicit form. The analysis will be carried out in the t–t'–t''–J^* model, which correctly reflects the strong correlation limit in the Hubbard model. In atomic approximation, the Hamiltonian of the t–t'–t''–J^* model can be written in the form [12]

$$H = \sum_{f\sigma}(\varepsilon-\mu)X_f^{\sigma\sigma} + \sum_{fm\sigma} t_{fm} X_f^{\sigma 0} X_m^{0\sigma}$$

$$+ \sum_{fm} J_{fm}(X_f^{+-}X_m^{-+} - X_f^{++}X_m^{--}) + \sum_{\substack{fmg\sigma \\ (f \neq g)}} \left(\frac{t_{fm}t_{mg}}{U}\right) \tag{1}$$

$$\times (X_f^{\sigma 0}X_m^{\bar{\sigma}\sigma}X_g^{0\bar{\sigma}} - X_f^{\sigma 0}X_m^{\bar{\sigma}\bar{\sigma}}X_g^{0\sigma}).$$

Here, X_f^{pq} are the Hubbard operators: $X_f^{0\sigma}$ ($X_f^{0\bar{\sigma}}$) describes the transition of an ion located at site f from an electron state with the spin momentum component σ ($\bar{\sigma} = -\sigma$) to a state without electrons, while $X_f^{\sigma 0}$ describes the reverse process. Single-site transitions associated with a change in the spin momentum component are reflected by operators X_f^{+-} and X_f^{-+}. Diagonal operators $X_f^{\sigma\sigma}$ and X_f^{00} are projection operators for one-electron and zero-electron sectors of the Hilbert subspace corresponding to site f. The energy of one-electron one-ion state is denoted by ε, μ is the chemical potential of the system, t_{fm} is the integral of electron hopping from site m to site f, and J_{fm} is the parameter of exchange coupling between electron states at sites m and f.

The first three terms of Hamiltonian (1) are known to correspond to the t–J model, while the last term ($H_{(3)}$) describes three-center interactions, which are sometimes referred to as correlated hoppings. Hamiltonian (1) can be derived from the Hubbard model in the strong electron correlation mode $|t_{fm}| \ll U$ if charge carrier concentration $n < 1$ [12]. The inclusion of $H_{(3)}$ is dictated by the fact that the effects induced by this component considerably influence the concentration dependence of superconducting transition temperature $T_c(n)$

[22]. Since the specific form of this dependence changes after the addition of hoppings between sites from remote coordination spheres, we will not confine our further analysis to the nearest neighbor approximation and assume that three hopping parameters (t, t', and t'') differ from zero. Such a model is often referred to as the t–t'–t''–J^* model (the asterisk indicates the presence of term $H_{(3)}$ in the interaction Hamiltonian). It should be noted that the need to take into account three-center interactions in analyzing the properties of the Hubbard model has been demonstrated recently by many authors (see, for example, [23]).

It is well known that traditional superconductors can be described using the Gor'kov equations connecting Green's functions with normal $\Sigma_{0\uparrow,0\uparrow}(\mathbf{k}, i\omega_n)$ and anomalous $\Sigma_{0\uparrow,\downarrow 0}(\mathbf{k}, i\omega_n)$ components of self-energy operator $\hat{\Sigma}(\mathbf{k}, i\omega_n)$. It was noted in the Introduction that anomalous components $P_{0\uparrow,\downarrow 0}(\mathbf{k}, i\omega_n)$ and $P_{0\downarrow,\uparrow 0}(\mathbf{k}, i\omega_n)$ of strength operator $\hat{P}(\mathbf{k}, i\omega_n)$ must also be taken into account in analyzing electron systems with strong correlations on the basis of the graphic form of perturbation theory. In this connection, we will briefly discus the changes in the equations for the superconducting phase, which are associated with the inclusion of anomalous components $P_{0\sigma,\bar{\sigma}0}(\mathbf{k}, i\omega_n)$ and $P_{\bar{\sigma}0,0\sigma}(\mathbf{k}, i\omega_n)$.

Let us introduce the Matsubara Green's functions in atomic representation [16]:

$$D_{\alpha\beta}(f\tau; g\tau') = -\langle T_\tau \tilde{X}_f^{\alpha}(\tau)\tilde{X}_g^{-\beta}(\tau')\rangle. \quad (2)$$

Here, α and β are a pair of indices for one-site states, e.g., $(0\,\sigma)$, $(\bar{\sigma}\;0)$, or $(+\,-)$. In this case, if $\beta = (p\;q)$, then $-\beta = (q\;p)$. Operator T_τ is the ordering operator in Matsubara time. The Hubbard operators on the right-hand side of definition (2) are taken in the "Heisenberg" representation with Matsubara time τ,

$$\tilde{X}_f^{\alpha}(\tau) = \exp(\tau H)X_f^{\alpha}\exp(-\tau H), \quad 0 < \tau < 1/T, \quad (3)$$

where T is the temperature of the system and H is its Hamiltonian.

To derive the Gor'kov equations, let us consider normal ($D_{0\sigma,0\sigma}$ and $D_{\bar{\sigma}0,\bar{\sigma}0}$) and anomalous ($D_{0\sigma,\bar{\sigma}0}$ and $D_{\bar{\sigma}0,0\sigma}$) Green's functions. For brevity, we introduce the matrix electron function

$$\hat{D}_\sigma(f\tau; g\tau') = \begin{bmatrix} D_{0\sigma,0\sigma}(f\tau; g\tau'), & D_{0\sigma,\bar{\sigma}0}(f\tau; g\tau') \\ D_{\bar{\sigma}0,0\sigma}(f\tau; g\tau'), & D_{\bar{\sigma}0,\bar{\sigma}0}(f\tau; g\tau') \end{bmatrix} \quad (4)$$

and define its Fourier transform $\hat{D}_\sigma(\mathbf{k}, i\omega_m)$:

$$\hat{D}_\sigma(f\tau; g\tau') = \frac{T}{N}\sum_{\mathbf{k},\,\omega_m}\exp\{i\mathbf{k}(\mathbf{R}_f - \mathbf{R}_g) - i\omega_m(\tau-\tau')\}\hat{D}_\sigma(\mathbf{k}, i\omega_m). \quad (5)$$

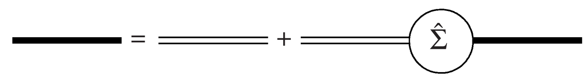
The graphic form for function $\hat{D}_\sigma(\mathbf{k}, i\omega_m)$ leads to the matrix relation

$$\hat{D}_\sigma(\mathbf{k}, i\omega_m) = \hat{G}_\sigma(\mathbf{k}, i\omega_m)\hat{P}_\sigma(\mathbf{k}, i\omega_m), \quad (6)$$

where $\hat{P}_\sigma(\mathbf{k}, i\omega_m)$ is the strength operator,

$$\hat{P}_\sigma(\mathbf{k}, i\omega_m) = \begin{bmatrix} P_{0\sigma,0\sigma}(\mathbf{k}, i\omega_m), & P_{0\sigma,\bar{\sigma}0}(\mathbf{k}, i\omega_m) \\ P_{\bar{\sigma}0,0\sigma}(\mathbf{k}, i\omega_m), & P_{\bar{\sigma}0,\bar{\sigma}0}(\mathbf{k}, i\omega_m) \end{bmatrix}, \quad (7)$$

and $\hat{G}_\sigma(\mathbf{k}, i\omega_m)$ is a function satisfying the Gor'kov equation



. (8)

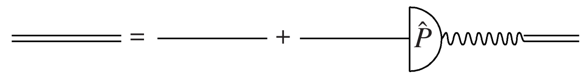
Here, the bold segment denotes the matrix Green function

$$\hat{G}_\sigma(\mathbf{k}, i\omega_m) = \begin{bmatrix} G_{0\sigma,0\sigma}(\mathbf{k}, i\omega_m), & G_{0\sigma,\bar{\sigma}0}(\mathbf{k}, i\omega_m) \\ G_{\bar{\sigma}0,0\sigma}(\mathbf{k}, i\omega_m), & G_{\bar{\sigma}0,\bar{\sigma}0}(\mathbf{k}, i\omega_m) \end{bmatrix}, \quad (9)$$

and symbol $\hat{\Sigma}$ inscribed in the circle denotes the matrix self-energy operator

$$\hat{\Sigma}_\sigma(\mathbf{k}, i\omega_m) = \begin{bmatrix} \Sigma_{0\sigma,0\sigma}(\mathbf{k}, i\omega_m), & \Sigma_{0\sigma,\bar{\sigma}0}(\mathbf{k}, i\omega_m) \\ \Sigma_{\bar{\sigma}0,0\sigma}(\mathbf{k}, i\omega_m), & \Sigma_{\bar{\sigma}0,\bar{\sigma}0}(\mathbf{k}, i\omega_m) \end{bmatrix}. \quad (10)$$

Double fine lines are juxtaposed to collective Green function $\hat{G}_\sigma^{(0)}(\mathbf{k}, i\omega_m)$ defined by the graphic equation



. (11)

The fine line correspond to the initial matrix Green function in atomic representation,

$$\hat{G}_0(i\omega_m) = \begin{bmatrix} 1/(i\omega_m - \varepsilon + \mu), & 0 \\ 0, & 1/(i\omega_m + \varepsilon - \mu) \end{bmatrix}, \quad (12)$$

while the semicircle with $\hat{P}$ is the strength operator introduced above, and the wavy line corresponds to the interaction operator

$$\hat{V}_\sigma(\mathbf{k}) = \begin{bmatrix} V_{0\sigma,0\sigma}(\mathbf{k}), & V_{0\sigma,\bar{\sigma}0}(\mathbf{k}) \\ V_{\bar{\sigma}0,0\sigma}(\mathbf{k}), & V_{\bar{\sigma}0,\bar{\sigma}0}(\mathbf{k}) \end{bmatrix} = \begin{pmatrix} t_{\mathbf{k}}, & 0 \\ 0, & -t_{\mathbf{k}} \end{pmatrix}. \quad (13)$$

Equations (8) and (11) can be written in analytic form

$$\begin{gathered} \hat{G}_\sigma(\mathbf{k}, i\omega_m) = \hat{G}_\sigma^{(0)}(\mathbf{k}, i\omega_m) \\ + \hat{G}_\sigma^{(0)}(\mathbf{k}, i\omega_m)\hat{\Sigma}_\sigma(\mathbf{k}, i\omega_m)\hat{G}_\sigma(\mathbf{k}, i\omega_m), \\ \hat{G}_\sigma^{(0)}(\mathbf{k}, i\omega_m) = \hat{G}_0(i\omega_m) \\ + \hat{G}_0(i\omega_m)\hat{P}_\sigma(\mathbf{k}, i\omega_m)\hat{V}_\sigma(\mathbf{k})\hat{G}_\sigma^{(0)}(\mathbf{k}, i\omega_m). \end{gathered} \quad (14)$$

It follows hence that

$$\begin{gathered} \hat{G}_\sigma(\mathbf{k}, i\omega_m) = \{\hat{G}_0^{-1}(i\omega_m) \\ - \hat{P}_\sigma(\mathbf{k}, i\omega_m)\hat{V}_\sigma(\mathbf{k}) - \hat{\Sigma}_\sigma(\mathbf{k}, i\omega_m)\}^{-1}. \end{gathered} \quad (15)$$

Considering that the anomalous components of both self-energy ($\Sigma_{0\sigma,\bar{\sigma}0}$) and strength ($P_{0\sigma,\bar{\sigma}0}$) operators differ from zero in the superconducting phase, we obtain from Eq. (15) the following expressions for Green's functions components $\hat{G}_\sigma(k, i\omega_m)$ that will be used in subsequent analysis:

$$\begin{gathered} G_{0\sigma,0\sigma}(\mathbf{k}, i\omega_m) \\ = \frac{i\omega_m + \varepsilon - \mu + t_k P_{\bar{\sigma}0,\bar{\sigma}0}(\mathbf{k}, i\omega_m) - \Sigma_{\bar{\sigma}0,\bar{\sigma}0}(\mathbf{k}, i\omega_m)}{\det(\mathbf{k}, i\omega_m)}, \\ G_{0\sigma,\bar{\sigma}0}(\mathbf{k}, i\omega_m) \\ = \frac{\Sigma_{0\sigma,\bar{\sigma}0}(\mathbf{k}, i\omega_m) - t_{\mathbf{k}} P_{0\sigma,\bar{\sigma}0}(\mathbf{k}, i\omega_m)}{\det(\mathbf{k}, i\omega_m)}, \end{gathered} \quad (16)$$

where

$$\begin{gathered} \det(\mathbf{k}, i\omega_m) = \{i\omega_m + \varepsilon - \mu + t_{\mathbf{k}} P_{\bar{\sigma}0,\bar{\sigma}0}(\mathbf{k}, i\omega_m) \\ - \Sigma_{\bar{\sigma}0,\bar{\sigma}0}(\mathbf{k}, i\omega_m)\} \\ \times \{i\omega_m - \varepsilon + \mu \\ - t_{\mathbf{k}} P_{0\sigma,0\sigma}(\mathbf{k}, i\omega_m) - \Sigma_{0\sigma,0\sigma}(\mathbf{k}, i\omega_m)\} \\ - \{\Sigma_{0\sigma,\bar{\sigma}0}(\mathbf{k}, i\omega_m) - t_{\mathbf{k}} P_{0\sigma,\bar{\sigma}0}(\mathbf{k}, i\omega_m)\} \\ \times \{\Sigma_{\bar{\sigma}0,0\sigma}(\mathbf{k}, i\omega_m) + t_{\mathbf{k}} P_{\bar{\sigma}0,0\sigma}(\mathbf{k}, i\omega_m)\}. \end{gathered} \quad (17)$$

It follows from these expressions that anomalous components $P_{0\sigma,\bar{\sigma}0}(\mathbf{k}, i\omega_m)$ of the strength operator are important for calculating anomalous thermodynamic averages. Indeed, taking into account relation (6), we obtain

$$\begin{gathered} D_{0\sigma,\bar{\sigma}0}(\mathbf{k}, i\omega_m) = G_{0\sigma,0\sigma}(\mathbf{k}, i\omega_m)P_{0\sigma,\bar{\sigma}0}(\mathbf{k}, i\omega_m) \\ + G_{0\sigma,\bar{\sigma}0}(\mathbf{k}, i\omega_m)P_{\bar{\sigma}0,\bar{\sigma}0}(\mathbf{k}, i\omega_m). \end{gathered} \quad (18)$$

Consequently, the expression for an anomalous one-time single-site mean is defined by two terms:

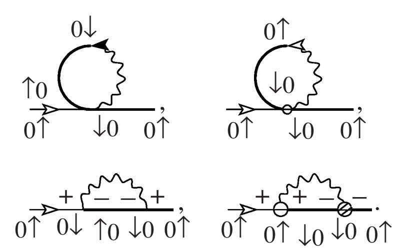
$$\begin{gathered} \langle X_f^{0\bar{\sigma}} X_f^{0\sigma} \rangle = \frac{T}{N}\sum_{\mathbf{k},\omega_m} \exp(i\omega_m\delta) \\ \times \left\{ \frac{\Sigma_{0\sigma,\bar{\sigma}0}(\mathbf{k}, i\omega_m)P_{\bar{\sigma}0,\bar{\sigma}0}(\mathbf{k}, i\omega_m)}{\det(\mathbf{k}, i\omega_m)} \right. \\ \left. + \frac{[i\omega_m + \varepsilon - \mu - \Sigma_{\bar{\sigma}0,\bar{\sigma}0}(\mathbf{k}, i\omega_m)]P_{0\sigma,\bar{\sigma}0}(\mathbf{k}, i\omega_m)}{\det(k, i\omega_m)} \right\} = 0, \\ \delta \longrightarrow +0. \end{gathered} \quad (19)$$

It can be seen that the anomalous average under investigation in strongly correlated systems is not a quantity proportional to only the anomalous component of the self-energy operator. In view of the presence of the anomalous component of the strength operator, an additional contribution (second term in the braces) appears. This means that the condition of vanishing (in accordance with the algebra of Hubbard operators) of the anomalous average considered here plays the role of an additional relation between normal and anomalous components of the self-energy and strength operators.

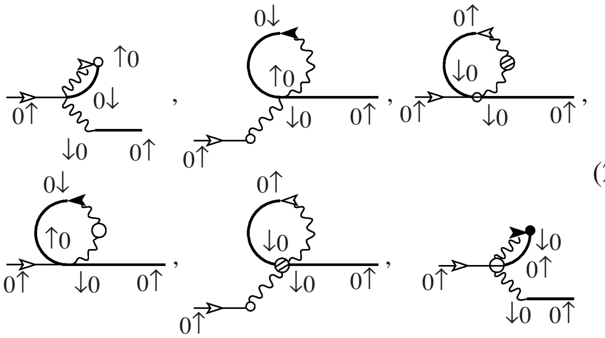
The above analysis shows that the description of the superconducting phase of Hubbard fermions must generally be based not on the single equation defining the anomalous self-energy operator, but on a system of equations which simultaneously define the anomalous components of the self-energy and strength operator.

3. ANOMALOUS COMPONENTS OF THE SELF-ENERGY AND STRENGTH OPERATORS IN THE ONE-LOOP APPROXIMATION

To derive explicit equations describing the superconducting phase, we will calculate anomalous quantities in the one-loop approximation. In this case, anomalous component $\Sigma_{0\uparrow,\downarrow 0}(\mathbf{k}, i\omega_m)$ of the self-energy operator is defined by ten diagrams. Four diagrams


(20)

are due to the interactions corresponding to the *t–J* model [10], while six diagrams



(21)

reflect the contributions from three-center interactions. The wavy lines with an arrow in diagrams (20) juxtapose hopping integral $t_{\mathbf{q}}$ in the momentum representation. The end of such a line with a light (dark) arrow forms a fragment of the diagram induced by operator $X_f^{0\uparrow}$ ($X_f^{0\downarrow}$). Wavy lines without arrows correspond to exchange integrals $J_{\mathbf{q}}$. In this case, the longitudinal interaction $J_{fm}X_f^{++}X_m^{--}$ is depicted by a wavy line with two large circles. The end with a light circle corresponds to the fragment of the diagram in which operator X_f^{++} participated in pairing. In this sense, the hatched circle corresponds to operator X_f^{--}. On the other hand, the transverse interaction $J_{fm}X_f^{+-}X_m^{-+}$ is juxtaposed to a wavy line with a sequence of two opposite values of the spin momentum projections indicated at its ends. This sequence unambiguously indicates one of the two operators participating in the description of the transverse interaction, the pairing with which induced the given fragment of the diagram. In diagrams (21), the matrix element of the three-center interaction in momentum representation corresponds to two wavy lines connected either by light (or hatched circle), or directly without a circle at an acute angle. The topological structure of the connection of the ends of such lines to fragments of diagrams is the same as for the interaction lines corresponding to hopping processes. The presence of a circle indicates that the diagonal operator participated in pairing during the application of the Wick theorem, while nondiagonal quasi-Bose operator $X_f^{\sigma\bar{\sigma}}$ participated in the case of connection at an angle.

Putting diagrams (20) and (21) in correspondence with analytic expressions, we obtain the components of the anomalous component of self-energy operator

$$\Sigma_{0\uparrow,\downarrow 0}^{(t-J)}(\mathbf{k}) = \frac{T}{N}\sum_{\mathbf{q},\,\omega_l}(t_{\mathbf{q}} + J_{\mathbf{k}-\mathbf{q}})\delta F(q),$$
$$\Sigma_{0\uparrow,\downarrow 0}^{(3)}(\mathbf{k}) = \frac{T}{N}\sum_{\mathbf{q},\,\omega_l}A_{\mathbf{k}}^{(3)}(\mathbf{q})\delta F(q), \tag{22}$$

where

$$A_{\mathbf{k}}^{(3)}(\mathbf{q}) = \left(1-\frac{n}{2}\right)\frac{2t_{\mathbf{k}}t_{\mathbf{q}}}{U}$$
$$-\left(1-\frac{n}{2}\right)J_{\mathbf{k}-\mathbf{q}} - \frac{n}{2}\left(\frac{2t_{\mathbf{q}}^2}{U} - J_0\right). \tag{23}$$

In formula (22), δF denotes the difference between anomalous Green's functions:

$$\delta F(q) = F_{\downarrow}(q) - F_{\uparrow}(q), \quad F_{\sigma}(q) = G_{0\sigma,\bar{\sigma}0}(q),$$
$$q \equiv (\mathbf{q}, i\omega_l), \quad \omega_l = (2l+1)\pi T. \tag{24}$$

Summing the components, we obtain the anomalous component of the self-energy operator,

$$\Sigma_{12}(\mathbf{k}) \equiv \Sigma_{0\uparrow,\downarrow 0}(\mathbf{k}) = \Sigma_{0\uparrow,\downarrow 0}^{(t-J)}(\mathbf{k}) + \Sigma_{0\uparrow,\downarrow 0}^{(3)}(\mathbf{k})$$
$$= \frac{T}{N}\sum_{\mathbf{q},\,\omega_m}A_{\mathbf{k}}(\mathbf{q})\delta F(q), \tag{25}$$

where

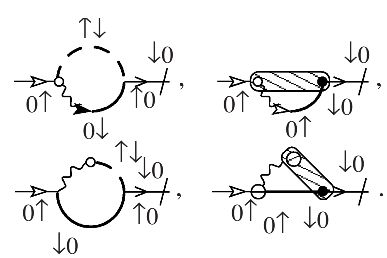
$$A_{\mathbf{k}}(\mathbf{q}) = t_{\mathbf{q}} + \frac{n}{2}J_{\mathbf{k}-\mathbf{q}}$$
$$+\left(1-\frac{n}{2}\right)\frac{2t_{\mathbf{k}}t_{\mathbf{q}}}{U} - \frac{n}{2}\left(\frac{2t_{\mathbf{q}}^2}{U} - J_0\right). \tag{26}$$

It can be seen that the coefficient of $J_{\mathbf{k}-\mathbf{q}}$ experienced the renormalization ($1 \longrightarrow 1-(1-n/2) = n/2$) obtained earlier using the method of irreducible Green's functions in [5]. It was shown in [22] that this renormalization is responsible for a decrease by more than an order of magnitude in the superconducting transition temperature of the superconducting phase with the $d_{x^2-y^2}$ symmetry of the order parameter.

Performing analogous calculations (with an obvious reversal of arrows and symbols denoting projections of spin moments and with the replacement of lines with light arrows by lines with dark arrows), we obtain the following relation that will be used below:

$$\Sigma_{0\uparrow,\downarrow 0}(\mathbf{k}) = -\Sigma_{0\downarrow,\uparrow 0}(\mathbf{k}). \tag{27}$$

Let us now calculate anomalous component $P_{0\uparrow,\downarrow 0}(k)$ of the strength operator. In the approximation used here, the interactions in the t–J model for this component make contributions defined by the following four diagrams:



(28)

Comparing the corresponding analytic expressions, we obtain

$$P^{(t-J)}_{0\uparrow,\downarrow0}(k) = -\frac{T}{N}\sum_q (t_{\mathbf{q}} + J_{\mathbf{q}-\mathbf{k}})\Lambda^{(a)}_{\uparrow}(q;\, q-k), \quad k \equiv (\mathbf{k}, i\omega_m), \quad q \equiv (\mathbf{q}, i\omega_l), \tag{29}$$

where $\Lambda^{(a)}_{\uparrow}(q,\, q-k)$ is defined by a combination of anomalous Green's functions with Fourier transforms of the Green's function of transverse ($D_\perp(q-k)$) and longitudinal ($D_\|(q-k)$) spin components, as well as Green's functions describing charge fluctuations ($C(q-k)$),

$$\Lambda^{(a)}_{\sigma}(q;\, q-k) = F_{\bar\sigma}(q)D_\perp(q-k) - F_\sigma(q) \times\left[D_\|(q-k) - \frac{1}{4}C(q-k)\right], \tag{30}$$

for $\sigma = \uparrow$. The Fourier transform of the Bose Green's function is defined in the conventional manner,

$$-\langle T_\tau \tilde{X}^{\uparrow\downarrow}_f(\tau)\tilde{X}^{\downarrow\uparrow}_g(\tau')\rangle$$

$$= \frac{T}{N}\sum_{\mathbf{q},\,\omega_s} \exp\{i[\mathbf{q}(\mathbf{R}_f - \mathbf{R}_g) - \omega_s(\tau-\tau')]\}D_\perp(\mathbf{q}, i\omega_s),$$

$$\omega_s = 2\pi sT,$$

$$-\langle T_\tau \tilde{S}^z_f(\tau)\tilde{S}^z_g(\tau')\rangle$$

$$= \frac{T}{N}\sum_{\mathbf{q},\,\omega_s} \exp\{i[\mathbf{q}(\mathbf{R}_f - \mathbf{R}_g) - \omega_s(\tau-\tau')]\}D_\|(\mathbf{q}, i\omega_s),$$

$$\omega_s = 2\pi sT,$$

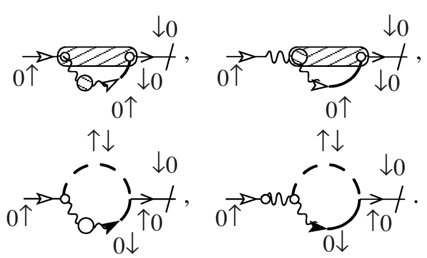
$$-\langle T_\tau \Delta\tilde{N}_f(\tau)\Delta\tilde{N}_g(\tau')\rangle$$

$$= \frac{T}{N}\sum_{\mathbf{q},\,\omega_s} \exp\{i[\mathbf{q}(\mathbf{R}_f - \mathbf{R}_g) - \omega_s(\tau-\tau')]\}C(\mathbf{q}, i\omega_s),$$

$$\omega_s = 2\pi sT.$$

In the last expression, $\Delta\tilde{N}_f(\tau) = \tilde{N}_f(\tau) - \langle N_f\rangle$, $\tilde{N}_f(\tau) = \tilde{X}^{\uparrow\uparrow}_f(\tau) + \tilde{X}^{\downarrow\downarrow}_f(\tau)$, where τ is the Matsubara time.

The following four diagrams define anomalous component $P^{(3)}_{0\uparrow,\downarrow0}(k)$ of the strength operator, which is associated with three-center interactions:



(31)

Their total analytic contribution is defined as

$$P^{(3)}_{0\uparrow,\downarrow0}(k) = -\frac{T}{2N}\sum_q A^{(3)}_{\mathbf{k}}(\mathbf{q})\Lambda^{(a)}_{\uparrow}(q;\, q-k), \quad k \equiv (\mathbf{k}, i\omega_m), \quad q \equiv (\mathbf{q}, i\omega_l). \tag{32}$$

Combining expressions (29) and (32), we obtain the complete form of the anomalous component of the strength operator,

$$P_{0\uparrow,\downarrow0}(k) = -\frac{T}{N}\sum_q B_{\mathbf{k}}(\mathbf{q})\Lambda^{(a)}_{\uparrow}(q;\, q-k), \quad k \equiv (\mathbf{k}, i\omega_m), \quad q \equiv (\mathbf{q}, i\omega_l), \tag{33}$$

where

$$B_{\mathbf{k}}(\mathbf{q}) = t_{\mathbf{q}} + \frac{1}{2}\left(1 + \frac{n}{2}\right)J_{\mathbf{k}-\mathbf{q}} + \left(1 - \frac{n}{2}\right)\frac{t_{\mathbf{k}}t_{\mathbf{q}}}{U} - \frac{n}{2}\left(\frac{t^2_{\mathbf{q}}}{U} - \frac{J_0}{2}\right). \tag{34}$$

It can be seen that kernel $B_{\mathbf{k}}(\mathbf{q})$ of the strength operator also contains the coefficient of $J_{\mathbf{k}-\mathbf{q}}$ renormalized by three-center interactions; however, in contrast to renormalization for $\Sigma_{0\uparrow,\downarrow0}(\mathbf{k})$, the renormalization for $P_{0\uparrow,\downarrow0}(\mathbf{k}, i\omega_m)$ is different:

$$1 \longrightarrow 1 - \frac{1}{2}\left(1 - \frac{n}{2}\right) = \frac{1}{2}\left(1 + \frac{n}{2}\right). \tag{35}$$

This means that if the contributions from the strength operator are taken into account, the description of the superconducting phase with the $d_{x^2-y^2}$ symmetry of the order parameter in the t–J^* model cannot be reduced to the description based on the t–J model, but with renormalized $J \longrightarrow \tilde{J} = (n/2)J$.

Another feature is associated with the dependence of $P_{0\uparrow,\downarrow0}(\mathbf{k}, i\omega_m)$ on the Matsubara frequency (anomalous component $\Sigma_{0\uparrow,\downarrow0}(\mathbf{k})$ of the self-energy operator depends only on the quasi-momentum). As a result, the superconducting phase in the approximation considered here is described by an infinite system of self-consistent integral equations.

4. SYSTEM OF SELF-CONSISTENT EQUATIONS FOR THE SUPERCONDUCTING PHASE

The derivation of self-consistent equations can be simplified using the symmetric combination of anomalous components of the strength operator:

$$P(k) = P_{0\uparrow,\downarrow0}(k) - P_{0\downarrow,\uparrow0}(k), \quad k \equiv (\mathbf{k}, i\omega_m).$$

The analytic expression for $P_{0\downarrow,\uparrow0}(k)$ can be derived from Eq. (33) by replacing $\Lambda^{a}_{\uparrow}(q;\, q-k)$ by $\Lambda^{(a)}_{\downarrow}(q;\, q-k)$. The validity of this statement can be verified using the diagram representation. It is advantageous to use $P(k)$ due to the fact that $P(k)$, as well as $\Sigma_{0\uparrow,\downarrow 0}(\mathbf{k})$, can be expressed in terms of difference $\delta F(q)$ between anomalous Green's functions. In this case, a symmetric combination of transverse and longitudinal spin Green's functions is formed [24, 25]:

$$P(k) = -\frac{T}{N}\sum_q B_{\mathbf{k}}(\mathbf{q})\Big[D_\perp(q-k) + D_\parallel(q-k) - \frac{1}{4}C(q-k)\Big]\delta F(q), \quad q \equiv (\mathbf{q}, i\omega_l). \tag{36}$$

Using the expressions for the anomalous components of the self-energy and strength operators, representation (16), and relation (27), we obtain a system of self-consistent equations in $\Sigma_{12}(\mathbf{k})$ and $P(\mathbf{k}, i\omega_m)$:

$$\Sigma_{12}(\mathbf{k}) = -\frac{T}{N}\sum_{\mathbf{q},\,\omega_l} A_{\mathbf{k}}(\mathbf{q})\frac{2\Sigma_{12}(\mathbf{q}) - t_{\mathbf{q}}P(\mathbf{q}, i\omega_l)}{\det(\mathbf{q}, i\omega_l)},$$

$$P(\mathbf{k}, i\omega_m) = -\frac{T}{N}\sum_{\mathbf{q},\,\omega_l} B_{\mathbf{k}}(\mathbf{q})\chi_C^-(\mathbf{q}-\mathbf{k}, i\omega_l - i\omega_m) \times \frac{2\Sigma_{12}(\mathbf{q}) - t_{\mathbf{q}}P(\mathbf{q}, i\omega_l)}{\det(\mathbf{q}, i\omega_l)}. \tag{37}$$

Introducing the spin–charge susceptibility

$$\chi_C^-(\mathbf{q}, i\omega_s) = -\Big[3D_\parallel(\mathbf{q}, i\omega_s) - \frac{1}{4}C(\mathbf{q}, i\omega_s)\Big], \tag{38}$$

we take into account the spherical symmetry of spin correlation functions [24, 25].

If we set $P(\mathbf{q}, i\omega_l) = 0$ in the first equation of the system and disregard the contributions to the normal components of the strength operators, which are functions of the Matsubara frequencies, we can carry out summation over ω_l. In this case, we arrive at the well-known equation defining the solutions for $\Sigma_{12}(\mathbf{k})$ in the superconducting phase in the mean-field approximation both for the *s*- and *d*-type symmetry of the superconducting order parameter. In fact, it can be seen from the second equation of system (37) that this case takes place only for $\chi_C^- \longrightarrow 0$. For finite values of χ_C^-, the self-consistent solution of the system is observed only for $P(\mathbf{q}, i\omega_l) \neq 0$, and the superconducting phase is described by an infinitely large number of integral equations defining $\Sigma_{12}(\mathbf{k})$ and $P(\mathbf{k}, i\omega_m)$. If we replace dynamic susceptibility χ_C^- by the static susceptibility, the equation for T_c for the *s* phase for $U = \infty$, which follows from system (37), has exactly the same form as in [26, 27]. It should be noted that the equation for T_c in these publications was derived from analysis of the scattering amplitude in the Cooper channel calculated in the paramagnetic phase taking into account scattering from spin fluctuations. This means that the inclusion of anomalous components of the strength operator in the one-loop approximation corresponds to the inclusion of spin-fluctuation scattering processes. The validity of this statement for the *d*-type symmetry of the order parameter can be demonstrated by introducing the anomalous Dyson self-energy operator, which is reducible in the Larkin sense (the self-energy operator irreducible in the Dyson sense is reducible in the Larkin sense [20]):

$$\Delta(\mathbf{k}, i\omega_m) = \Sigma_{12}(\mathbf{k}) - \frac{1}{2}t_{\mathbf{k}}P(\mathbf{k}, i\omega_m). \tag{39}$$

In this case, the system of self-consistent equations for $\Delta(\mathbf{k}, i\omega_m)$ can be written in the form

$$\Delta(\mathbf{k}, i\omega_m) = -\frac{T}{N}\sum_{\mathbf{q},\,\omega_l}\{2A_{\mathbf{k}}(\mathbf{q}) - t_{\mathbf{k}}B_{\mathbf{k}}(\mathbf{q})\chi_C^-(\mathbf{q}-\mathbf{k}, i\omega_l - i\omega_m)\}\frac{\Delta(\mathbf{q}, i\omega_l)}{\det(\mathbf{q}, i\omega_l)}. \tag{40}$$

The first term of the kernel of this integral equation corresponds to the mean field approximation. The second term defines the spin-fluctuation mechanism of Cooper pairing. Such a representation of the equations for the superconducting order parameter was introduced in [28] using the Hubbard diagram technique. Superconducting phases were described in [24] using the method of irreducible Green's functions in the *t–J* model taking into account the spin-fluctuation mechanism of pairing. It was also shown that the effect of spin fluctuations is reflected analytically in the emergence of a term containing the dynamic susceptibility in the integral kernel of the equation for the order parameter [24, 25]. In this connection, we must mention a series of publications based on the phenomenological approach to the spin-fluctuation mechanism of superconducting pairing in spin-fermion models (see, for example, [29, 30] and the literature cited therein). In these publications, only one term proportional to dynamic susceptibility is phenomenologically introduced into the kernel of the integral equation in the description of the superconducting phase. The multiplicative coefficients, which generally appear in the theory and are associated with the features of the model, are lost when this approach is used.

In our case, Eq. (40) was derived on the basis of the microscopic approach for the *t–J** model taking into account three-center interactions. It is significant that these interactions (e.g., for the *d*-type symmetry) renormalize the term corresponding to the mean-field approximation [5] in accordance with a certain scenario, while the multiplicative factor appearing in front of the susceptibility renormalizes it in accordance with a different scenario.

In the subsequent analysis, we will confine ourselves to the superconducting phase with the $d_{x^2-y^2}$ symmetry of the order parameter.

5. ALGORITHM FOR CALCULATING SUPERCONDUCTING TRANSITION TEMPERATURE

To solve the self-consistent equations, we must find function $\chi_C^-(\mathbf{q}, i\omega_m)$. Following [24], we will use the model approach, in which spin-charge susceptibility $\chi_C^-(\mathbf{q}, i\omega_m)$ can be represented by the product

$$\chi_{\text{mod}}(\mathbf{q}, i\omega_m) = \chi_s(\mathbf{q})\chi(i\omega_m); \tag{41}$$

as in [24], we assume that charge fluctuations can be neglected. The form of the model function can be determined by comparing with the susceptibility obtained in the generalized approximation of chaotic phases [10],

$$\begin{aligned}\chi_{\text{GRPA}}(\mathbf{k}, i\omega_l) &= -\Pi(\mathbf{k}, i\omega_l)\\ &\times\{[1-\Lambda(\mathbf{k}, i\omega_l)][1-Q(\mathbf{k}, i\omega_l)]-\Pi(\mathbf{k}, i\omega_l)\\ &\times[\Phi(\mathbf{k}, i\omega_l)+J(\mathbf{k})]\}^{-1},\end{aligned} \tag{42}$$

taking into account long-range hoppings (notation used here is the same as in [10]). Figure 1 shows the dependence of the susceptibility on the wavevector calculated using this formula for the following model parameters: $t' = 0.2|t|$, $t'' = 0.3|t|$, $J = 0.4|t|$, $n = 0.75$, $T = 0.03|t|$, and $\omega_m = 2\pi T$. It can be seen that a clearly manifested peak corresponding to experimental data is observed in the vicinity of point $\mathbf{q} = \mathbf{Q} = (\pi, \pi)$. Bearing this circumstance in mind, we will henceforth approximate the quasi-momentum dependence by the δ function:

$$\chi_s(\mathbf{q}) = 4\pi^2\delta(q-Q). \tag{43}$$

With such an approach, the dependence on the Matsubara frequency is correctly described by the function used in [24]. As a result, we obtain the following representation for susceptibility:

$$\begin{aligned}\chi_{\text{mod}}(\mathbf{q}, i\omega_m) &= \left(\frac{2\pi}{a}\right)^2\delta(q-Q)\frac{3n}{2\Omega}\\ &\times\tanh\left(\frac{\Omega}{2T}\right)\frac{1}{1-(i\omega_m/\Omega)^2}.\end{aligned} \tag{44}$$

The Matsubara susceptibility written in this form satisfies the sum rule:

$$T\sum_{\mathbf{q}, i\omega_m}\chi_{\text{mod}}(\mathbf{q}, i\omega_m) = \frac{3n}{4}. \tag{45}$$

Parameter Ω was chosen from the condition of the best coincidence of the peak height in the vicinity $\mathbf{q} = \mathbf{Q}$ at different Matsubara frequencies, i.e., from the equation

$$\begin{aligned}&\frac{1}{N}\sum_k\chi_{\text{GRPA}}(\mathbf{k}, i\omega_l)\\ &= n\Omega\tanh\left(\frac{\Omega}{2T}\right)\frac{1}{1-(i\omega_m/\Omega)^2} = \chi(i\omega_l).\end{aligned} \tag{46}$$

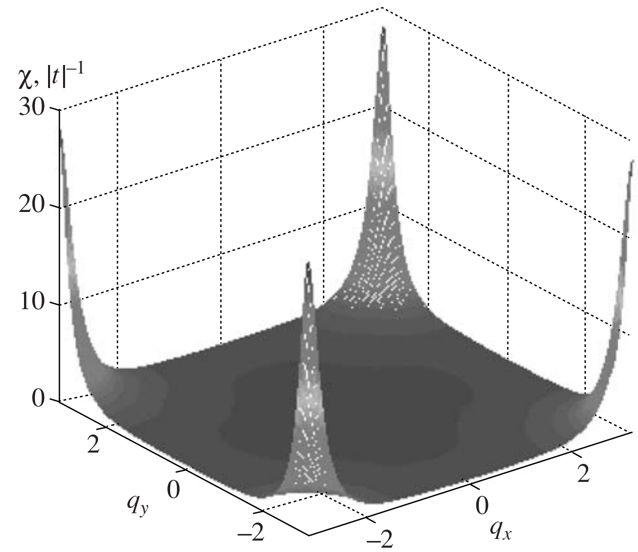


Fig. 1. Dependence of the transverse susceptibility component on quasi-momentum in the generalized random-phase approximation (GRPA).

It was found as a result of calculations that the best agreement is reached for $\Omega = 2|t|$.

We will solve system (37) taking into account electron hoppings between the sites lying within three coordination spheres. In this case, the Fourier transforms $t_{\mathbf{q}}$ and $J_{\mathbf{q}}$ can be written in the form ($t_1 \equiv t$, $t_2 \equiv t'$, $t_3 \equiv t''$)

$$t_{\mathbf{q}} = \sum_{n=1}^{3}4t_n\gamma_n(\mathbf{q}), \quad J_{\mathbf{q}} = \sum_{n=1}^{3}4J_n\gamma_n(\mathbf{q}), \tag{47}$$

where $\gamma_n(\mathbf{q})$ are invariants for the square mesh,

$$\gamma_1(\mathbf{q}) = \frac{1}{2}(\cos q_x + \cos q_y), \quad \gamma_2(\mathbf{q}) = \cos q_x \cos q_y,$$

$$\gamma_3(\mathbf{q}) = \frac{1}{2}(\cos 2q_x + \cos 2q_y).$$

For the $d_{x^2-y^2}$-type symmetry of the order parameter, contributions come only from J_1 and J_3. Considering that $J_3 = 2t_3^2/U$ and J_3 is smaller than J_1, we can confine the solution of the self-consistent equations only to the terms from the main invariant,

$$\begin{aligned}\Sigma_{12}(\mathbf{k}) &= \Delta(\cos k_x - \cos k_y),\\ P(\mathbf{k}, i\omega_l) &= P(i\omega_l)(\cos k_x - \cos k_y).\end{aligned} \tag{48}$$

In this case, the system of self-consistent equations can be reduced to the following equations for amplitudes Δ and $P(i\omega_l)$:

$$\left[\mathbf{1} + nJ_1T\sum_{\omega_l}a_{11}^{(0)}(i\omega_l)\right]\Delta$$

$$= \frac{nJ_1}{2}T\sum_{\omega_l} a_{11}^{(1)}(i\omega_l)P(i\omega_l),$$

$$P(i\omega_m) + 8\tilde{J}_1 T\sum_{\omega_l}\chi(i\omega_l - i\omega_m)a_{11}^{(0)}(i\omega_l)\Delta \tag{49}$$

$$= 4\tilde{J}_1 T\sum_{\omega_l}\chi(i\omega_l - i\omega_m)a_{11}^{(1)}(i\omega_l)P(i\omega_l),$$

where

$$\tilde{J}_1 = \frac{1+n/2}{2}J_1, \quad a_{11}^{(r)}(i\omega_m)$$
$$= \frac{1}{N}\sum_{\mathbf{q}}\frac{(\cos q_x - \cos q_y)^2}{\det(\mathbf{q}, i\omega_m)}(t_{\mathbf{q}})^r, \quad r = 0, 1. \tag{50}$$

At $T = T_c$, parameters Δ and $P(i\omega_l)$ vanish, but their ratio remains finite. Introducing function $\varphi(i\omega_l) = P(i\omega_l)/\Delta$ and setting $T = T_c$, we arrive at the system of nonhomogeneous equations

$$\varphi(i\omega_m^c) - 4\tilde{J}_1 T\sum_{\omega_l^c}\chi(i\omega_l^c - i\omega_m^c)a_{11}^{(1)}(i\omega_l^c)\varphi(i\omega_l^c)$$
$$= -8\tilde{J}_1 T_c\sum_{\omega_l}\chi(i\omega_l^c - i\omega_m^c)a_{11}^{(0)}(i\omega_l), \tag{51}$$

which are used for determining $\varphi(i\omega_l)$. Superscript "c" on the Matsubara frequencies indicates that the temperature appearing in their definition is equal to the superconducting transition temperature.

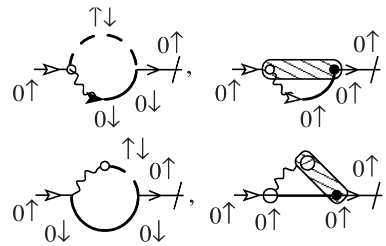
The closing equation can be written in the form of the sum rule following directly from system (49):

$$T_c\sum_{\omega_m^c}\varphi(i\omega_m^c) = 3\left(1+\frac{n}{2}\right). \tag{52}$$

Equations (51) and (52) were used in numerical calculations for determining the concentration dependence of superconducting transition temperature.

6. NORMAL COMPONENTS OF SELF-ENERGY AND STRENGTH OPERATORS. SUPERCONDUCTING TRANSITION TEMPERATURE

The effect of normal components $\Sigma_{11}(k) \equiv \Sigma_{0\uparrow,0\uparrow}(k) = \Sigma_{0\downarrow,0\downarrow}(k)$ and $P_{11} \equiv P_{0\uparrow,0\uparrow} = P_{0\downarrow,0\downarrow}(k)$ ($k \equiv (\mathbf{k}, i\omega_m)$) of the self-energy and strength operators on the conditions of realization of the superconducting phase will be considered in the same one-loop approximation. Separating the correction corresponding to the Hubbard I approximation in explicit form ($P_{11} = 1 - n/2 + \delta P_{11}(k)$), we find that correction $\delta P_{11}^{(tJ)}(k)$ associated with interactions in the t–J model is defined by four diagrams,



(53)

and can be represented analytically, taking into account the independence of normal Green's functions (in zero magnetic field) of the projection of spin angular momentum, in the form

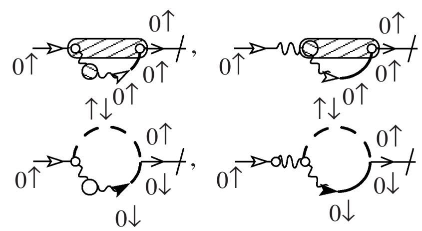
$$\delta P_{11}^{(tJ)}(k) = \frac{T}{N}\sum_q (t_{\mathbf{q}} + J_{\mathbf{q}-\mathbf{k}})G(q)\chi_C^+(q),$$
$$k \equiv (\mathbf{k}, i\omega_m), \quad q \equiv (\mathbf{q}, i\omega_l), \tag{54}$$

where

$$\chi_C^+(\mathbf{q}, i\omega_s) = -\left[3D_\parallel(\mathbf{q}, i\omega_s) + \frac{1}{4}C(\mathbf{q}, i\omega_s)\right],$$
$$\omega_s = 2\pi sT. \tag{55}$$

Here, as before, the spherical symmetry of spin correlation functions is taken into account. Normal component $G_{0\sigma,0\sigma}(q)$ of the Green function, in which spin indices are omitted, is denoted by $G(q)$.

The contribution to the normal component of the strength operator, which is associated with three-center interactions, is defined by the following four diagrams:



(56)

This contribution can be represented analytically in the form

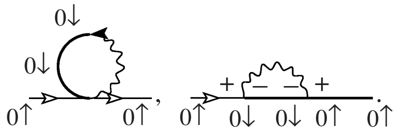
$$\delta P_{11}^{(3)}(k) = \frac{T}{2N}\sum_q A_{\mathbf{k}}^{(3)}(\mathbf{q})G(q)\chi_C^+(q-k),$$
$$k \equiv (\mathbf{k}, i\omega_m), \quad q \equiv (\mathbf{q}, i\omega_l). \tag{57}$$

Summing expressions (54) and (57), we derive the following analytic expression for the total correction:

$$\delta P_{11}(k) = \frac{T}{N}\sum_q B_{\mathbf{k}}(\mathbf{q})G(q)\chi_C^+(q-k),$$
$$k \equiv (\mathbf{k}, i\omega_m), \quad q \equiv (\mathbf{q}, i\omega_l). \tag{58}$$

As in the case of the anomalous component, three-center interactions renormalize the coefficient of $J_{\mathbf{k}-\mathbf{q}}$ appearing in the expression for $B_{\mathbf{k}}(\mathbf{q})$ in accordance with rule (35). The normal component of the strength operator in this approximation is a complex-valued quantity. To find this component in explicit form, we must use representation (16) obtained for Green's functions. This leads to a system of integral equations, which was solved numerically. Since representation (16) also contains the normal components of the self-energy operator, we will briefly consider the calculation of these components.

The contribution to the normal component Σ_{11} of the self-energy operator due to interactions in the *t–J* model is defined by the following two diagrams:

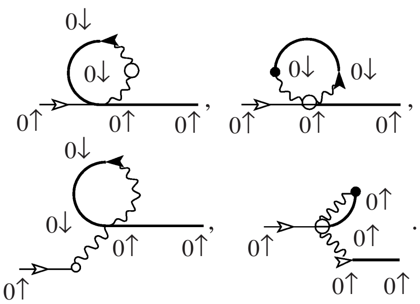


(59)

The corresponding analytic expression has the form

$$\Sigma_{11}^{(tJ)}(\mathbf{k}) = -\frac{T}{N}\sum_{\mathbf{q},\,\omega_l}(t_{\mathbf{q}} + J_{\mathbf{k}-\mathbf{q}})G(\mathbf{q}, i\omega_m) \times \exp(i\omega_l\delta), \quad \delta \longrightarrow +0. \tag{60}$$

The effect of three-center interactions on the correction to the normal component of the self-energy operator is defined by four diagrams:



(61)

In analytic form, we can write

$$\Sigma_{11}^{(3)}(\mathbf{k}) = \frac{T}{N}\sum_{\mathbf{q},\,\omega_l}\left\{(1-n)\left(\frac{J_0}{2} - \frac{t_{\mathbf{q}}^2}{U}\right) + \left(1-\frac{n}{2}\right)\left(J_{\mathbf{k}-\mathbf{q}} - \frac{2t_{\mathbf{k}}t_{\mathbf{q}}}{U}\right)\right\}G(\mathbf{q}, i\omega_l)\exp(i\omega_l\delta). \tag{62}$$

Using these expressions we obtain the total normal component of the self-energy operator:

$$\Sigma_{11}(\mathbf{k}) = -\frac{T}{N}\sum_{\mathbf{q},\,\omega_l}\left\{t_{\mathbf{q}} + \frac{n}{2}J_{\mathbf{k}-\mathbf{q}} + (2-n)\frac{t_{\mathbf{k}}t_{\mathbf{q}}}{U} + (1-n)\left(\frac{t_{\mathbf{q}}^2}{U} - \frac{J_0}{2}\right)\right\}G(\mathbf{q}, i\omega_l)\exp(i\omega_l\delta). \tag{63}$$

Substituting expression (44) for the model susceptibility, we obtain a simplified system of equations for calculating the normal components of the strength and self-energy operators (the terms leading to renormalization of chemical potential are omitted):

$$\delta P_{11}(\mathbf{k}, \omega_m) = T\sum_{i\omega_l}(t_{\mathbf{k}+\mathbf{Q}} - 4\tilde{J}_1)\chi(i\omega_l - i\omega_m) \times \left\{i\omega_l - \varepsilon + \mu - t_{\mathbf{k}+\mathbf{Q}} \times \left[\left(1-\frac{n}{2}\right) + \delta P_{11}(\mathbf{k}+\mathbf{Q}, \omega_l)\right] + \Sigma_{11}(\mathbf{k})\right\}^{-1}, \tag{64}$$

$$\Sigma_{11}(\mathbf{k}) = -\gamma_1(\mathbf{k})\frac{nT}{2N}\sum_{\mathbf{q},\,\omega_l}J_{\mathbf{q}}\left\{i\omega_l - \varepsilon + \mu - t_{\mathbf{q}}\left[\left(1-\frac{n}{2}\right) + \delta P_{11}(\mathbf{q}, \omega_l)\right] - \Sigma_{11}(\mathbf{q})\right\}^{-1}.$$

In the numerical solution of these equations, we also used the equation for chemical potential, which was written taking into account the renormalizations associated with contributions Σ_{11} and P_{11}:

$$\frac{n}{2} = \frac{T}{N}\sum_{q,\,\omega_m}e^{i\omega_m\delta} \times \frac{P_{11}(\mathbf{q}, i\omega_m)}{i\omega_m - \varepsilon + \mu - P_{11}(\mathbf{q}, i\omega_m)t_{\mathbf{q}} - \Sigma_{11}(\mathbf{q})}, \quad \delta \longrightarrow +0. \tag{65}$$

Here, in the summation over Matsubara frequencies, we used the self-consistently determined dependence $P_{11}(\mathbf{q}, i\omega_m)$.

By way of example, Fig. 2 shows the results of numerical calculations for the imaginary and real parts of the strength operator for the following set of variables: $t' = -0.1|t|$, $t'' = -0.1|t|$, $J = 0.4|t|$, $n = 0.8$, and $T = 0.01|t|$. The features of the dependence of P_{11} on ω_m remain qualitatively the same upon variation of the model parameters. It can be seen that P_{11} is a strongly varying function of the Matsubara frequency in the range $|\omega_m| \le 40|t|$. For $|\omega_m| \gg |t|$, the imaginary part of P_{11} rapidly decreases to zero, while the real part tends to the value corresponding to the Hubbard I approximation (i.e., $P_{11} \longrightarrow 1 - n/2$). Consequently, in the range of frequencies commensurate with the absolute value of the hopping integral, we must take into account the difference between P_{11} and the simplest Hubbard I approximation.

After self-consistent calculation of the normal and anomalous components of the self-energy and strength operators, we calculated the concentration dependences of the superconducting transition temperature using Eq. (52). Figure 3 shows the dependences of T_c on electron concentration n, which were obtained using two

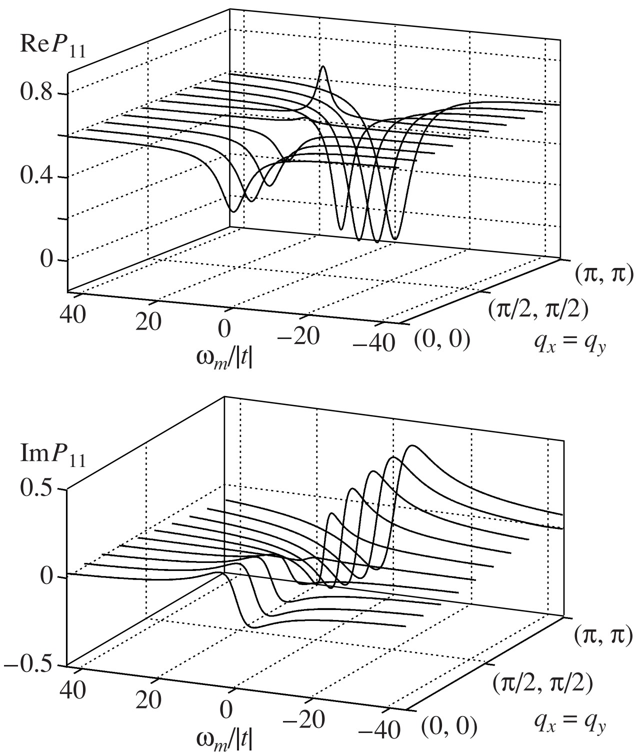


Fig. 2. Dependences of the real and imaginary parts of normal components of the strength operator on the Matsubara frequency and wavevector.

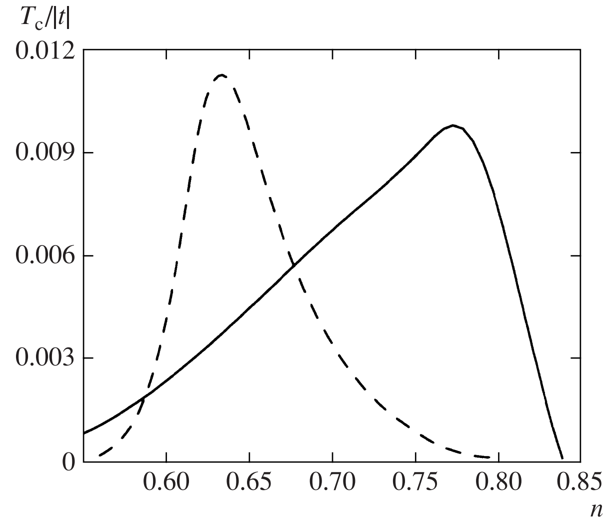


Fig. 3. Dependence of superconducting transition temperature T_c on electron concentration n.

approximations for the following values of parameters: $t' = -0.1|t_1|$, $t'' = -0.1|t_1|$, and $J_1 = 0.4|t_1|$. The dashed curve shows the dependence corresponding to the mean field approximation, while the solid curve is obtained taking into account the components of dynamic processes of spin-fluctuation scattering. The parameters were chosen in such a way that the value of concentration at the peak of the curve corresponded to the optimal doping level. It can be seen from the figure that the inclusion of strength operator components noticeably modifies the shape of the concentration dependence. For instance, the point corresponding to the peak on concentration dependence $T_c(n)$ is displaced to the range of higher electron concentrations and is in the best conformity with experimental data. Thus, the conditions for the formation of the superconducting phase with the d-type symmetry of the order parameter noticeably change when spin-fluctuation scattering is taken into account. It should be noted that in a certain range of parameters, the mean field approximation gives a qualitatively satisfactory agreement with experimental data. At the same time, the inclusion of spin-fluctuation scattering processes radically changed the range in which the superconducting phase under investigation was formed. In particular, not only the displacement of the concentration dependence took place, but the superconducting transition temperature became noticeably lower. We do not consider here such dependences because of the lack of practical interest and limited volume of this article. It should be noted, however, that such results emphasize one again the limitations of the mean field approximation and the important role of spin-fluctuation scattering processes, which are reflected in the approach used here in the normal and anomalous components of the self-energy and strength operators.

7. CONCLUSIONS

The results of calculations presented in this article demonstrate that the superconducting phase of strongly correlated electrons (Hubbard fermions) can be described by a system of self-consistent equations containing a new element, viz., the anomalous component $P_{0\sigma,\bar{\sigma}0}(\mathbf{k}, i\omega_m)$ of the strength operator. The inclusion of this quantity not only modifies the formal structure of the self-consistent equations, but also considerably affects the concentration dependence of the superconducting transition temperature to the phase with the $d_{x^2-y^2}$-type symmetry of the order parameter. In this connection, we formulate the following conclusions.

(1) In this study, we have analyzed only the d-type symmetry of the superconducting phase. The solution for a superconducting phase with the s-type symmetry can also be obtained from the system of self-consistent equations presented here. In particular, the equation for the superconducting transition temperature following from this system coincides with the corresponding equations derived earlier in [26, 27], where the scattering amplitude in the Cooper channel was analyzed. In these publications, a significant role of spin-fluctuation scattering in the computation of T_c was noted. The coincidence of the equations for T_c derived from analysis of the scattering amplitude in the paramagnetic phase and

on the basis of equations in the superconducting phase confirms the regulation concerning the inclusion of physically equivalent processes described by different analytic constructions. An analogous coincidence is also observed for the *d*-type symmetry of the order parameter.

(2) The inclusion of three-center interactions and long-range hoppings is due to the following factors. First, three-center interactions considerably affect the superconducting transition temperature even in the mean field approximation [22]. In [23], these interactions were taken into account. On the other hand, the inclusion of long hoppings affects both the form of the equation for T_c [31], and the value of charge carrier concentration, for which the highest superconducting transition temperature is observed. The above analysis of the role of spin-fluctuation scattering shows that the simultaneous inclusion of three-center interactions and electron hoppings between the sites lying within three coordination spheres is important for interpreting experimental data. It should be emphasized that three-center interaction renormalize the coupling constant in the expressions for components of the self-energy and strength operator in different manners. This circumstance becomes important for the following reason. If we disregard the corrections to the strength operator, the role of three-center interactions for the *d* phase is reduced to the substitution of the effective parameter for the exchange parameter. However, since the renormalization in the strength operator is different, the consistent inclusion of three center interactions cannot be reduced to a renormalization of the coupling constant.

(3) The form of self-consistent equations is modified due to only anomalous components of the strength operator, while the normal components of this operator were also found to be significant for calculating specific values of superconducting transition temperature. Thus, spin-fluctuation processes in the theory of the superconducting phase in the one-loop approximation are reflected in anomalous and normal components of the strength operator. In this case, the problem of computation of magnetic susceptibility becomes of considerable importance. In this study, peculiar features of this function were determined from a comparison with the susceptibility calculated earlier [10] in the generalized random-phase approximation (GRPA).

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