High-temperature superconductivity and normal state in the Holstein-t-J model

E.E. Zubov

O.O. Galkin Institute for Physics and Engineering NASU
72, R. Luxemburg Str., Donetsk, 83114, Ukraine
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I. INTRODUCTION

In the 21st century a phenomenon of the high-temperature superconductivity in cuprates continues to attract the attention of many researches [1]. There are a tremendous number of suggested mechanisms of this phenomenon. In any case there is not a such theory which would describe all properties of this complicated state. In this work we have centered on the main peculiarity which in our opinion might help to illuminate the origin of high-T \textsubscript{SC} in cuprates. The electron-phonon coupling is supposed to be not essential in the Cooper electron pairings. But this interaction forms the polaron excitations which play an important role in the correlation narrowing of the electron band. In that case it is necessary to differentiate the collectivized electrons in metals and ones in doped cuprates. Indeed, in metals there is wave electron states with a possibility of the site double occupancy. But their hole states is virtual. And that’s why we have the partition function \( \exp(\varepsilon_{k\sigma}/T) + \exp(\varepsilon_{-k\sigma}/T) \) for electron excitations \( \varepsilon_{k\pm\sigma} \). In cuprates a coordinate representation is realized for electron wave functions and we have the partition function \( 1 + \exp(\varepsilon_{\sigma}/T) + \exp(\varepsilon_{-\sigma}/T) \) with electron levels \( \varepsilon_{\pm\sigma} \) and hole state.

The cuprates belong to class of the strongly correlated electron system. In work [2] an effective Hamiltonian of the t-J model was suggested based on the use of Gutzwiller projection operator. It allowed to exclude the upper Hubbard band with double site occupancy by electrons and essentially to simplify an investigation of the strongly correlated electron systems. In work [3] a mean field approximation of the t-J model was developed to study the high-temperature superconductivity. In this work a fundamental idea about spin pairing via electron exchange interaction was formulated. Unfortunately, authors were not taken into account the essential difference between metal and strongly correlated electrons. Using Bogolyubov’s u-v transform of the Hamiltonian they obtained the equation for gap function to be similar in BCS theory.

In this work we propose to divide the mean field BCS type Hamiltonian into uniform and nonuniform parts. The perturbation theory was built with uniform unperturbed Hamiltonian. The nonuniform part is neglected since it has a weak influence on the hopping integral. A hopping term of the total t-J Hamiltonian is considered as perturbation in the limit of a weak doping with \( u-v \) transformed creation and destruction operators. The anormal mean values to be proportional the superconducting gap function were calculated. It has been obtained the condition on values of the chemical potential and exchange parameter. With account of the correlation band narrowing we make the conclusion about impossibility of HTSC in the pure t-J model.

In what follow we include into consideration the electron-phonon interaction. The evidences for a presence of one and its important role in the strongly correlated systems was emphasised in works [4–6]. In view of the fact that Hamiltonian of electron-phonon coupling is nonuniform many authors simplify the kinematic part by simple renormalization of the hopping integral [6] or use the theory of Eliashberg for collectivized metal electrons [4]. In former case it gives rise to drastic supression of the electron band and is responsible for the absence of HTSC in a system without interaction of polarons. The simplest form of the Holstein Hamiltonian for polarons needs to be considered with uniform electron-phonon interaction and Einstein phonon mode. One can provide the exact unitary transform to separate fermion and boson degree of freedom. It allows to build the subsequent perturbation theory of the strongly correlated electron system with Holstein’s polarons.

The structure of the paper is as follows. In Sec.II we consider the Hamiltonian of pure t-J model in the superconducting state. It was separated the uniform mean field part with correpsonding coefficients of u-v transform. It enables us in Sec.III to build the perturbation theory for strongly correlated electrons in the superconducting state. In particular, it was obtained the transformed Hubbard operators in coordinate representation using the Bogolyubov’s u-v transform. As a result, the equation for gap function and conditions for superconducting
state were presented. In Sec. IV the properties of normal state without electron-phonon coupling are considered. In the framework of the developed diagrammatic method it was shown the absence of superconductivity in a pure t-J model. In Sec.V, a normal state of the cuprate d-electrons with polaron excitations is investigated to find the critical temperature of superconducting state. In this section it has been solved the problem of a frequency summation with infinity number of poles as implicit functions. The suggested method of an inverse function allowed to calculate the diagrammatic contributions for all polaron bands. In Sec.V the obtained equations are solved numerically that allowed to find the concentration dependences of the critical temperature \( T_{SC} \) and gap function \( \Delta \) versus temperature. The theoretical values of \( T_{SC} \) and \( \Delta \) are in good agreement with experiment that supports the model to put forward by us.

II. HAMILTONIAN OF THE SYSTEM

The Hamiltonian of the Holstein model with strongly correlated electrons takes the form:

\[
\hat{H} = \hat{H}_f + \hat{H}_b, \tag{1}
\]

where the Fermi part, \( \hat{H}_f \), is expressed as follows:

\[
\hat{H}_f = \sum_{i,j} J_{ij} \left( S_i S_j - \frac{1}{4} n_i n_j \right) - \mu \sum_{i} n_{i\sigma} + \hat{V} \tag{2}
\]

Here, \( J_{ij} \) is the indirect exchange of the collectivized d-electrons with spins \( S_i \) and \( S_j \), \( n_i = n_{i\sigma} + n_{i-\sigma} \) is the electron concentration on \( i \)-site, \( \mu \) is the chemical potential. The perturbation \( \hat{V} \) is written as

\[
\hat{V} = \sum_{i,j,\sigma} v_{ij} c^+_i c_j (1 - n_{i-\sigma})(1 - n_{j-\sigma}), \tag{3}
\]

where \( c^+_i (c_i) \) creates (annihilates) an electron of spin \( \sigma \) on lattice site \( i \) and \( v_{ij} \) is the hopping integral to be equal to \( t \) for nearest neighbours. The Hamiltonian \( \hat{H}_f \) of t-J model reflects the strong electron correlations. In a weak doping level we will consider the part \( \hat{H}_b \) as a perturbation.

The boson part of Hamiltonian \( \hat{H}_b \) has a form similar to that used in the Holstein model of a small polaron:

\[
\hat{H}_b = -\frac{g}{2} \sum_{i} n_i (b_i^+ + b_i) + \omega_0 \sum_{i} b_i^+ b_i, \tag{4}
\]

where \( g \) is the electron-phonon coupling strength, \( b_i^+ \) and \( b_i \) are the phonon creation and destruction operators. We will use the Einstein model where the phonon frequency \( \omega_0 \) is assumed to be dispersion-free.

The Lang-Firsov unitary transform \( \tilde{U} = \exp \left( \hat{S} \right) \) of Hamiltonian \( \hat{H}_b \) allows to separate the boson and fermion operators in \( \hat{H}_b \), where \( \tilde{S} = -\frac{g}{2} \sum_{i} n_i (b_i^+ - b_i) \).

As a result we have

\[
\hat{H}_b = \tilde{U}^{-1} \hat{H}_b \tilde{U} = \omega_0 \sum_{i} b_i^+ b_i - \xi \sum_{i} n_i, \tag{5}
\]

where \( \xi = g^2 / \omega_0 \) is the polaron binding energy. The unitary transformed perturbation \( \tilde{V} \) is presented as

\[
\tilde{V} = \sum_{<ij>,\sigma} t_{ij} \tilde{c}^+_i \tilde{c}_j (1 - n_{i-\sigma})(1 - n_{j-\sigma}), \tag{6}
\]

Here, the unitary transformed Fermi operators

\[
\tilde{c}_{i\sigma} = Y_{i\sigma} c_{i\sigma} \tag{7}
\]

are product of Bose \( Y_i = e^{H(b_i^+ - b_i)} \) and corresponding Fermi destruction operators, where \( \lambda = g / \omega_0 \). It is necessary to point out that first and second terms of the Hamiltonian \( \hat{H}_b \) are not changed under transform \( \tilde{U} \).

One can separate in a Heisenberg part of the Hamiltonian \( \hat{H}_f \) by standard manner a mean field to be connected with anomalous averages \( \tilde{\mu} \). Then an unperturbed Hamiltonian takes the form

\[
\hat{H}_0f = \sum_{<ij>,\sigma} \{ \Delta_{ij\sigma} c^+_{i\sigma} c_{j-\sigma}^{\sigma} + \Delta_{ij\sigma}^* c_{i-\sigma} c_{j\sigma} \} - \sum_{i\sigma} \tilde{\mu}_{i\sigma} n_{i\sigma}, \tag{8}
\]

where \( \tilde{\mu}_{i\sigma} = \bar{\mu} - \sigma J(0) < S_z >, \) \( \bar{\mu} = \mu + \xi, < S_z > \) is a mean electron spin and \( \sigma = \pm 1 \). The gap functions are expressed via exchange parameters:

\[
\Delta_{ij\sigma} = -J_{ij} < c_{i\sigma} c_{j-\sigma} >, \quad \Delta_{ij\sigma}^* = -J_{ij} < c_{i-\sigma}^+ c_{j\sigma}^+ > \tag{9}
\]

In a wave space the Hamiltonian \( \hat{H}_0f \) takes the form

\[
\hat{H}_0f = \sum_{k\sigma} \{ \Delta_{k\sigma} c^+_{k\sigma} c_{-k-\sigma}^{\sigma} + \Delta_{k\sigma}^* c_{-k-\sigma} c_{k\sigma} \} - \sum_{k\sigma} \tilde{\mu}_{k\sigma} n_{k\sigma}, \tag{10}
\]

where the gap functions \( \Delta_{k\sigma} \) can be presented as

\[
\Delta_{k\sigma} = -\frac{1}{N} \sum_{q} J(q + k) < c_{q-\sigma} c_{q\sigma} > \tag{11}
\]

de and \( \Delta_{k\sigma}^* \) is conjugate function \( \Delta_{k\sigma} \). One can point out that in Eqs. \( \hat{H}_0f \) and \( \hat{H}_f \) the operators of creation and destruction are not transformed by operator \( Y_i \) from \( \hat{V} \).

The Bogolyubov’s u-v transform

\[
c_{k\sigma} = u_{k\sigma} \alpha_{k\sigma} + u_{k\sigma}^* \alpha_{-k-\sigma}^+, \quad c^+_{k\sigma} = u_{k\sigma}^* \alpha_{k\sigma} + u_{k\sigma} \alpha_{-k-\sigma}^- \tag{12}
\]

to new operators \( \alpha_{k\sigma} \) and \( \alpha_{-k-\sigma}^- \) allows to diagonalize \( \hat{H}_0f \) with the next conditions

\[
u_{k\sigma} = -v_{-k-\sigma}, \quad |u_{k\sigma}|^2 + |v_{k\sigma}|^2 = 1 \tag{13}
\]
Then we have

$$\hat{H}_{0f} = \sum_{k\sigma} \hat{E}_{k\sigma} \alpha_{k\sigma}^+ \alpha_{k\sigma}, \quad (14)$$

where

$$\hat{E}_{k\sigma} = -\tilde{\mu} \sqrt{1 + \left(\frac{\Delta_k}{\tilde{\mu}}\right)^2} \quad (15)$$

In what follows we will consider a paramagnetic state when $< S^z > = 0$. Then one can put

$$\tilde{\mu}_\sigma = \tilde{\mu}, \quad |\Delta_{k\sigma}| = |\Delta_{-k-\sigma}| = \Delta_k \quad (16)$$

So far it has been obtained that the BCS Hamiltonian coincides with similar Hamiltonian of Baskaran-Zou-Anderson. Unfortunately, the authors of work do not separate perturbation $\hat{V}$ from $\hat{H_0}$. Instead of this they narrow band multiplying the hopping integral $t$ by factor $x$ to be equal to hole concentration. It does not allow to find the rigorous statement relatively an appearance of the superconductivity since the band energy at $x \approx 0$ has finite quantity. That’s why we will expand Eq. (14) in terms of the small parameter up to third order:

$$\hat{E}_{k\sigma} = -\tilde{\mu} \left\{1 + \frac{\Delta_k^2}{2 \tilde{\mu}^2} - \frac{\Delta_k^4}{8 \tilde{\mu}^4} + \frac{\Delta_k^6}{48 \tilde{\mu}^6} - \ldots\right\} \quad (17)$$

Apparently, the corrections to chemical potential in Eq. (17) will produce the additional nonuniform part $\Delta H$ to perturbation $\hat{V}$ from (3) in the coordinate space:

$$\Delta H = \sum_{ij} \delta t_{ij} \alpha_{i\sigma}^+ \alpha_{j\sigma}, \quad (18)$$

where

$$\delta t_{ij} \approx \frac{1}{N} \sum_k \left\{-\frac{\Delta_k^2}{2 \tilde{\mu}^2} + \frac{\Delta_k^4}{8 \tilde{\mu}^4} - \frac{\Delta_k^6}{48 \tilde{\mu}^6}\right\} e^{i(k \cdot R_j - R_i)} \quad (19)$$

In what follows our consideration is limited by the square lattice and s- or d- symmetry of order parameter $\Delta_k = \Delta (\cos k_x a \pm \cos k_y a)$. In (17) we will extract one site part of $\Delta H_1$:

$$\Delta H_1 = \sum_{ij} \delta t_{ij} \alpha_{i\sigma}^+ \alpha_{i\sigma} \quad (20)$$

The rest $\Delta H_2$ of (18) may be presented as

$$\sum_{i \neq j} \delta t_{ij} < \alpha_{i\sigma}^+ \alpha_{j\sigma}> + \sum_{i \neq j} \delta t_{ij} \alpha_{i\sigma}^+ \alpha_{j\sigma}^- - \sum_{i \neq j} \delta t_{ij} < \alpha_{i\sigma}^+ \alpha_{j\sigma}> \quad (21)$$

The first term of (21) is a nonoperator part and last two are connected with correlation corrections to superconducting state. In our mean field theory this corrections are not considered.

Therefore, we have

$$\Delta H = \Delta H_1, \quad (22)$$

where

$$\frac{1}{N} \sum_k \Delta_k^{2p} = \frac{\Delta_{2p}}{\pi^2} \int_0^\pi dx \int_0^\pi dy (\cos x \pm \cos y)^{2p}$$

and

$$\delta t_{ij} = -\frac{\Delta^2}{2 \tilde{\mu}} + \frac{9 \Delta^4}{32 \tilde{\mu}^3} - \frac{75 \Delta^6}{192 \tilde{\mu}^5} + \ldots \quad (23)$$

Finally, an unperturbed BCS Hamiltonian in coordinate space takes the simple form

$$\hat{H}_{0f} = -\sum_i \mu_g \alpha_{i\sigma}^+ \alpha_{i\sigma}, \quad (24)$$

where the renormalized chemical potential $\mu_g$ looks as

$$\mu_g = \tilde{\mu} - \delta t_{ii} \quad (25)$$

In view of the unitary transformed Hamiltonian one can build the perturbation theory with operator $\hat{V}$ from (6) in which $\tilde{c}_{i\sigma}$ and $\tilde{\sigma}_{i\sigma}$ replaced by $\tilde{c}_{i\sigma}^+$ and $\tilde{c}_{i\sigma}$, respectively, where

$$\tilde{c}_{i\sigma} = \sum_{k_{\rho\sigma}} \exp(i(k \cdot R_i - R_\rho)) \left\{u_k^\dagger \alpha_{\rho\sigma} + v_k \alpha_{\rho\sigma}^+\right\}$$

$$\tilde{c}_{i\sigma}^+ = \sum_{k_{\rho\sigma}} \exp(-i(k \cdot R_i - R_\rho)) \left\{u_k^\dagger \alpha_{\rho\sigma}^+ + v_k \alpha_{\rho\sigma}\right\} \quad (26)$$

Here the coefficients of the u-v transform are

$$u_k = -\frac{\tilde{\mu} - \hat{E}_k}{\sqrt{2 \hat{E}_k (\hat{E}_k - \tilde{\mu})}} = \frac{\Delta_k}{\sqrt{2 \hat{E}_k (\hat{E}_k - \tilde{\mu})}} \quad (27)$$

III. PERTURBATION THEORY FOR ELECTRON SYSTEM IN A SUPERCONDUCTING STATE

The scattering matrix formalism for a system with strongly correlated electrons differs from that in the band theory of metals. Indeed, in our case we must exclude the upper Hubbard’s band by Gutzwiller’s projection operator. As a result one can not use the wave representation at disentanglement of correlators arising from series of the perturbation theory. Unfortunately, the BCS Hamiltonian is diagonalized if and only if we work in $k$-space. That’s why, the coordinate representation is introduced to connect the coordinate and $k$-spaces of transformed Hamiltonian. There is a powerful method.
of Hubbard operators to account for excluding of double electron site occupancy. In works [8,10] the general diagram method for Hubbard operator was presented. Let us dwell on the main statements related to our model.

Let us introduce the Hubbard’s operators $X^{ik} = |\psi_i\rangle \langle \psi_k|$, where we have three electron wave functions $|\psi_i\rangle = |0\rangle$, $|\psi_\sigma\rangle = |\sigma\rangle$, corresponding to hole, spin up ($\sigma = +$) and spin down ($\sigma = -$) electron states, respectively. Apparently, in a normal state operators $X^{0\sigma}$ and unperturbed Fermi Green’s functions and anticommutator $\{X^{0\sigma}, X^{0\sigma}\} = F^{0\sigma} = X^{0\sigma}_+ + X^{0\sigma}_-$, which differs from unit as for destruction and creation operators. It is a result of neglecting the upper Hubbard’s band. The main task is to find the average of operators $F^{0\sigma}$ and $e^{i\sigma\sigma}$.

In the first case we obtain the self-consistent equation for chemical potential of the para-electric state. Apparently, from condition $\Delta/\mu \ll 1$ one can neglect the influence of order parameter $\Delta$ on $\mu$. In the second case we will have the equation for a gap function. Since the fermion and boson subsystems are divided in accordance with Hamiltonian [8] now we will consider creation and destruction operators with one tilda corresponding to u-v transform. The second tilda will reflect an unitary transform (7). The average of operator $A$ is determined by a standard manner:

$$<A> = \frac{1}{\sigma(\beta)} <A\sigma(\beta)>_0,$$  

(28)

where the symbol $<\rangle_0 = Sp(exp(-\beta H_{0\ldots})) / Sp(exp(-\beta H_0))$ denotes a statistical averaging over the unperturbed Hamiltonian with temperature $1/\beta = T$, $Sp$ is a trace of the operator. The $S$ matrix is written as [11]

$$\sigma(\beta) = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \int_0^{\beta} \cdots \int_0^{\beta} dt_1 \cdots dt_n T_\tau \{V(t_1) \cdots V(t_n)\}$$  

(29)

In expression for $\sigma(\beta)$ the symbols $V(t_\tau) = e^{iH_{\tau\tau}V} e^{-iH_{\tau\tau}}$ and $T_\tau$ are operator in interaction representation and time-ordering operator, respectively. Now the task is to calculate all possible averages of the product of $A$ operators for different sites. Using the Vick’s theorem for Hubbard’s operators this correlators can be reduced to product of semi-invariants of the diagonal operators and unperturbed Fermi Green’s functions $G_{\alpha\beta}(\tau) = <X^{0\beta}(\tau) X^{0\alpha}(0)> / <F^{0\alpha}_0>$. The Fourier transform of these functions has the form

$$G_{\alpha\beta}(i\omega_n) = \frac{1}{2\beta} \int_{-\beta}^{\beta} e^{-i\omega_\tau} G_{\alpha\beta}(\tau)d\tau = \frac{1}{\beta} \frac{1}{i\omega_n + \varepsilon_{\alpha\beta}},$$  

(30)

where $\omega_n = (2n + 1)\pi/\beta$, $\varepsilon_{\alpha\beta} = \varepsilon_\alpha - \varepsilon_\beta$ and $\varepsilon_\alpha$ is the energy level of unperturbed Hamiltonian $H_{0f}$. In the case where is account of the electron-phonon interaction the unperturbed Fermi-Bose Green’s function is written as

$$\tilde{G}_{\alpha\beta}(\tau) = -<T_\tau X^{\alpha\beta} Y(\tau) X^{\beta\alpha}(0) Y^+(0)> / <F^{0\alpha}_0>. $$

The Fourier component $\tilde{G}_{\alpha\beta}(i\omega_n)$ of $\tilde{G}_{\alpha\beta}(\tau)$ is expressed as follows [10]:

$$\tilde{G}_{\alpha\beta}(i\omega_n) = \frac{1}{\beta} f(\varepsilon_{\alpha\beta}) \sum_{m=-\infty}^{\infty} d_m e^{\beta\varepsilon_{\alpha\beta} + i\frac{\beta}{2} m \omega_0} e^{-\frac{\beta}{2} m \omega_0} (\omega_n + m \omega_0 + \varepsilon_{\alpha\beta}),$$  

(31)

where $f(x) = 1/(e^{\beta x} + 1)$ and $B = 1/(e^{\beta \omega_0} - 1)$ are the Fermi and Bose distributions, respectively, $d_m = e^{-\lambda^2 (2\beta + 1)} I_m(2\lambda \sqrt{\beta(B+1)})$. $I_m(x)$ are the Bessel functions of complex argument and $\omega_n$ is the same as in [30].

Unfortunately, the Vick’s theorem cannot be used for transformed Hubbard’s operators in accordance with [7]. That’s why, for averaging we have to separate the boson subsystem from fermion. In case of isolated pairings such separation is not needed. As it will be seen later a similar situation is realized for effective kinematic interaction and diagrams to be formed by one effective line of interactions and one unperturbed Green’s function. Further, we denote by $U_{cp}(\tau_1 - \tau_j) = <T_\tau Y(\tau_j) Y^+(\tau_1)>_0$.

Let us write the possible pairings between creation and destruction operators. The normal operator pairing has the form

$$T_\tau \tilde{G}_{\alpha\beta}(\tau) \tilde{G}_{\sigma\sigma}(0) = \frac{1}{N^2} \sum_{k_1,k_2} e^{i(k_1 R_1 - i k_2 R_2)} e^{i(k_1 - k_2) R_0},$$

$$\cdot \{ -u^{*}_{k_1} u^{*}_{k_2} \tilde{G}_{\alpha\beta}(\tau) F_{\sigma\sigma}^{00} - u_{k_1} u_{k_2} \tilde{G}_{\beta\beta}(\sigma^0) F_{\sigma\sigma}^{00} \}$$  

(32)

and an average over the Hamiltonian $H_{0f}$ gives the next unperturbed Green’s functions:

$$\tilde{G}_{\alpha\beta}(\tau) = -<T_\tau \tilde{G}_{\alpha\beta}(\tau) \tilde{G}_{\beta\beta}(0)>_0 = \frac{1}{N} \sum_{k} e^{i(k R_1 - R_2)}.$$  

$$\left| u_k \right|^2 \tilde{G}_{\alpha\beta}(\tau) <F^{0\sigma}_0 >_0 + |v_k|^2 \tilde{G}_{\beta\beta}(\sigma^0) <F_{\sigma\sigma}^{0)} >_0,$$  

(33)

where $\tilde{G}_{\alpha\beta}(i\omega_n)$ is unperturbed Green’s function from [31]. The anomalous operator pairing is presented as

$$T_\tau \tilde{G}_{\alpha\beta}(\tau) \tilde{G}_{\sigma\sigma}(0) = \frac{1}{N^2} \sum_{k_1,k_2} e^{i(k_1 R_1 + i k_2 R_2)} e^{-i(k_1 + k_2) R_0},$$

$$\cdot \{ -u_{k_1} u_{k_2} \tilde{G}_{\alpha\beta}(\tau) F_{\sigma\sigma}^{00} - u^{*}_{k_1} u^{*}_{k_2} \tilde{G}_{\beta\beta}(\sigma^0) F_{\sigma\sigma}^{00} \}$$  

(34)

Here the arrows are directed from “active” operator to “passive” with the use of Vick’s theorem. In particular, the average of [34] at $\tau \rightarrow 0$ gives unperturbed gap functions:

$$<\tilde{c}_1 \sigma \tilde{c}_m \sigma >_0 = -\frac{1}{N} \sum_{k} e^{i(k (R_1 - R_m))} u^{*}_{k_1} u_{k_2} <F^{0\sigma}_0 >_0 =$$

$$= \frac{1}{N} \sum_{k} e^{i(k (R_1 - R_m))} \varphi^{11}_{k\sigma}(0)$$  

(35)
The pairing with diagonal operator takes the form:

\[ T_\tau \hat{c}_{l\sigma}(\tau) F^{\sigma 0}_{m\sigma} = - \frac{1}{N} \sum_{k} e^{i \mathbf{k} \cdot (\mathbf{R}_m - \mathbf{R}_n)} v_k \tilde{G}_{-\sigma 0}(\tau) \alpha_{l\sigma}^+ \]

The similar expressions can be presented for other pairings. One can point out that anticommutator

\[ \{ \hat{c}_{l\sigma} \hat{c}_{m\sigma}^+ \} = \tilde{F}_{l\sigma}^{0} = - \frac{1}{N} \sum_{k_1 k_2} e^{i (k_1 - k_2) \cdot (\mathbf{R}_m - \mathbf{R}_n)} \cdot (u_{k_1}^* u_{k_2} F^{\sigma 0}_p + v_{k_1} v_{k_2} F^{\sigma 0}_p) \]

We shall calculate the average value \(< \hat{c}_{l\sigma} \hat{c}_{m\sigma} >\). This average is conveniently calculated by replacement

\[ < \hat{c}_{l\sigma} \hat{c}_{m\sigma} > = \lim_{\tau \to +0} < T_\tau \hat{c}_{l\sigma}(\tau) \hat{c}_{m\sigma}(0) > \]

Let \( B_{0\sigma}(\tau_j - \tau_i, \mathbf{k}) \) is the Fourier components of the effective kinetic interaction caused by perturbation \( V \) from (3). Then it is necessary to find an average of the following expression:

\[ \int_{0}^{\beta} d\tau_j \int_{0}^{\beta} d\tau_i \frac{1}{N} \sum_{\mathbf{k}} B_{0\sigma}(\tau_j - \tau_i, \mathbf{k}) e^{i \mathbf{k} \cdot (\mathbf{R}_j - \mathbf{R}_l)} \cdot \left( T_\tau \hat{c}_{l\sigma}(\tau) \hat{c}_{m\sigma}(0) \right) \]

And the high-order perturbation with pairings of type (30) renormalize the combined occupancy, \(< F^{\sigma 0}_{m\sigma} >\) to \(< F^{\sigma 0}_{m\sigma} >\) in accordance with the following function

\[ \beta \delta \tilde{\mu}_\sigma = \frac{1}{N} \sum_{q, \omega_n} \beta B_{0\sigma}(q, i \omega_n) \tilde{G}_{0\sigma}(i \omega_n) \]

The high orders of perturbation theory with pairings of type (30) renormalize the combined occupancy, \(< F^{\sigma 0}_{m\sigma} >\) to \(< F^{\sigma 0}_{m\sigma} >\) in accordance with expanding function

\[ < F^{\sigma 0}_{m\sigma} > = e^{-\beta \delta \mu_\sigma} \frac{e^{-\beta (\lambda + \varepsilon + \varepsilon_\sigma)}}{e^{-\beta \delta \mu_\sigma} + e^{-\beta (\lambda + \varepsilon + \varepsilon_\sigma)} + 1} \]

Thus, on summing (33), (34) and so on, we obtain

\[ \varphi_{(\tau \to +0)}^{11}(\tau) = u_{k} v_{-k} G_{0\sigma}(\tau) < F^{-\sigma 0}_{0} > + u_{-k} v_{k} G_{0\sigma}(\tau) < F^{\sigma 0}_{0} > \]

The next more complicated pairings appear as

\[ \int_{0}^{\beta} d\tau_j \int_{0}^{\beta} d\tau_i \frac{1}{N} \sum_{\mathbf{k}} B_{0\sigma}(\tau_j - \tau_i, \mathbf{k}) e^{i \mathbf{k} \cdot (\mathbf{R}_j - \mathbf{R}_l)} \cdot \left( T_\tau \hat{c}_{l\sigma}(\tau) \hat{c}_{m\sigma}(0) \right) \]

where

\[ \varphi_{(\tau \to +0)}^{12}(\tau) = \int_{0}^{\beta} d\tau_j \int_{0}^{\beta} d\tau_i \frac{1}{N} \sum_{\mathbf{k}} B_{0\sigma}(\tau_j - \tau_i, \mathbf{k}') \cdot \left( u_{k}' v_{k} v_{k} v_{-k} G_{0\sigma}(\tau_i - \tau_j) G_{0\sigma}(\tau_j - \tau_i) G_{0\sigma}(\tau_j \to \tau_i) - \right. \]

\[ \left. \int_{0}^{\beta} d\tau_j \int_{0}^{\beta} d\tau_i \frac{1}{N} \sum_{\mathbf{k}} B_{0\sigma}(\tau_j - \tau_i, \mathbf{k}') U_{0\sigma}(\tau_i - \tau_j) \cdot \left( u_{k}' v_{k} v_{k} v_{-k} G_{0\sigma}(\tau_i - \tau_j) G_{0\sigma}(\tau_j - \tau_i) G_{0\sigma}(\tau_j \to \tau_i) - \right. \]

Here, the cumulants \(< F^{\sigma 0}_{m\sigma} F^{\sigma 0}_{m\sigma} >\) and \(< F^{\sigma 0}_{m\sigma} F^{\sigma 0}_{m\sigma} >\) correspond to linked diagrams expressed in the terms of derivatives \( \partial_{\sigma} < F^{\sigma 0}_{m\sigma} > \) and \( \partial_{-\sigma} < F^{\sigma 0}_{m\sigma} > \), respectively, where \( \partial_{\sigma} = \partial / \partial (-\beta \varepsilon_\sigma) \).
Also, we have to evaluate the mean value
\[ K_2 = \langle T_{\tau} c_{1-\sigma}(\tau) \bar{c}_{m\sigma}(0) \bar{c}_{1-\sigma}(\tau) c_{m\sigma}(\tau) \rangle_0 \] at \( \tau \to +0 \). If we make in previous correlator
\[ K_1 = \langle T_{\tau} \bar{c}_{1-\sigma}(\tau) \bar{c}_{m\sigma}(0) \bar{c}_{1-\sigma}(\tau) \bar{c}_{m\sigma}(\tau) \rangle_0 \] the replacement \( \sigma \to -\sigma \) and \( m \leftrightarrow l \), we obtain \(-K_2\) in the limit for \( \tau \to -0 \). Thus, it follows from \( K_1 \):
\[ \varphi_{k\sigma}^{21}(0) = -\varphi_{-k-\sigma}^{12}(\tau \to -0) \]
One can point out that Fourier transform of \( \langle \bar{c}_{1-\sigma} \bar{c}_{m\sigma} \rangle \) is \( \varphi_{k\sigma} \), i.e.
\[ \langle \bar{c}_{1-\sigma} \bar{c}_{m\sigma} \rangle = \frac{1}{N} \sum_k e^{ik(R_l - R_m)} \varphi_{k\sigma} \]

\[ \varphi_{k\sigma}^{12}(0) + \varphi_{k\sigma}^{21}(0) = \int_0^\beta d\tau_j \int_0^\beta d\tau_i \frac{1}{N} \sum_{k'} \frac{1}{B_{0\sigma}}(\tau_j - \tau_i, k')U_{ep}(\tau_i - \tau_j) < F_{\sigma 0} >_0 \cdot \{ v_{k'} u_{k'} (u_k^2)^2 G_{-\sigma 0}(\tau_i) G_{\sigma 0}(\tau_j) + u_k v_k v_{-k} G_{0-\sigma}(\tau_i) G_{\sigma 0}(\tau_j) \} \]

Apparently, that integrals
\[ \int_0^\beta d\tau_j \int_0^\beta d\tau_i \frac{1}{N} \sum_{k'} \frac{1}{B_{0\sigma}}(\tau_j - \tau_i, k')U_{ep}(\tau_i - \tau_j) < F_{\sigma 0} >_0 \]

Thus, the left hand of Eq. (1) does not depend on wave vector \( k \) because of relations (27) and this contribution in gap function (11) is equal zero. Then we have for gap function
\[ \langle \bar{c}_{-k-\sigma} \bar{c}_{k\sigma} \rangle = -u_{-k} v_k < F^{\sigma 0} >_1 \]

Using Eqs. (27) we obtain the equation for gap
\[ \Delta_k = \frac{1}{N} \sum_q J(q + k) \frac{\Delta_q}{2|E_q|} < F^{\sigma 0} >_1 \]

This equation in the limit \( T \to 0 \) coincides practically with a similar equation obtained by G.Baskaran Z. Zou and P.W. Anderson in Ref. [3]. There is one essential difference. In Ref. [3] the temperature factor depends on wave vector and tends to 1 at \( T \to 0 \). In our case the electron-hole presence is accounted for. As a result we have \( k \) -independent factor \( < F^{\sigma 0} >_1 \) to be equal to 1/2 at temperature \( T \to 0 \). This factor is determined by Eq. (38). Here we can put \( \delta \mu_{\sigma} = \delta \mu_{-\sigma} \) when finding the critical temperature of superconducting state. Then one can write
\[ < F^{\sigma 0} >_1 = \frac{e^{\beta E_{\mu} + 1}}{1 + e^{\beta E_{\mu} + e^{\beta E_{-\mu}}}} \]

where \( E_{\mu} = -\varepsilon_{\sigma} + \delta \mu_{-\sigma} \) and
\[ \delta \mu_{\sigma} = \frac{1}{N} \sum_{q \neq 0} \beta B_{0\sigma}(q, \varepsilon_{\omega n}) \tilde{G}_{\sigma 0}(\varepsilon_{\omega n}) \]

with \( \tilde{G}_{\sigma 0}(\varepsilon_{\omega n}) \) from (31). The solution of (41) at temperature \( T_{SC} \) when \( \Delta = 0 \) gives the self-consistent equation for temperature of the superconducting transition:
\[ T_{SC} = \frac{\tilde{\mu} + \delta \mu_{\sigma}}{\ln \frac{2\pi}{\mu_{\sigma}}} \]

From (44) follows the next requirement on the chemical potential:
\[ J/4 \leq \tilde{\mu} \leq J/3 \]
This condition is rigorous and that’s why the preceding spin-fluctuation theories are failed in the explanation of high-temperature superconductivity. As will be seen from a next section the chemical potential of paramagnetic state of the strongly correlated electrons substantially exceed an exchange parameter $J$, i.e. the strong charge-spin fluctuations destroy the Cooper’s pairs.

**IV. NORMAL STATE OF ELECTRONS IN THE ABSENCE OF ELECTRON-PHONON INTERACTION**

The theory of effective self-consistent field and phase transition in a system of the strongly correlated d-electrons of cuprates was developed by us in works [12, 13]. In particular, the equation for chemical potential in paramagnetic state is written as

$$<F_{\sigma}^0> = 1 - \frac{n}{2} = <F_{\sigma}^0 >_1 - \tilde{\nu}_\sigma <F_{-\sigma}^0> _1,$$  \hspace{0.5cm} (46)

where $<F_{\sigma}^0> _1$ is determined by Eq. (12) and at $g=0$

$$\delta \tilde{\mu}_\sigma = \delta \mu_\sigma = \frac{1}{N} \sum_q t(q) f(E_{q\sigma})$$  \hspace{0.5cm} (47)

$$\tilde{\nu}_\sigma = \nu_\sigma = \frac{1}{<F_{\sigma}^0> } \left\{ \frac{1}{N} \sum_q f(E_{q\sigma}) - f(\varepsilon_\sigma) \right\}$$  \hspace{0.5cm} (48)

Here, the band energy $E_{q\sigma} = \varepsilon_\sigma + t(q) <F_{\sigma}^0>$ and Fourier components of hoping integral $t(q) = \sum_{ij} t_{ij} e^{-iq(r_i-r_j)} = 2t(cos(q_x a)+cos(q_y a))$ for rectangular lattice with constant $a$. Let the function $I(x)$ be given by formula:

$$I(x) = \int_{-2}^{x} D_C(x) dx,$$  \hspace{0.5cm} (49)

where the electron density of state $D_C(x)$ has a form for rectangular lattice

$$D_C(x) = \frac{1}{\pi^2} K \left( \sqrt{1 - (x/2)^2} \right)$$  \hspace{0.5cm} (50)

and $K(x)$ is a complete elliptic integral of the first order. At $T = 0$ and $\tilde{\mu} + \delta \mu_\sigma > 0$ it is easy to write the solution of Eq.(48) for chemical potential of paramagnetic (PM-2) phase:

$$\tilde{\mu}/W = \frac{2 - n}{8} I^{-1} \left( 1 - \frac{1}{2}(1 - n)(2 - n) \right),$$  \hspace{0.5cm} (51)

where $I^{-1}(x)$ is an inverse function of $I(x)$. It corresponds to gas limit in a hole concentration $I$-n, when $<F_{\sigma}^0> _1 = 1/2$. Indeed, $<F_{\sigma}^0> = 1 - n/2$, i.e. at $n \sim 1$ we have $<F_{\sigma}^0> \sim 1/2$. At $T = 0$ and $\tilde{\mu} + \delta \mu_\sigma < 0$ we obtain for paramagnetic (PM-1) phase:

$$\tilde{\mu}_{PM1}/W = \frac{2 - n}{8} I^{-1} \left( \frac{n}{2} \left( 1 - \frac{n}{2} \right) \right),$$

that corresponds to gas limit in electron concentration $n$: $<F_{\sigma}^0> _1 = 1$ and $<F_{\sigma}^0> \sim 1$. In Fig.4 the concentration dependence of the chemical potential in units of bandwidth $W$ in PM-1 and PM-2 phases is presented. One can see the disrupt of $\tilde{\mu}$ at $n = n_{cr.} = 0.5714$. From Fig.1 it is easy to see the correlation narrowing of band $W$ in PM-2 phase. Indeed, at $n = 1$ we have $\tilde{\mu}/W = 0.25$ that it less then $\tilde{\mu}/W = 0.5$ for ferromagnetic state when a such narrowing is absent [14]. In work [12] a similar narrowing of PM is also observed. Unfortunately, this narrowing is unsuffient to fulfill the condition of PM even at $n = n_{cr.}$ when $\tilde{\mu}(n_{cr.})/W \approx 0.09$. With an increase in temperature the chemical potential is also increased.

![FIG. 1: The concentration dependence of the chemical potential in PM-1 and PM-2 phases in units of bandwidth $W$. At $n=0.5714$ there is a disrupt of $\tilde{\mu}$.](image)

In Fig. 2 the temperature dependencies of the chemical potential at electron concentration $n=0.8, 0.9, 0.95$ and 0.99 (curves 1-4, respectively) are presented. These curves were obtained by numerical solving of the Eq. (16). It turns out that the inclusion of electron-phonon interaction may enforce essentially the correlation narrowing of band at which the conditions can be fulfilled.

**V. NORMAL STATE OF THE CUPRATES WITH POLARON EXCITATIONS**

The problem of the polaron excitations in a system of d-electrons was considered by many authors [4, 5, 16]. We will not analyze these works in detail but point out on the main their limitations. Unfortunately, the authors...
simplify the Hamiltonian $\hat{V}$ renormalizing a hopping integral $t$ by factor $e^{-\lambda^2}$. As a result we obtain a drastic decrease in temperature of the superconducting state $\Omega$ and authors would have to use the effects of interactions of more high order of smallness. In fact the situation is more complicated. It is connected with properties of the unperturbed Green’s functions $G_{\alpha\beta}(i\omega_n)$. In series expansion of Eq. (31) for $m$-th order we have product $e^{-\lambda^2}$ and $\lambda^{2m}/m!$. As was proved by G.D. Mahan in book [11] there is a Gaussian $\frac{1}{\sqrt{2\pi m}} \exp \left\{- (\lambda^2 - m)/(2m) \right\}$ instead of $e^{-\lambda^2}$. Thus, with increasing $\lambda$ a number $m$ of the polaron band, where the spectral function has a maximum, is increased.

Let us consider this question more thoroughly. In zeroth order of effective field for total Green’s function $\Lambda_{0\sigma}(i\omega_n, q)$ the graphic equation is presented in Fig. 3 where the bold, thin straight and wave lines correspond to $\beta\Lambda_{0\sigma}(i\omega_n, q)$, $\beta\tilde{G}_{0\sigma}(i\omega_n)$ and $t(q)$, respectively. The solution of this equation is written as

$$\beta\Lambda_{0\sigma}(i\omega_n, q) = \frac{\beta\tilde{G}_{0\sigma}(i\omega_n) < F^{\sigma 0} >}{1 - \beta t(q)\tilde{G}_{0\sigma}(i\omega_n) < F^{\sigma 0} >} \quad (52)$$

In this equation we have replaced $< F^{\sigma 0} >_0$ on the total average $< F^{\sigma 0} >$ to obtain the self-consistent parameter for effective kinematic field. The main problem in Eq. (52) is connected with determination of poles which are defined by equation

$$1 - \beta t(q)\tilde{G}_{0\sigma}(i\omega_n) < F^{\sigma 0} > = 0 \quad (53)$$

Indeed, in diagram methods one must often evaluate frequency summations. The traditional methods solve this problem if the poles of Matsubara Green’s functions are known [11]. Unfortunately, Eq. (53) for $i\omega_n$ gives the algebraic equation of infinity order and the task becomes unsolved. It turn out that one can overcome this difficulty by method of inverse function. To understand the essence of a question we will simplify the Green’s function $\tilde{G}_{0\sigma}(i\omega_n)$, where

$$\tilde{G}_{0\sigma}(i\omega_n) \approx \delta(i\omega_n - \sigma \epsilon) \exp \left\{- (\lambda^2 - m)/(2m) \right\} \quad (54)$$

Let $\beta \tilde{G}_{0\sigma}(w) = \frac{1}{\omega_n} (M(1,1 + w, -\lambda^2)(1 - f(\epsilon_\sigma)),$ (55)

where $M(a,b,z)$ is the confluent hypergeometric function of Kummer [17]. In Fig. 4 the $\beta \tilde{G}_{0\sigma}(w)$ as function of $w$ is presented at $T=0$ when $\epsilon_\sigma = -\mu < 0$, $g/W=0.07$ and phonon frequency $\omega_0/W=0.01875$. As illustrated in Fig. 4 this function has monotonous behaviour between poles $m$ and $m+1$. It allows to find the inverse function $\beta \tilde{G}_{0\sigma}(\Omega)$ in this area. Let us denote by $E_{n\sigma\sigma}$ the $n$-th root of the Eq. (53). In the vicinity of $E_{n\sigma\sigma}$ one can expand $\beta \tilde{G}_{0\sigma}(\Omega)$ in powers $\Omega - E_{n\sigma\sigma}$ and we have

$$\beta \Lambda_{0\sigma}(\Omega, q) \approx \sum_n \frac{\beta \tilde{G}_{0\sigma}(E_{n\sigma\sigma}) < F^{\sigma 0} >}{\Omega - E_{n\sigma\sigma}}$$

After analytic continuation $\Omega > \Omega + i\delta$ we obtain the imaginary part of the $\beta \Lambda_{0\sigma}(\Omega, q)$:

$$Im(\beta \Lambda_{0\sigma}(\Omega, q)) = \pi \sum_n \frac{\beta \tilde{G}_{0\sigma}(E_{n\sigma\sigma}) \delta(\Omega - E_{n\sigma\sigma})}{t(q) \beta \delta \tilde{G}_{0\sigma}(\Omega) d\Omega}$$

where $\delta(x)$ is the Dirac delta function. The uniform spec-
where $n\omega_0 < \Omega < (n+1)\omega_0$ and $\left| F'(\hat{\Omega}) \right| / F'(\hat{\Omega}) = -1$ (see Eq. (54)). We have to combine all $n$ bands into one that gives the uniform electron spectral density throughout the whole frequency interval:

$$R_\sigma(\Omega, 0) = \frac{8\pi}{W} D_C(\psi(\Omega))$$

where $\psi(\Omega) = 4/(\beta W\hat{G}_{0\sigma}(\Omega) < F^{\sigma 0}>)$.

In Fig. 5 the frequency dependences of the electron spectral density $R_\sigma(w, 0)$ at temperature $T=0$ in units $W$ are presented. In the absence of an electron-phonon interaction it is observed the typical 2d-dimensional spectral density with van Hove singularity. With increase the constant of electron-phonon interaction $g$ the polaron bands are formed, each of which has a pointed singularity. Also, a whole band is shifted to the left edge and its bandwidth depends on $g$ weakly.

Now we will calculate the functions $\tilde{\nu}_\sigma$ and $\delta\tilde{\mu}_\sigma$ in Eq. (39) for $\tilde{\mu}$ with account of the electron-phonon interactions. These functions correspond to diagrams $a$ and $b$ in Fig. 6 where the straight and wave lines denote
\[ \tilde{G}_{0\sigma}(\omega_n) \] from (51) and effective kinematic interaction
\[ B_{0\sigma}(\omega_n, \mathbf{q}) \], respectively, and presented as
\[ \beta B_{0\sigma}(\omega_n, \mathbf{q}) = \frac{\beta(q)}{1 - \beta(tq)\tilde{G}_{0\sigma}(\omega_n)} < F_{\sigma 0} > \]

Then one can write

FIG. 6: Diagrams for functions \( \beta \delta \tilde{\nu}_\sigma \) (a) and \( \tilde{\nu}_\sigma < F_{\sigma 0} > \) (b) from Eq. (63).

\[ \beta \delta \tilde{\nu}_\sigma = \frac{1}{N} \sum_{q^m} \beta B_{0\sigma}(\omega_n, \mathbf{q})\tilde{G}_{0\sigma}(\omega_n) \]
\[ = \frac{1}{N} \sum_{q_{nm}} \beta B_{0\sigma}(\omega_n, \mathbf{q})U_{ep}(\omega_n - \omega_m) \cdot (\tilde{G}_{0\sigma}(\omega_m))^2 < F_{\sigma 0} > , \quad (59) \]

where the Fourier component \( U_{ep}(\omega_n) \) of boson unperturbed Green’s function \( U_{ep}(\tau_\tau) \) has a form
\[ U_{ep}(\omega_n) = \frac{1}{\beta} \sum_{m=-\infty}^{+\infty} d_m \frac{2 \sinh(\beta m \omega_n / 2)}{\omega_n + m \omega_n} \]

and \( \omega_n = 4 \pi n T \). Also, \( \tilde{\nu}_\sigma \) in (59) depends on unperturbed pure electron Green’s function \( \tilde{G}_{0\sigma} \), whereas \( \delta \tilde{\nu}_\sigma \)

is determined by \( \tilde{G}_{0\sigma}(\omega_n) \) from (51). The method of inverse function can be used to Eq. (59) to make a frequency summation. Indeed, in accordance with formula from (11) one can evaluate the summation by integration over contour \( C \) to be a circle of radius \( R \to \infty \). Then we have
\[ \delta \tilde{\nu}_\sigma = \frac{1}{2} \sum_{q_{nm}} \frac{1}{2\pi i} \oint_C \beta B_{0\sigma}(\omega, \mathbf{q})\tilde{G}_{0\sigma}(\omega) f(\omega) d\omega = \]
\[ = \frac{1}{2} \sum_{q_{nm}} \frac{1}{2\pi i} \sum_{k} \text{Res} \left[ \beta B_{0\sigma}(\omega, \mathbf{q})\tilde{G}_{0\sigma}(\omega) \right]_{\omega_k} \]

where \( \text{Res} f(\omega) \) is the residue of \( f(\omega) \) in pole \( \omega_k \).

On then applying the similar procedure as for \( R_\sigma(\Omega, 0) \) above, we obtain
\[ \delta \tilde{\nu}_\sigma = \int_{-\infty}^{+\infty} d\Omega f(\Omega) \frac{4 \text{Res}_{\Omega} f(\Omega)}{W < F_{\sigma 0} > W < F_{\sigma 0} > ^2} = \]
\[ \delta \tilde{\nu}_\sigma = \int_{-\infty}^{+\infty} d\Omega f(\Omega) \frac{4 \text{Res}_{\Omega} f(\Omega)}{W < F_{\sigma 0} > W < F_{\sigma 0} > } \quad (60) \]

The expressions for \( \tilde{\nu}_\sigma \) is more complicated:
\[ \tilde{\nu}_\sigma = \tilde{\nu}_{\sigma 1} + \tilde{\nu}_{\sigma 2} + \tilde{\nu}_{\sigma} \quad (61) \]

where \( \tilde{\nu}_{\sigma 1} \) and \( \tilde{\nu}_{\sigma 2} \) are equal
\[ \tilde{\nu}_{\sigma 1} = \int_{-\infty}^{+\infty} d\Omega f(\Omega) \frac{4 \text{Res}_{\Omega} f(\Omega)}{W < F_{\sigma 0} > W < F_{\sigma 0} > } \]
\[ r_{\sigma} = - \frac{1}{\pi F_{\sigma 0}} \sum_{m=-\infty}^{+\infty} f(\epsilon_{\sigma} - m \omega_0) \quad (62) \]

Here,
\[ \varphi_{0\sigma}^1(\Omega) = - \frac{1}{4} \sum_{m=-\infty}^{+\infty} \frac{2 d_m f(\epsilon_{\sigma})(1 - f(\epsilon_{\sigma}))}{\omega_0 + m \omega_0} \text{ sinh}(\beta m \omega_0 / 2) \approx \]
\[ \approx - \frac{1}{\beta \omega_0} f(\epsilon_{\sigma})(1 - f(\epsilon_{\sigma})) \{ M(1, 1 + \Omega / \omega_0, -\lambda^2) - M(1, 1 - \Omega / \omega_0, -\lambda^2) \} \]
\[ \varphi_{0\sigma}^2(\Omega) = \frac{1}{\beta \omega_0} \frac{\partial \tilde{G}_{0\sigma}(\omega)}{\partial \omega} = - \frac{1}{\beta \omega_0} \frac{\partial \tilde{G}_{0\sigma}(\omega)}{\partial \omega} \]

where the integral on \( m \)-th segment has a form
\[ R_m = \int_{m-1}^{m} dw f(w \omega_0 + \epsilon_{\sigma}) \frac{\partial}{\partial w} (\psi(w)) D_C (\psi(w)) \quad (64) \]

Let \( w_{lm} \) and \( w_{rm} \) be the left and right edges of the segment with \( m \)-th singularity, respectively. They are determined by equations:
\[ \frac{4}{W \beta \tilde{G}_{0\sigma}(w_{lm})} < F_{\sigma 0} > = \pm 2, \]

where upper and lower signs correspond to \( w_{lm} \) and \( w_{rm} \), respectively. On now carrying out the partial integration
In SC phase the contribution of the polaron excitation in function of $T$ of superconducting state (SC) is determined by $\omega$ of phonons \[ \text{(19)} \]. Finally, we have $\omega \sim 2$ corresponds the cuprate YBa$_2$Cu$_3$O$_6$ (see Fig. 5, c) for considered temperature area and $g/W < 0.085$. Finally, the Eqs. (60), (61) and (65) allow to find the numerical solution of a set of equations (44) and (46) without any difficulties.

VI. RESULTS OF THE NUMERICAL CALCULATIONS

To calculate the temperature of superconducting state \[ \text{[44]} \] we take the value of hopping integral $t \sim 0.5$ eV and exchange parameter $J \sim 0.023$ eV \[ \text{[4, 18]} \]. It corresponds the cuprate YBa$_2$Cu$_3$O$_6$ with Neel temperature $T_N = 420$ K. The parameter $J$ is determined with account of $\sim 30\%$ contribution of the spin fluctuations. Then we have the bandwidth $W = 4$ eV. Also, we take the frequency $\omega = 75$ meV to be typical for cuprates in Einstein model for phonons \[ \text{[10]} \]. Finally, we have $\omega_0/W = 0.01875$ and $J/W = 0.058$.

Let us consider the solutions of Eq. (44) at temperature $T = 0$. At $T \sim 0$ one can rewrite Eq. (46) as

$$
\tilde{\mu} + \delta \tilde{\sigma} = T \ln \frac{n/2 - \tilde{\nu}_\sigma}{1/2 - n/2 + \tilde{\nu}_\sigma/2}
$$

It follows from \[ \text{[60]} \] that at $T = 0$ for PM-2 phase, when $\tilde{\mu} + \delta \tilde{\sigma} > 0$, the chemical potential obeys the equation $1/2 - n/2 + \tilde{\nu}_\sigma/2 = 0$. Surprisingly, but there is a situation, when $\tilde{\mu} + \delta \tilde{\sigma} = 0$ and $1/2 - n/2 + \tilde{\nu}_\sigma/2 \neq 0$, $n/2 - \tilde{\nu}_\sigma \neq 0$.

In Fig. 6 the curves of $\tilde{\mu}$ as function of $g$ at different electron concentrations are presented. On curves 2-4 at $g = g_{cr}$, one can observe the kinks. When $g > g_{cr}$, the chemical potential obeys the equation $\tilde{\mu} + \delta \tilde{\sigma} = 0$ and at $g < g_{cr}$ for $\tilde{\mu}$ we have $1/2 - n/2 + \tilde{\nu}_\sigma/2 = 0$. At critical concentration $n = n_{cr}$, of transition in PM-1 phase we have $g_{cr} = 0$. In inset the influence of temperature is shown.

In Fig. 5 the phase diagram in coordinate $g-n$ at $T = 0$ is presented. The upper and lower parts of boundary of superconducting state (SC) is determined by $g_{cr}$, as function of $n$ and value of $g$ at which $\tilde{\mu} = 0$ (see Fig. 5). In SC phase the contribution of the polaron excitation in the narrowing of electron band is essential. The chemical potential is decreased up to zero. Thus, the condition \[ \text{[18]} \] for appearance of SC state can be realized. In the area of localized state we can not obtain the solution for $\tilde{\mu}$ corresponding to hole doped electron system (PM-2 phase).

In Fig. 6 the concentration dependences of the chemical potential for different parameters of electron-phonon coupling are presented at $T = 0$. The straight lines shows a region of acceptability of $\tilde{\mu}$ at different values of $g$ and $n$. One can see that at small values of $g$ the bandwidth is insufficiently narrow. At large values of $g$ the pointed
FIG. 9: The concentration dependences of the chemical potential at $T=0$ and parameters of electron-phonon coupling $g/W=0.07$, 0.0655, 0.065 and 0.06 (curves 1-4, respectively).

Now we will calculate the temperature of superconducting state $T_{SC}$. In accordance with Eq. (44) it is necessary to find $\tilde{\mu}$ and $\delta \tilde{\mu}_\sigma$ as functions of $T$ and electron concentration. In Fig. 10 the temperature dependences of $\tilde{\mu}$ and $\delta \tilde{\mu}_\sigma$ at $g/W=0.07$ and different electron concentration were obtained by solving the Eq.(46). From Fig. 10 a it easy to see that chemical potential in a definite temperature and concentration area meets the condition (45) and as a result one can solve the Eq.(44) for $T_{SC}$.

FIG. 10: The temperature dependences of $\tilde{\mu}$ (a) and $\delta \tilde{\mu}_\sigma$ (b) at $g/W=0.07$ and $n=0.86, 0.92, 0.96$ and 0.98 (curves 1-4, respectively).

In Fig. 11 the concentration dependence of the temperature of superconducting state is presented for $g/W=0.07$ and $W=4eV$. We observe the high-temperature superconductivity with left and right edge of superconducting phase on axis $n$. The area between straight lines determines $\tilde{\mu}$ in accordance with requirement (45) for SC phase. Indeed, the left edge of SC phase $n_{LSC}=0.858$ when $T_{SC}(n_{LSC})=0$ is determined from equation $J/4+\delta \tilde{\mu}_\sigma=0$ (see Eq.[60], i.e.

$$
\frac{4(\omega_0/W)^2}{(1-n/2)^2} \int_{\tilde{\mu}/\omega_0}^{\infty} dw \cdot w^4 D_C \left( \frac{4w\omega_0/W}{(1-n/2)M(1+w,-\lambda^2)} \right) = -J/(4W)
$$

The right edge $n=1$ when $T_{SC}=0$ follows from condition $\delta \tilde{\mu}_\sigma/W \rightarrow 0$ at $n \rightarrow 1$(see Fig. 10, b). It reflects the weakening of effective kinematic field at half filling of the band near $T_{SC}$. Since $\tilde{\mu} \rightarrow J/4$ then $\ln J - \frac{2}{4} \tilde{\mu} - \frac{J}{2\tilde{\mu}} \rightarrow +\infty$ and $T_{SC} \rightarrow 0$. The maximum of $T_{SC}$ from Fig. 11 is in a good agreement with experimental value $T_{SC} \approx 100K$ for cuprate YBa$_2$Cu$_3$O$_7$. [4].

FIG. 11: The temperature of superconducting state $T_{SC}$ versus electron concentration $n$ with strength of electron-phonon coupling $g/W=0.07$ and bandwidth $W=4 eV$.

It is interesting to find the gap as a functions of $n$ at $T=0$ and its temperature dependence for fixed $n$. The gap $\Delta$ is determined from Eq.(41) by expansion $|\tilde{E}_q|$ into a series in $\Delta/\tilde{\mu}$. It is easy to find that

$$
\Delta_k = <F_\sigma> \frac{1}{2\tilde{\mu}} \left\{ \frac{9}{8} \Delta^2 + \frac{75}{32} \Delta^4 - \ldots \right\},
$$

where $<F_\sigma> \frac{1}{2\tilde{\mu}}$ is determined by (42) with $\varepsilon_\sigma = -\mu_\sigma$. At $T=0$ we have $<F_\sigma> >1/2$ and it gives the algebraic equations for $\Delta/\tilde{\mu}$. For example, at $n=0.9$ and $g/W=0.07$ from Fig. 12 (curve 4) we have $\tilde{\mu}/W=0.0114$ and $\Delta/W=0.0055$. With account of $T_{SC}/W=0.00215$ at $n=0.9$ we obtain $2\Delta/T_{SC}=5.15$. By similar manner the gap $\Delta$ versus $T$ was calculated.
In Fig. 12 the concentration (a) and temperature (b) dependencies of the relationship $2\Delta/T_{SC}$ are presented. An optimal doping gives the maximal value of $2\Delta/T_{SC} \approx 5$ that also corresponds to experimental results for cuprates [4].

VII. CONCLUSIONS

In the present work, an influence of the electron-phonon interaction on normal and superconducting properties of the strongly correlated electrons has been studied. The strong kinematic interactions in a doped system were shown to destroy the singlet pairs of electrons formed by indirect exchange. The inclusion of the sufficiently strong electron-phonon coupling stabilizes these pairs by virtue of correlation band narrowing manifested in a drastic decrease of the chemical potential. It was built the phase diagram of ground states in coordinates the constant of electron-phonon coupling $g$ and electron concentration $n$. At optimal value of $g$ and $n$ for cuprate YBa$_2$Cu$_3$O$_7$ the calculated critical temperature of superconductivity $T_{SC}$ and $2\Delta/T_{SC}$ are very close to experimentally observed. This value $g/W=0.07$ corresponds to energy of the Holstein’s polaron $E_p = g^2/\omega_0 \approx 1.05$ eV and its radius $R_p = a(W/E_p) \approx 4a$. A new method of the frequency summation with infinite number of poles of unperturbed Green’s function was suggested. The exact analytic expressions of diagrams in the first nonvanishing approximation of perturbation theory were obtained to find the contribution of polarons in the chemical potential.

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