Eliashberg–type equations for correlated superconductors

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Abstract

The derivation of the Eliashberg type equations for a superconductor with strong electron correlations and electron–phonon interaction has been presented. The proper account of short range Coulomb interactions results in strongly anisotropic equations. Possible symmetries of the order parameter include s,p and d-wave. We found the carrier concentration dependence of the coupling constants corresponding to these symmetries. At low hole doping the d-wave component is the largest one.

PACS: 71.27.+a, 74.20.-z, 74.25.Kc, 75.10.Lp
I. INTRODUCTION

Recently there appeared in the literature a number of papers dealing with the problem of electron–phonon interaction in strongly correlated superconductors\textsuperscript{1–9}. It turns out that interplay between Coulomb and electron–phonon interactions is very subtle and may result in an unexpected behaviour of various quantities\textsuperscript{10–13}.

The main motivation for all these studies come from experiments on high $T_c$ superconductors which in one or other way have pointed out the importance of electron–phonon interaction. There have been found Raman and infrared–active modes\textsuperscript{14} with strongly temperature dependent linewidth. Small, but nonzero, isotope shift exponent $\alpha$ ($T_c \propto M^\alpha$, where $M$ the ion isotope mass)\textsuperscript{15,16} is the strong indication of the electron–phonon coupling. Similar conclusions can be inferred from tunneling and photoemission\textsuperscript{17}, neutron\textsuperscript{18,19}, specific heat\textsuperscript{20}, thermal conductivity\textsuperscript{21,22} and other experiments.

It is the purpose of this paper to derive Eliashberg type\textsuperscript{23} equations valid for the strongly correlated superconductor with electron–phonon interaction. To this end we assume the validity of Migdal\textsuperscript{24} theorem which means that we assume relatively weak electron–phonon interaction. The strong correlations described by the Hubbard model will be treated via slave boson method. The derived equations are strongly anisotropic and lead to the possibility of various types of symmetries of order parameter. The relative stability of various symmetries does depend on the carrier concentration and other parameters.

In Section II we present the model Hamiltonian for strongly correlated systems and discuss the application of slave boson approximation to it in the $U = \infty$ limit, both in mean field and beyond it. The derivation of the Eliashberg equations on the real frequency axis is described in considerable detail in Section III. Section IV contains presentation of results and discussion.

II. THE MODEL

We start with the one band Hubbard model with general form of electron–phonon interaction term

$$H = \sum_{ij\sigma} (t_{ij} - \mu \delta_{ij}) \tilde{c}_{i\sigma}^+ \tilde{c}_{j\sigma} + \sum_{ij\sigma} T_{ij\sigma}^a u^a_{\alpha,\sigma} \tilde{c}_{i\sigma}^+ \tilde{c}_{j\sigma} + U \sum_i \tilde{n}_{i\uparrow} \tilde{n}_{i\downarrow} + H_{\text{ph}}. \quad (1)$$
Here $\tilde{c}_{i\sigma}^+(\tilde{c}_{i\sigma})$ is the creation (annihilation) operator for a spin $\sigma$ electron at site $i$ of the lattice, $u_i^\alpha$ is the $\alpha$–th component of the displacement vector of the ion, $\tilde{n}_{i\sigma} = \tilde{c}_{i\sigma}^+\tilde{c}_{i\sigma}$, $\mu$ denotes chemical potential, $t_{ij}$ is the hopping integral assumed to take on nonzero value $-t$ for $i, j$ being nearest neighbour sites, $U$ is the Hubbard on–site repulsion of carriers. $H_{ph}$ denotes the Hamiltonian of the lattice. The electron–lattice interaction described by the second term in (1) has two components

$$T_{ij}^\alpha = T_{ij}^\alpha + V_{ij}^\alpha \delta_{ij},$$

the first of which, $T_{ij}^\alpha$ has been derived from modulation of the hopping integral $t_{ij}$ in the deformed lattice. It is related to the derivative of $t_{ij}$ taken at equilibrium position of an ion

$$T_{ij}^\alpha = \frac{\partial t_{ij}}{\partial R_{ij}} \delta_{is} - \frac{\partial t_{ij}}{\partial R_{ij}} \delta_{js}.$$

The second part of the interaction i.e. the term $V_{ij}^\alpha$ is connected with fluctuations of the crystal field. Due to ionic character of high temperature superconductors this term is expected to be more important and has to be taken into account even if we have assumed the equilibrium value of crystal field $\varepsilon_i = t_{ii}$ to be zero. The systematic derivation and the discussion of the electron–ion interaction in context of superconducting oxides can be found in Ref. 26.

We are interested in the strong correlation limit, characterised by the large $U$ values ($U \gg W$, where $W = 8t$ is the width of electron band in a two dimensional square lattice). In this limit and for less than half filled band (i.e. concentration of carriers $n < 1$) it is very inconvenient for two carriers to occupy the same site $i$. It means that double occupation of sites is prohibited and the dynamics of carriers is limited to empty and singly occupied states. Thus we have to project out all the doubly occupied states of the system. This procedure is most conveniently carried out with the help of auxiliary particles and in the $U = \infty$ limit. One rewrites the electron operators in (1) in terms of new fermion operators $c_{i\sigma}^+(c_{i\sigma})$ and auxiliary boson operator $b_{i}^+(b_{i})$ as $\tilde{c}_{i\sigma}^+\tilde{c}_{j\sigma} \rightarrow c_{i\sigma}^+c_{j\sigma}b_{i}b_{j}^+$. The term $U$ may then be dropped out at the expense of introducing at each site a constraint

$$\sum_{\sigma} c_{i\sigma}^+c_{i\sigma} + b_{i}^+b_{i} = 1 \quad (2)$$

via Lagrange multiplier $\Lambda_i$. The constraint allows for at most single occupation of each size.

The Hamiltonian (1) then becomes

$$H = \sum_{ijs\alpha} t_{ij} c_{i\sigma}^+c_{j\sigma}b_{i}b_{j}^+ - \mu \sum_{i\sigma} c_{i\sigma}^+c_{i\sigma} + \sum_{ijs\alpha} T_{ij}^\alpha u_{i\alpha}^s c_{i\sigma}^+c_{j\sigma}b_{i}b_{j}^+$$

$$+ \sum_{i\sigma} V_{i\sigma}^\alpha u_{i\alpha}^s c_{i\sigma}^+c_{i\sigma} + \sum_{i} \Lambda_i (\sum_{\sigma} c_{i\sigma}^+c_{i\sigma} + b_{i}^+b_{i} - 1) + H_{ph}. \quad (3)$$
Note that on-site terms are not modified. It is connected with the meaning of the boson operators $b_i^+$ as operators creating empty states at site $i$. The hopping of a real electron from occupied state $j$ to an empty state at $i$, described by term $\tilde{c}_i^{+\sigma} \tilde{c}_j^{\sigma}$ in (1) consists of motion of a fermion between these sites ($c_i^{+\sigma} c_j^{\sigma}$) and at the same time the empty site moves from site $i$ to $j$ ($b_i^+ b_j^+$).

It has been shown that mean field description can be obtained by assuming average values $\langle b_i \rangle = \langle b_j^+ \rangle = r$ and $\Lambda_i = \Lambda$ at each site. Two parameters $r$ and $\Lambda$ entering the mean field Hamiltonian can be choosen so as to make minimal the ground state energy $E_{GS} = \langle H \rangle$. One gets:

\[
    r^2 = 1 - n
\]

\[
    -\Lambda = \frac{1}{N} \sum_{ij} t_{ij} \langle c_i^{+\sigma} c_j^{\sigma} \rangle + \frac{1}{N} \sum_{ij\sigma\sigma} T_{ij\sigma}^{\prime\prime} \langle u_s^{\alpha} c_i^{+\sigma} c_j^{\sigma} \rangle.
\]

Here $n = \frac{1}{N} \sum_{i\sigma} \langle c_i^{\sigma} c_i^{\sigma} \rangle$ denotes the concentration of electrons in the band ($n < 1$). There are two modifications of the spectrum of electrons encountered on the mean field level. First is the band narrowing described by $r^2$ and its shift described by $\Lambda$. The spectrum of noninteracting fermions in the mean field is given by $(r^2 \epsilon_k - \mu + \Lambda)$ instead of $(\epsilon_k - \mu)$ of original electrons (at $U = 0$). For the half filled band $n = 1$ the system is localised ($r = 0$). Here $\epsilon_k$ is the Fourier transform of $t_{ij}$.

To go beyond mean field approximation for slave bosons it is convenient to define boson fluctuating fields via: $b_i^+ = r + \delta b_i^+$, $b_i = r + \delta b_i$.

In view of our main goal in next section which is derivation of the Eliashberg equations, we shall write down the Hamiltonian in terms of Gorkov–Nambu field operators:

\[
    \psi_i = \begin{pmatrix} c_i^{\uparrow} \\ c_i^{\downarrow} \end{pmatrix} \quad \text{and} \quad \psi_j^+ = (c_j^{\uparrow}, c_j^{\downarrow}).
\]

Using this in (1) we obtain

\[
    H = H_{MF} + H' + H'',
\]

where in site representation

\[
    H_{MF} = \sum_{ij} (r^2 t_{ij} - \mu \delta_{ij}) \psi_i^+ \hat{\tau}_3 \psi_j + \sum_{ij\sigma} (r^2 T_{ij\sigma}^{\prime\prime} + V_{ij\sigma}^{\prime\prime}) u_s^{\alpha} \psi_i^+ \hat{\tau}_3 \psi_j
\]

\[
    + \Lambda \sum_i (\psi_i^+ \hat{\tau}_3 \psi_i + r^2 - 1) + H_{ph},
\]

\[
    H' = \sum_{ij} [r t_{ij} \psi_i^+ \hat{\tau}_3 \psi_j + \Lambda \delta_{ij}] (\delta b_i + \delta b_j^+) + \sum_{ij\sigma} r T_{ij\sigma}^{\prime\prime} u_s^{\alpha} \psi_i^+ \hat{\tau}_3 \psi_j (\delta b_i + \delta b_j^+) ,
\]

\[
    H'' = \Lambda \sum_i \delta b_i^+ \delta b_i + \sum_{ij} t_{ij} \psi_i^+ \hat{\tau}_3 \psi_j \delta b_i \delta b_j^+ + \sum_{ij\alpha s} T_{ij\sigma}^{\prime\prime} u_s^{\alpha} \psi_i^+ \hat{\tau}_3 \psi_j \delta b_i \delta b_j^+.
\]
First term of $H'$ describes fermion–boson interaction, while the last one fermion–phonon–boson interaction. More complicated interactions are contained in $H''$. They will be treated in a mean field type of approximation. The important point is that $H''$ significantly contributes to dynamics of fluctuating boson field. In the mean field approximation for electrons the boson fluctuations are described by effective Hamiltonian

$$H_B = \sum_i (\Lambda \delta_{ij} + t_{ij} \langle c_{i\sigma}^+ c_{j\sigma} \rangle) \delta b_j^+ \delta b_i$$  \hspace{1cm} (6)$$

For the sake of completeness we write down the Hamiltonian for phonons which we assume to be described in the harmonic approximation. In the second quantised form it reads

$$H_{ph} = \sum_{q\nu} \hbar \omega_{q\nu} (a_{q\nu}^+ a_{q\nu} + \frac{1}{2}).$$  \hspace{1cm} (7)$$

III. EQUATIONS OF SUPERCONDUCTIVITY

To properly describe the superconducting state in the system at hand one has to work in site representation. The important point is that in considered $U = \infty$ limit the double occupation of a given site is strictly forbidden. This means inter alia that correlation functions $\langle c_{i\uparrow}^+ c_{j\downarrow} \rangle$ describing superconducting pairs vanish exactly for $i = j$, i.e. the on–site pairing is forbidden. On the other hand the correlations of the type $\langle c_{i\sigma}^+ c_{i\sigma} \rangle$ measure the average number of carriers at site $i$, and are allowed to enter into formula. This important fact has first been noted by Zieliński and coworkers and leads, as we shall see, to severe changes in the form of Eliashberg equations.

To derive them we use the equation of motion method for the double time thermodynamic Green’s functions. For arbitrary operators $A$ an $B$ it reads (we employ here the Zubarev notation)

$$\omega \ll A|B \gg_\omega = \langle [A, B]_\pm \rangle + \ll [A, H]_-|B \gg_\omega$$

$$= \langle [A, B]_\pm \rangle - \ll A|[B, H]_- \gg_\omega,$$

where $\ll A|B \gg_\omega$ is the Fourier transformed, frequency dependent, retarded Green’s function. $[A, B]_\pm$ denotes anticommutator (+) or commutator (−).

Standard procedure leads to the following equation for the matrix Green’s function (GF)
\[
\sum_{l}\{\omega \hat{\tau}_0 + (\mu - \Lambda) \hat{\tau}_3\} \delta_{ij} - (r^2 + (\delta b_i \delta b_j^+)) t_{ij} \hat{\tau}_3 - \tilde{M}_d(\omega) \ll \psi_l |\psi_j^+ \gg_{\omega} = \delta_{ij} \hat{\tau}_0. \tag{8}
\]

Here \( \hat{\tau}_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \), \( \hat{\tau}_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \), \( \hat{\tau}_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \) are Pauli matrices and \( \tilde{M}_d \) denotes the matrix self-energy. Due to complicated interactions in the Hamiltonian \( \tilde{M}_d \) contains a number of terms. Here we write down few most important contributions.

The contribution from fermion–phonon scattering is given by

\[
\tilde{M}^{ph}_{ij}(\omega) = \sum_{i'} \sum_{\alpha' \alpha s} (r^2 T_{ij's}^\alpha + V_{js}^\alpha \delta_{ij}) (r^2 T_{i'j's'}^{\alpha'}) + V_{js'}^{\alpha'} \delta_{i'j'}) \hat{\tau}_3 \ll u_s^\alpha \psi_j^+ |u_{s'}^{\alpha'} \psi_j^+ \gg_{\omega} \hat{\tau}_3. \tag{9}
\]

The contribution from linear boson–fermion scattering reads

\[
\tilde{M}^B_{ij}(\omega) = \sum_{i'} t_{ij} t_{i'j'} \hat{\tau}_3 \ll \phi_{ij'}^B \psi_j^+ |\phi_{i'j'}^B \psi_j^+ \gg_{\omega} \hat{\tau}_3, \tag{10}
\]

with \( \phi_{ij}^B = \delta b_i + \delta b_j^+ \).

Related, but probably less important contribution from quadratic boson–fermion scattering (from \( H'' \))

\[
\tilde{M}^{Q}_{ij}(\omega) = \sum_{i'} t_{ij} t_{i'j'} \hat{\tau}_3 \ll \delta b_i \delta b_j^+ \psi_j^+ |\delta b_{i'} \delta b_{j'}^+ \psi_{j'}^+ \gg_{\omega} \hat{\tau}_3. \tag{11}
\]

This contribution is absent if one approximates \( H'' \) in mean field like manner.

There are also two contributions from three particle scattering events: fermion–phonon–slave boson. From \( H' \) part of the Hamiltonian we get

\[
\tilde{M}^{ph-B}_{ij}(\omega) = \sum_{i'} \sum_{\alpha' \alpha s} r^2 T_{ij's}^\alpha T_{i'j's'}^{\alpha'} \hat{\tau}_3 \ll \phi_{ij'}^B u_s^\alpha \psi_j^+ |\phi_{i'j'}^B u_{s'}^{\alpha'} \psi_j^+ \gg_{\omega} \hat{\tau}_3, \tag{12}
\]

while from second term in \( H'' \)

\[
\tilde{M}^{ph-B}_{ij}(\omega) = \sum_{i'} \sum_{\alpha' \alpha s} T_{ij's}^{\alpha} T_{i'j's'}^{\alpha'} \hat{\tau}_3 \ll u_s^\alpha \delta b_i \delta b_j^+ \psi_j^+ |u_{s'}^{\alpha'} \delta b_{i'} \delta b_{j'}^+ \psi_{j'}^+ \gg_{\omega} \hat{\tau}_3. \]

To get real frequency axis Eliashberg equations in a standard form\(^2\) one has to express the higher order Green’s function appearing on the rhs’ of various selfenergy pieces by the GF’s of fermions \( \ll \psi_l |\psi_k^+ \gg_{\omega} \), bosons \( \ll \delta b_p |\delta b_p^+ \gg_{\omega} \) and ,,phonons” \( \ll \phi_{q\nu} |\phi_{-q\nu} \gg_{\omega} \). This is easily achieved with help of spectral representation and decoupling of various time correlation functions as e.g.

\[
\langle \delta b_p(t) \phi_{q\nu}(t) \psi_k(t) \delta b_p^+(0) \phi_{q\nu}(0) \psi_k^+(0) \rangle \approx \langle \delta b_p(t) \delta b_p^+(0) \rangle \langle \phi_{q\nu}(t) \phi_{-q\nu}(0) \rangle \langle \psi_k(t) \psi_k^+(0) \rangle.
\]
This approximation neglects vertex corrections. In the present situations the vertex corrections stem from fermion–phonon, fermion–boson and also more complicated interactions. As already mentioned the assumption of small electron–phonon coupling allows us to neglect fermion–phonon vertex corrections. The same is not true for the fermion–boson vertices. They do not contain small parameters and should be taken into account. Their importance has also been stressed in previous studies. We shall postpone discussion of vertex corrections and concentrate on the anisotropy of Eliashberg equations.

The next step is Fourier transform of the various selfenergy parts. Defining the Fourier components of \( \hat{M}_{ij} \) by

\[
\hat{\Sigma}_k(\omega) = \frac{1}{N} \sum_{ij} e^{-ik(R_i-R_j)} \hat{M}_{ij}(\omega),
\]

we get

\[
\hat{\Sigma}_{k}^{\text{ph}}(\omega) = \frac{1}{N^2} \sum_{\vec{k},\vec{q},\nu} |M_{k,q}^{\nu}|^2 \tilde{\tau}_3 \ll \delta b^\nu _{\vec{q},\vec{k}} |\delta b^+ _{\vec{q},\vec{k}}| \gg \omega \tilde{\tau}_3 \frac{1}{N} \sum_{ij'} e^{-i(\vec{k}+\vec{q}-\vec{R}) (\vec{R}_{i'} - \vec{R}_{j'})},
\]

\[
\hat{\Sigma}_{k}^{B}(\omega) = \frac{1}{N^2} \sum_{\vec{k},\vec{q},\nu} \left\{ e^2_{\vec{k}-\vec{q}} \tilde{\tau}_3 \ll \delta b^\nu _{\vec{q},\vec{k}} |\delta b^+ _{\vec{q},\vec{k}}| \gg \omega \tilde{\tau}_3 \frac{1}{N} \sum_{ij'} e^{i(\vec{k}-\vec{q}-\vec{R})(\vec{R}_{i'} - \vec{R}_{j'})} \right\},
\]

\[
\hat{\Sigma}_{k}^{\text{ph-B}} = \frac{1}{N^3} \sum_{\vec{k},\vec{q},\vec{p}} \left\{ r^2 |\hat{M}_{k,q,p}^{\nu}|^2 \tilde{\tau}_3 \ll \delta b^\nu _{\vec{q},\vec{k}} |\delta b^+ _{\vec{q},\vec{k}}| \gg \omega \tilde{\tau}_3 \frac{1}{N} \sum_{ij'} e^{i(\vec{k}-\vec{q}-\vec{R})(\vec{R}_{i'} - \vec{R}_{j'})} + r^2 |\hat{M}_{k,q,p}^{\nu}|^2 \tilde{\tau}_3 \ll \delta b^\nu _{\vec{q},\vec{k}} |\delta b^+ _{\vec{q},\vec{k}}| \gg \omega \tilde{\tau}_3 \frac{1}{N} \sum_{ij'} e^{i(\vec{k}+\vec{p}-\vec{q})(\vec{R}_{i'} - \vec{R}_{j'})} \right\}. \tag{14}
\]

Here \( \phi_{\nu} = a_{\nu} + a^+_{-\nu} \) denotes the phonon field, \( a^+_{\nu} \) is creation operator of the \( q \nu \) phonon.

Electron–phonon matrix elements \( M_{kq}^{\nu} \) and \( \hat{M}_{k,q,p}^{\nu} \) are defined as

\[
|M_{k,q}^{\nu}|^2 = |g_{\nu}(\vec{q})|^2 |\sum_{\alpha} e_{\nu}^\alpha(\vec{q}) [r^2 V_{\nu}(\vec{v}^\alpha_{k-q} - \vec{v}^\alpha_{k}) + V_{\nu}(\vec{v}^\alpha_{q})]|^2,
\]

\[
|\hat{M}_{k,q,p}^{\nu}|^2 = V_{\nu}^2 |g_{\nu}(\vec{q})|^2 |\sum_{\alpha} e_{\nu}^\alpha(\vec{q}) (\vec{v}^\alpha_{k-q-p} - \vec{v}^\alpha_{k-p})|^2, \tag{15}
\]

and \( g_{\nu}(\vec{q}) = (\hbar/2\omega_{\nu}(\vec{q}) \cdot M)^{1/2} \), \( \vec{v}^\alpha_{k} = \frac{\partial \vec{v}^\alpha_{k}}{\partial \alpha} \), \( e_{\nu}^\alpha(\vec{q}) \) is the \( \alpha \)–th component of the phonon polarisation operator, while \( V_{\nu}^\alpha_{\vec{q}} \) is the Fourier transform of the ionic part of electron–phonon
interaction, $\omega_\nu(\vec{q})$ denotes the phonon dispersion and $M$ — the ionic mass. $V_c$ ($V_i$) denotes the strength of the covalent (ionic) part of electron–phonon interaction.

The factors of the type
\[
\frac{1}{N} \sum_{i'j'} e^{i\vec{k}_i' - \vec{k}_{j'}}
\]
are to be treated very carefully. As already mentioned the sum goes over all sites $i'$ and $j'$ if we evaluate the normal contributions to the self-energy matrix i.e. components (1,1) and (2,2) of the self–energy matrix which are proportional to the GF of the type $\langle \hat{O}_{c'\sigma} | \hat{O}' c_{j'\sigma}^+ \rangle$ ($\hat{O}, \hat{O}'$ are arbitrary operators). In such a case the above sum reduces to $N\delta_{k,0}$. When calculating off–diagonal elements of the selfenergy which depends on the GF's like $\langle \hat{O}_{c'\beta} | \hat{O}' c_{j'\gamma}^\dagger \rangle$ it is reasonable to assume $i'$ and $j'$ to be nearest neighbours, as in the $U = \infty$ limit only nearest neighbour pairs will probably survive. In this situation the sum reduces to $\gamma(\vec{k}) = -\epsilon(\vec{k})/2t$.

The approximation of the sum to $(i', j')$ being nearest neighbour sites relies on the experimental fact that the superconducting coherence length is small: of order of lattice spacing. In an effective theory like the one presented here it translates to nearest neighbour pairs.

To proceed we expand matrix selfenergy $\hat{\Sigma}_k(\omega)$ as
\[
\hat{\Sigma}_k(\omega) = \omega[1 - Z_k(\omega)]\hat{\tau}_0 + \phi_k(\omega)\hat{\tau}_1 + \chi_k(\omega)\hat{\tau}_3
\]
and write down the equations for various parts of it. We get
\[
\omega[1 - Z_k^{ph}(\omega)] = \frac{1}{2} \int d\omega_1 \int d\omega_2 \frac{t_h \delta_{\omega_1}}{2 \omega - \omega_1 - \omega_2} \frac{1}{N} \sum_{\vec{k}'} k^{ph}_{k\vec{k}'}(\omega_2) \cdot \left(-\frac{1}{\pi} \text{Im} \frac{\omega_1 Z_{\vec{k}}(\omega_1)}{D_{\vec{k}}(\omega_1)} \right)
\]
\[
\phi_k^{ph}(\omega) = \frac{1}{2} \int d\omega_1 \int d\omega_2 \frac{t_h \delta_{\omega_1}}{2 \omega - \omega_1 - \omega_2} \frac{1}{N} \sum_{\vec{k}'} k^{ph}_{k\vec{k}'}(\omega_2) \cdot \left(-\frac{1}{\pi} \text{Im} \frac{-\phi_{\vec{k}}(\omega_1)}{D_{\vec{k}}(\omega_1)} \right)
\]
\[
\chi_k^{ph}(\omega) = \frac{1}{2} \int d\omega_1 \int d\omega_2 \frac{t_h \delta_{\omega_1}}{2 \omega - \omega_1 - \omega_2} \frac{1}{N} \sum_{\vec{k}'} k^{ph}_{k\vec{k}'}(\omega_2) \cdot \left(-\frac{1}{\pi} \text{Im} \frac{r^2 \epsilon_{\vec{k}} - \mu + \Lambda + \sum_q \delta_{\vec{k}'-q} \delta_{b_q^\dagger b_q} + \chi_{\vec{k}}(\omega_1)}{D_{\vec{k}}(\omega_1)} \right)
\]
where we denoted $D_{\vec{k}}(\omega_1) = [\omega_1 Z_{\vec{k}}(\omega_1)]^2 - [\phi_{\vec{k}}(\omega_1)]^2 - [r^2 \epsilon_{\vec{k}} - \mu + \Lambda + \sum_q \delta_{\vec{k}'-q} \delta_{b_q^\dagger b_q} + \chi_{\vec{k}}(\omega_1)]^2$ and
\( K^{ph}_{kk'}(\omega_2) = \sum_{\nu} |M^{\nu}_{kk'}|^2 (-\frac{1}{\pi}) Im \ll \phi_{k-k',\nu} |\phi_{-k+k',\nu} \gg \omega_{2+i\omega} \),
(18)

\( \tilde{K}^{ph}_{kk'}(\omega_2) = \frac{1}{N} \sum_{q,\nu} |M^{\nu}_{kk'}|^2 (-\frac{1}{\pi}) Im \ll \phi_{q,\nu} |\phi_{-q,\nu} \gg \omega_{2+i\omega} \gamma(\vec{k} - \vec{q} - \vec{k}'). \)
(19)

Completely analogous set of equations is obtained for contributions to \( \tilde{\Sigma}_k^B(\omega) \). The only difference is that \( K^{ph}_{kk'} \) and \( \tilde{K}^{ph}_{kk'} \) will be replaced by \( K^B_{kk'} \) and \( \tilde{K}^B_{kk'} \), given by

\[ K^B_{kk'}(\omega_2) = \epsilon^2_k (-\frac{1}{\pi}) Im \ll \delta b_{k-k'}|\delta b^+_k \gg \omega_{2+i\omega} + \epsilon^2_k (-\frac{1}{\pi}) Im \ll \delta b_{-k+k'}|\delta b^+_k \gg \omega_{2+i\omega} , \]
(20)

and

\[ \tilde{K}^B_{kk'}(\omega_2) = \frac{1}{N} \sum_q \epsilon^2_k (-\frac{1}{\pi}) Im \ll \delta b_{q,\nu}|\delta b^+_q \gg \omega_{2+i\omega} \gamma(\vec{k} - \vec{q} - \vec{k}') + \epsilon^2_k \frac{1}{N} \sum_q \left(-\frac{1}{\pi}\right) Im \ll \delta b^+_q|\delta b_q \gg \omega_{2+i\omega} \gamma(\vec{k} - \vec{q} - \vec{k}') . \]
(21)

Due to complicated structure of the GF entering the expression for \( \tilde{M}^{ph,B}_k(\omega) \) the corresponding 

Eliasashberg equations on the real frequency axis have more complicated form

\[ \omega [1 - Z^{ph,B}_k(\omega)] = \frac{1}{4} \int d\omega_1 \int d\omega_2 \int d\omega_3 \frac{\mathcal{F}_{c\omega_1}(c\omega_2) + c\omega_2 c\omega_3 + 1}{\omega - \omega_1 - \omega_2 - \omega_3} \]
\[ \frac{1}{N} \sum_{k'} K^{ph,B}_{kk'}(\omega_2, \omega_3) (-\frac{1}{\pi}) Im \frac{\omega_1 Z_{k'}(\omega_1)}{D_{k'}(\omega_1)} \]

\[ \phi^{ph,B}_k(\omega) = \frac{1}{4} \int d\omega_1 \int d\omega_2 \int d\omega_3 \frac{\mathcal{F}_{c\omega_1}(c\omega_2) + c\omega_2 c\omega_3 + 1}{\omega - \omega_1 - \omega_2 - \omega_3} \]
\[ \frac{1}{N} \sum_{k'} \tilde{K}^{ph,B}_{kk'}(\omega_2, \omega_3) (-\frac{1}{\pi}) Im \frac{-\phi_{k'}(\omega_1)}{D_{k'}(\omega_1)} \]

\[ \chi^{ph,B}_k(\omega) = \frac{1}{4} \int d\omega_1 \int d\omega_2 \int d\omega_3 \frac{r^2 \epsilon^2_{k'}}{\omega - \omega_1 - \omega_2 - \omega_3} \]
\[ \frac{1}{N} \sum_{k'} K^{ph,B}_{kk'}(\omega_2, \omega_3) (-\frac{1}{\pi}) Im \frac{r^2 \epsilon^2_{k'} - \mu + \Lambda + \sum_q \epsilon^{-2}_{q,\nu}\langle \delta b_{q,\nu} \delta b^+_{q} \rangle + \chi'(\omega_1)}{D_{k'}(\omega_1)}, \]
(22)

with

\[ K^{ph,B}_{kk'}(\omega_2, \omega_3) = \frac{1}{N} \sum_{\rho,\nu} \left\{ r^2 |\tilde{M}^{\nu}_{kk',\rho}|^2 (-\frac{1}{\pi}) Im \ll \phi_{k',\nu} |\phi_{-k-k',\nu} \gg \omega_{2+i\omega} \right\} \]
\[ + r^2 |\tilde{M}^{\nu}_{kk',\rho}|^2 (-\frac{1}{\pi}) Im \ll \phi_{k',\nu} |\phi_{-k-k',\nu} \gg \omega_{2+i\omega} \gamma(\vec{k} \pm \vec{p} - \vec{q}) \]
\[ + r^2 |\tilde{M}^{\nu}_{kk',\rho}|^2 (-\frac{1}{\pi}) Im \ll \phi_{k',\nu} |\phi_{-k-k',\nu} \gg \omega_{2+i\omega} \gamma(\vec{k} + \vec{p} - \vec{q}) \]
\[ + r^2 |\tilde{M}^{\nu}_{kk',\rho}|^2 (-\frac{1}{\pi}) Im \ll \phi_{k',\nu} |\phi_{-k-k',\nu} \gg \omega_{2+i\omega} \gamma(\vec{k} - \vec{q}) \]
(23)
Equations (17–24) supplemented with expressions for phonon and slave–boson Greens functions form a complete set and have to be solved selfconsistently.

There are few differences between them and usual Eliashberg equations for superconductors. The most important is the presence of two different types of kernels $K_{kk'}$ and $\tilde{K}_{kk'}$ determining normal ($Z_{k'}, \chi_{k'}$) and anomalous ($\phi_{k'}$) parts of the self–energy, respectively.

Other point worth to mention is strong renormalisation of the bare electron spectrum $\epsilon_{\vec{k}} = -2t\gamma(\vec{k})$. At the mean field level of the theory it is both shifted and mass renormalised to $\vec{r}^2\epsilon_{\vec{k}} + \Lambda$. Beyond mean field level for bosons the nontrivial energy dependence comes from renormalisation of the fermion (matrix) Greens function given by the $\chi^B_{\vec{k}}(\omega)$ factor. Note, that from the equation for $\chi^B_{\vec{k}}(\omega)$ and definition (20) of $K^B_{\vec{k}\vec{k}'}(\omega)$ we have

$$\chi^B_{\vec{k}}(\omega) = C(\omega) + \epsilon_{\vec{k}}^2 C_1(\omega),$$

where $C(\omega)$ and $C_1(\omega)$ are weakly $\vec{k}$ dependent functions to be calculated from equation (17). To take this effect into account one has to solve the equations at each point of the Brillouin zone — a very difficult task.

**IV. RESULTS AND DISCUSSION**

The complete solution of Eliashberg equations which are integral equations with complicated kernels would require finding all functions $Z_{k}(\omega), \phi_{k}(\omega), \chi_{k}(\omega)$ at all frequencies and all points in the Brillouin zone. In the standard approach the valid argument was that most important changes are to be expected at the Fermi level. The various pieces of selfenergies were thus averaged over the wave vectors lying on the Fermi surface. In this way it was possible to reduce the equations to the integral equation of the single variable: the frequency. It is not obvious that the same arguments do apply in the present case especially to the boson contribution to self–energy.

Sticking to the mean field approximation for slave bosons leads to $\delta b_\vec{q} = \delta b^+_{\vec{q}} \equiv 0$. In this approximation only phonon contribution to $\Sigma_{\vec{k}}$ survives, $\hat{\Sigma}_{k}(\omega) = \Sigma^\text{ph}_k(\omega)$. In this case most of arguments developed previously[13] apply and one can use known parametrisations of solutions to Eliashberg equations. The relevant parameters describing superconducting transition temperature $T_c$ are the typical phonon frequency $\omega_D$ and electron–phonon parameter $\lambda_{e-ph}$. The
last parameter is determined by the kernel $K^{\text{ph}}$. In our theory we do have two different kernels as also found previously by Zieliński and coworkers.\[44x730]

We thus define two coupling constants $\lambda_{e-ph}$ and $\tilde{\lambda}_{e-ph}$. The first one is related to wave function renormalisation and other describes genuine superconducting coupling in strongly correlated system. We define $\lambda_{e-ph}$ by $\[44x687\]$.

$$\lambda_{e-ph} = 2 \int \frac{d\omega}{\omega} \alpha^2 F(\omega)$$

(26)

where

$$\alpha^2 F(\omega) = \frac{1}{N} \sum_{kk'} R^{\text{ph}}_{kk'}(\omega) \delta(\epsilon_k^2 - \mu + \Lambda) \delta(\epsilon_{k'}^2 - \mu + \Lambda) \sum_k \delta(\epsilon_k^2 - \mu + \Lambda)$$

Similar expression defines $\tilde{\lambda}_{e-ph}$ except that $\tilde{R}^{\text{ph}}_{kk'}(\omega)$ enters. In the general case there exist four more parameters: $\lambda_{e-B}, \tilde{\lambda}_{e-B}, \lambda_{e-ph-B}$ and $\tilde{\lambda}_{e-ph-B}$.

For numerical purposes it is convenient to take optical phonons with $\omega_{q\nu} = \omega_o$. In this case the frequency integral in (26) can be calculated very easily.

Strong wave vector dependence of the kernels $\tilde{R}^{\text{ph}}_{kk'}(\omega)$ makes the question of symmetry of the order parameter very important. To get some information on this point we calculate various symmetry components $\lambda_{i-e-ph}$ of the pairing interaction. We define them as $\[44x323\]$

$$\tilde{\lambda}_{i-e-ph}^i = \frac{1}{N} \sum_{kk'} \tilde{R}^{\text{ph}}_{kk'} \delta(\epsilon_k^2 - \mu + \Lambda) \delta(\epsilon_{k'}^2 - \mu + \Lambda) \delta_g(\epsilon_k) \delta_g(\epsilon_{k'}) / A_i$$

We have taken $g_1 = \cos k_x a + \cos k_y a$, $g_2 = \cos k_x a - \cos k_y a$, $g_3 = \sin k_x a + \sin k_y a$ and $g_4 = \sin k_x a - \sin k_y a$; $A_i = \sum_k g_i^2(\epsilon_k^2 - \mu + \Lambda)$.

There are few parameters which control the behaviour of the system. These are: carrier concentration $n$, strength of the electron – phonon interaction parameters $V_c$ and $V_i$, the frequency $\omega_0$ of the optical phonon etc. All the energies are measured in units of $D = 2t$, and for numerical purposes we have taken $\omega_0 = 0.02$, and the value of the ionic mass $M$ appropriate for oxygen.

In this work we shall concentrate on the results obtained from the kernel $\tilde{R}^{\text{ph}}_{kk'}$, describing anomalous part of the self–energy. In the previous work\[44x332\] we have analysed in some detail the properties of the system resulting from the kernel entering normal self–energy.

We start the discussion by showing the results obtained for $V_i = 0$. The covalent part of the interaction is strongly $\tilde{k}$ dependent. It is described by the matrix element $|M_{\tilde{k}q}|^2$ in equation (15). In figure (1a) we show the results obtained by making the same approximation as in previous treatment of the similar model\[44x381\] where $|M_{\tilde{k}q}|^2$ has been replaced by wave vector.
independent constant multiplied by \( r^4 \). The concentration dependence of \( s, p \) and \( d \) components of the coupling constant are shown by solid, dotted and dashed lines, respectively. It is the factor \( r^4 = (1-n)^2 \), which strongly supresses the values of \( \tilde{\lambda}_i \) at higher electron concentrations. The important point is that for small doping of holes the d-wave component is the largest one. This signals the possibility of the d-wave pairing in this parameter range. For \( \delta = 1-n > 0.3 \) the p-wave pairing takes over. At quite small electron concentrations extended s-wave seem to be most stable pairing.

In figure (1b) we show similar set of data obtained with \(|M_{\vec{k}\vec{q}}|^2\) replaced by its Fermi surface average \( M^2 \). Due to oscillatory dependence of \(|M_{\vec{k}\vec{q}}|^2\) on wave vectors the average value of it is strongly concentration dependent (solid line in figure (1b)) and reduced in comparison to 1 (the value arbitrarily assumed for data shown in Fig.(1a)). Small values of \( M_F \) at large \( n \) are due again to \( r^4 \) factor, while at small \( n \) to phase space restrictions.

Taking the full wave vector dependence of \(|M_{\vec{k}\vec{q}}|^2\) leads to the results shown in figure (1c). Solid line in this figure shows total coupling \( \tilde{\lambda}_{el-ph} \) calculated from (26). Other lines represent the symmetry components \( \tilde{\lambda}_i \) as indicated. The values of all couplings are very small. Thus in the mean field approximation for slave bosons one is not able to get realistic values of the superconducting transition temperature from covalent part of the electron-phonon interaction. Let us look at the relative values of the various couplings. At large electron concentration (small hole doping) the d-wave component of \( \tilde{\lambda} \) exceeds by far all other components.

Bigger values of coupling constants are obtained when ionic part of the electron–phonon interaction is taken into account. Figure (2a) shows the concentration dependence of \( \tilde{\lambda} \) (solid line) and \( \tilde{\lambda}_i \) (dashed lines) obtained for \( V_c = 0 \) and \( V_i = 1 \) (in units of \( D \)). The values of the coupling parameters are quite realistic now. The nice feature of this result is the possibility of d symmetry pairing at small hole concentration. The presence of both ionic and covalent parts of electron-phonon interaction leads to small changes of the phase diagram (cf. Fig.2(b)) . The d symmetry remains most probable at small hole dopings \( \delta < 0.3 \). For intermediate carrier concentrations p-wave pairing is most stable, while extended s-wave is stable at small electron concentration \( n < 0.3 \). The slight decrease of the values of couplings as compared to figure (2a) is due to interference effects between interaction channels (cf. expression (15) for \(|M_{\vec{k}\vec{q}}|^2\)). In this work we have concentrated on the calculation of the electron–phonon coupling constants. To obtain realistic estimations of the concentration dependence of the superconducting transition temperature one has to take simultaneously into account the condensation of the (slave) bosons. Boson condensation temperature \( T^B_c \) of the 3d massive bosons is proportional to the
2/3 power of the boson concentration \((1 - n)\). For the massless bosons the power changes to 1/3 in 3d case and 1/2 for interesting case of two dimensional system. Because superconducting transition temperature, in the systems with covalent coupling (c.f. figures 1a,1b,1c), also vanishes for \(n \to 1\), the additional condition for Bose – Einstein condensation can change the phase diagram in quantitative way only. The situation is different in systems with ionic or mixed (covalent plus ionic) interactions and especially for the phase with \(d\)-wave symmetry of the order parameter. The coupling constant \(\lambda_d\) takes on sizeable values (c.f. figs. 2a and 2b) at low hole concentration. In this case the additional condition will modify the \(T_c vs. n\) phase diagram making it qualitatively more similar to that obtained for covalent electron – phonon interaction.

In conclusion we have presented the derivation of the Eliashberg equations for the system with strong electron – electron and electron – phonon interactions. The results show the importance of the correlations which make the superconducting order parameter very anisotropic. Its symmetry depends on the carrier concentration. We have illustrated the theory by showing the results of calculations of coupling constants in the mean field approximation for slave bosons.

As already mentioned beyond mean field level there are important changes of the structure of the theory. The mixed fermion – phonon – slave boson contribution to the selfenergy and corresponding coupling constants will overtake the fermion – phonon contributions considered here. The \(\chi\) component of the selfenergy due to fermion – slave boson scattering acquires nontrivial energy \(\epsilon_{\vec{k}}\) dependence. The study of both these effects will be reported in the forthcoming paper.

**Acknowledgements:** This work has been supported by KNB grant No. 2P 302 070 06. Stimulated discussions with profs. M. Grilli, J. Ranninger, R. Zeyher and J. Zieliński done during acknowledged. Part of the work has been done during author’s stay in ISI Torino sponsored by the European Community.
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FIGURES

FIG. 1. The concentration dependence of the coupling constants \( \tilde{\lambda}_i \) calculated for a model with \( V_i = 0, V_c = 1 \) and: (a) constant value of the electron – phonon matrix element \( |M_{\vec{k}\vec{q}}| = 1.0 \), (b) \( |M_{\vec{k}\vec{q}}| \) averaged over the Fermi surface and (c) the actual value \( |M_{\vec{k}\vec{q}}| \) with full wave vector dependence taken into account.

FIG. 2. The pairing coupling constants vs \( n \) for a model with: (a) ionic electron – phonon interaction \( (V_i = 1, V_c = 0) \) and (b) both ionic and covalent interactions \( (V_i = 1, V_c = 1) \)
