Superconductivity in two-band non-adiabatic systems.

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Theory of superconductivity in two-band non-adiabatic systems with strong electron correlations in the linear approximation over non-adiabaticity is built in the article. Having assumed weak electron-phonon interaction analytical expressions for the vertex functions $P_{Vn}$ and “intersecting” functions $P_{Cn}$ for each energy band ($n = 1, 2$) are obtained. Mass operators of Green functions with account of diagrams with intersection of two lines of electron-phonon interaction (exceeding the frameworks of Migdal theorem) are derived as well as main equations of theory of superconductivity in two-band systems. Analytical formulas for the temperature of superconducting transition $T_C$ are obtained as well as renormalization of the quantities which enter these formulas because of effects of non-adiabaticity and strong electron correlations. Dependence of $T_C$ and coefficient of isotope effect $\alpha$ on Migdal parameter $m = \omega_0/\varepsilon_F$ is studied. Overlapping of energy bands on Fermi surface with effects of non-adiabaticity at low values of transferred momentum ($q \ll 2p_F$) is shown to obtain high values of $T_c$ even assuming weak electron-phonon interaction.

1. Introduction

There have been 20 years since the discovery of high-$T_c$ materials [1]. There have been made thorough experimental and theoretical studies of properties of these materials in normal and superconducting state. It is established the significant distinction of physical properties in comparison with the case of ordinary superconductors. New high-$T_c$ materials have some peculiarities such as strong anisotropy of crystalline properties (layered structure), strong electron correlations, strong electron-phonon interaction, presence of the points with high symmetry in the momentum space, overlapping of energy bands on Fermi surface, small values of Fermi energy. Sophisticated nature of these systems makes it difficult to solve one the main problems of modern physics - to find the real mechanism of high-$T_c$ superconductivity. Thorough consideration of all peculiarities in these materials is one of the possible solutions of this problem as well as study of their influence on thermodynamic and magnetic properties of system.

In order to study effect of overlapping of energy bands on Fermi surface, for example, which results in two energy gaps there was used the model proposed by Moscalenco [2].
(see also Suhl et al. [3]). Theory of superconductivity for ordinary superconductors (pure and doped) which is based on this model was build long before the discovery of high-$T_C$ materials (see history of this development in [4], [5]).

The application of this theory to the high-$T_C$ materials was done by us and other authors (see references in [6]). A great number of experimental data over superconducting properties of the metal-oxide compounds are showed to be understood in the frameworks of this theory [6].

From the other hand, there are some questions and the role of non-adiabaticity should be explained as well as of strong electron correlations in high-$T_C$ materials. More specifically, we have the case with low values of Fermi energy ($\varepsilon_F \ll \omega_D$) or when it is compared with Debye energy ($\varepsilon_F \sim \omega_D$), and great values of Coulomb interaction between electrons. These factors can not favor the high-$T_C$ superconductivity within the frameworks of the BCS-Bogolyubov-Eliashberg-Migdal theory. In addition, this theory is not valid to describe non-adiabatic systems when Migdal theorem is broken down [7]. That is why there is necessity to take into consideration vertex and "intersecting" diagrams over electron-phonon interaction (additional multi-particle effects) at determining Green functions.

There is great number of works which study superconductivity in non-adiabatic systems and build the theory of superconductivity by going beyond Migdal theorem (see review [8]). The vertex functions at ($\varepsilon_F \sim \omega_D$) is followed from these studies to be negative and as result to decrease the coupling of electron-phonon interaction which in its turn does not give the high values of the temperature of superconducting transition $T_C$. The opposite picture we have when the transferred momentum of electron-phonon interaction is small ($q \ll 2p_F$). Such a specific case arises when strong electron correlation are taken into account [9], [10]. A non-adiabatic system with half-filling of energy band have been studied in works [11], [12] where the cutoff of the electron-phonon interaction over the transferred momentum $q_c \ll 2p_F$. In this way the vertex $P_V$ and intersecting $P_C$ functions are positive and favor the significant increase of the coupling of electron-phonon interaction, rising as a result the temperature of superconducting transition up to the values of high-$T_C$ materials. Positive values of $P_V$ and $P_C$ are also possible in the non-adiabatic systems with van Hove singularities in the electron energy spectrum. This is observed clearly, for instance, in the case of the "extended" singularity in electron energy spectrum [13], which is found experimentally in yttrium ceramics [14].

Note that studies of thermodynamic properties of one-band superconducting non-adiabatic system with variable density of charge carriers (pure and with magnetic impurity) have been performed by one of the authors [15], [16]. These studies show that non-adiabaticity favors the superconductivity of one-band systems as well as strong electron correlations.
Intensive investigations of new superconducting materials have been made for last five years. Compound $MgB_2$ with $T_c \sim 40k$ [17] is of great interest. This compound has some anomalies amongst its physical properties (see, for example, reviews [18], [19]). These anomalies are established to be caused by properties of system anisotropy and, in particular, by overlapping of energy bands on Fermi surface. The theory of superconductivity with energy bands that overlap on Fermi surface[2], [18] - [22] has been put into the kernel of description of the properties of $MgB_2$ compound. The effects of non-adiabaticity can play significant role in establishing properties of $MgB_2$ compound because Migdal parameter in these compounds $m = \frac{\omega D}{\varepsilon_F} \approx 0.1$ [23].

Therefore, modern high-$T_C$ superconductors (oxide metals, fullerenes, organic systems, boride magnesium) are non-adiabatic systems. In addition to this electron energy spectrum has essential peculiarity - overlapping of energy bands on Fermi surface what is proved by band calculations (see, for example, 24 -27). All this encourages us to build theory of superconductivity in two-band non-adiabatic systems. This article is aimed to perform this task. The article is designed in the following way:

Having based on the Hamiltonian of Frolich type the equations for temperature electron Green functions are obtained in section 2 as well as equations for mass operators $M$ and $\Sigma$. Transition to the band representation has been performed as well $n\vec{k}\tilde{\Omega}$ - representation. Definitions of vertex $P_{Vn}$ and ”intersecting” $P_{Cn}$ functions of each energy band are given in section 3. The system of equation for order parameters of two-band system is also derived here.

The equation for the temperature of superconducting temperature $T_C$ has been obtained in section 4 and its solution have been found as well. In addition the coefficient of isotope effect $\alpha$ is determined also.

Numerical calculations are performed in section 5 as well as the analysis of results.

2. Hamiltonian of the system and Green functions.

We start with Frolich type Hamiltonian

$$H = H_0 + H_1,$$

where $H_0$ is Hamiltonian of non-interacting electrons and phonons, and $H_1$ is electron-phonon interaction determined by expression

$$H_1 = \sum_{\sigma} \int d\vec{x} \psi_\sigma^+(\vec{x}) \psi_\sigma(\vec{x}) \varphi(\vec{x}).$$
Here $\psi_\sigma^+(\vec{x})$ and $\psi_\sigma(\vec{x})$ are creation and annihilation operators of electrons with spin $\sigma$ at the point $\vec{x}$. Having based on the Hamiltonian (1) and using diagrammatic method of the perturbation theory [28] we obtain the system of equations for normal $G(x, x')$ and abnormal $\tilde{F}(x, x')$ Green function:

\[
G(x, x') = G^0(x, x') + \int \int dx_1 dx_2 G^0(x, x_1)M(x_1, x_2)G(x_2, x') - \int \int dx_1 dx_2 G^0(x, x_1)\Sigma(x_1, x_2)\tilde{F}(x_2, x'),
\]

\[
\tilde{F}(x, x') = \int dx_1 dx_2 G^0(x_1, x)\tilde{\Sigma}(x_1, x_2)G(x_2, x') + \int dx_1 dx_2 G^0(x_1, x)M(x_2, x_1)\tilde{F}(x_2, x').
\] (3)

Because of absence of spin interactions in (1) to obtain the system (3) we used the following relationships:

\[
G_{\alpha\beta}(x, x') = \delta_{\alpha\beta}G(x, x'); \quad \tilde{F}_{\alpha\alpha'}(x, x') = -g_{\alpha,\alpha'}\tilde{F}(x, x'),
\] (4)

where

\[
g_{\alpha,\alpha'} = \delta_{\alpha,-\alpha'}(\delta_{\alpha\uparrow} - \delta_{\alpha\downarrow}) = -g_{\alpha',\alpha}.\] (5)

Mass operators diagonal $M$ and non-diagonal $\Sigma$ at temperatures close to the critical ($T \sim T_C$) have the following form:

\[
M(x_1, x_2) = -D(x_1, x_2)G(x_1, x_2) + \int \int dx_3 dx_4 D(x_4, x_2)D(x_1, x_3)\times
\]

\[
\times G(x_1, x_4)G(x_4, x_3)G(x_3, x_2),\] (6)

\[
\Sigma(x_1, x_2) = -D(x_1, x_2)F(x_1, x_2) + \int \int dx_3 dx_4 D(x_1, x_3)D(x_4, x_2)\times
\]

\[
\times [G(x_1, x_4)G(x_2, x_3)F(x_4, x_3) + G(x_3, x_4)F(x_1, x_4)G(x_2, x_3) +
\]

\[
+ F(x_3, x_2)G(x_1, x_4)G(x_4, x_3)] - F(x_1, x_3)\tilde{F}(x_3, x_4)F(x_4, x_2).\] (7)

As follows from (6) and (7) there are diagrams with intersection of two lines of electron-phonon interaction as well as diagrams that enter the mass operators in adiabatic systems. Account of these terms represents the vertex corrections and exceedance beyond bounds.
of Migdal theorem [7]. We go in (3), (6) and (7) to \( n\vec{k}\Omega \) representation in accordance with decompositions of Green functions:

\[
G(x, x') = \frac{1}{\beta} \sum_{k k'} \sum_{n m} \sum_{\Omega} G_{n m}(\vec{k}, \vec{k}', \Omega) \psi_{n \vec{k}}(\vec{x}) \psi_{m \vec{k}'}^*(\vec{x}') e^{-i\Omega(\tau - \tau')},
\]

\[
F(x, x') = \frac{1}{\beta} \sum_{k k'} \sum_{n m} \sum_{\Omega} F_{n m}(\vec{k}, \vec{k}', \Omega) \psi_{n \vec{k}}(\vec{x}) \psi_{m \vec{k}'}^*(\vec{x}') e^{-i\Omega(\tau - \tau')},
\]

\[
\tilde{F}(x, x') = \frac{1}{\beta} \sum_{k k'} \sum_{n m} \sum_{\Omega} \tilde{F}_{n m}(\vec{k}, \vec{k}', \Omega) \psi_{n \vec{k}}^*(\vec{x}) \psi_{m \vec{k}'}^*(\vec{x}') e^{-i\Omega(\tau - \tau')},
\]

and for mass operators as well

\[
M(x, x') = \frac{1}{\beta} \sum_{k k'} \sum_{n m} \sum_{\Omega} M_{n m}(\vec{k}, \vec{k}', \Omega) \psi_{n \vec{k}}(\vec{x}) \psi_{m \vec{k}'}^*(\vec{x}') e^{-i\Omega(\tau - \tau')},
\]

\[
\Sigma(x, x') = \frac{1}{\beta} \sum_{k k'} \sum_{n m} \sum_{\Omega} \Sigma_{n m}(\vec{k}, \vec{k}', \Omega) \psi_{n \vec{k}}(\vec{x}) \psi_{m \vec{k}'}^*(\vec{x}') e^{-i\Omega(\tau - \tau')},
\]

\[
\tilde{\Sigma}(x, x') = \frac{1}{\beta} \sum_{k k'} \sum_{n m} \sum_{\Omega} \tilde{\Sigma}_{n m}(\vec{k}, \vec{k}', \Omega) \psi_{n \vec{k}}^*(\vec{x}) \psi_{m \vec{k}'}^*(\vec{x}') e^{-i\Omega(\tau - \tau')},
\]

where \( \psi_{n \vec{k}}(\vec{x}) = e^{i\vec{k}\vec{x}} U_{n \vec{k}}(\vec{x}) \) is Bloch function.

Having substituted (8) and (9) in (3) and performed all necessary actions we obtain the system of equations for \( G_{n m}(\vec{k}, \vec{k}', \Omega) \) and \( \tilde{F}_{n m}(\vec{k}, \vec{k}', \Omega) \). Solution of this system of equations and thermodynamic properties of two-band superconductors without effects of non-adiabaticity are presented in works [29], [30]. In this way all possible superconducting pairings between electrons in each energy band and between electrons from different bands are taken into consideration.

Hereinafter we restrict ourselves by approximation diagonal indexes over bands:

\[
G_{n m}(\vec{k}, \vec{k}', \Omega) = \delta_{\vec{k}, \vec{k}'} \delta_{n m} G_n(\vec{k}, \Omega); \quad \tilde{F}_{n m}(\vec{k}, \vec{k}', \Omega) = \delta_{\vec{k}, -\vec{k}'} \delta_{n m} \tilde{F}_n(\vec{k}, \Omega).
\]

If we do not take into consideration the effects, connected with non-adiabaticity of a system this approximation leads to two-band model of Moscalenco [2]. This model corresponds to the formation of the cooper pairs inside each energy band and their tunneling from one energy band to another one. In approximation (10) solution of equation (3) can be presented in the form:

\[
G_n(\vec{k}, \Omega) = -\frac{iZ_n(\Omega) \Omega + \tilde{\varepsilon}_n(\vec{k})}{A_n(\vec{k}, \Omega)}, \quad \tilde{F}_n(\vec{k}, \Omega) = \frac{\Sigma_n(\vec{k}, \Omega)}{A_n(\vec{k}, \Omega)}, \quad F_n(\vec{k}, \Omega) = \frac{\Sigma_n(\vec{k}, \Omega)}{A_n(\vec{k}, \Omega)},
\]
where

\[ A_n(\vec{k}, \Omega) = \Omega^2 Z_n^2(\Omega) + \varepsilon_n^2(\vec{k}) + \Sigma_n(\vec{k}, \Omega) \Sigma_n(\vec{k}, \Omega), \]
\[ Z_n(\Omega) = 1 - \frac{1}{\Omega} Im M_n(\vec{k}, \Omega), \quad \varepsilon_n(\vec{k}) = \varepsilon_n(\vec{k}) + Re M_n(\vec{k}, \Omega). \]  

(12)

\[ M_n \text{ and } \Sigma_n \text{ are mass operators in } n\vec{k}\Omega \text{ representation that are determined by expressions (6) and (7) and take into account diagrams which breaks down Migdal theorem.} \]

3. Mass operators and vertex functions.

Having gone to \( n\vec{k}\Omega \) - representation in definitions of mass operators (6) and (7) in accordance with the decompositions (8) and (9) we obtain:

\[ M_m(\vec{p}, \Omega) = -\frac{1}{\beta} \sum_{\vec{p}_1} \sum_{\Omega_1} \sum_n D(\vec{p} - \vec{p}_1, \Omega - \Omega_1) g_{mn}^2(p, p_1) G_n(\vec{p}_1, \Omega_1) + \]
\[ + \frac{1}{\beta^2} \sum_{\vec{p}_1, \vec{p}_2} \sum_{\Omega_1, \Omega_2} D(\vec{p} - \vec{p}_1, \Omega - \Omega_1) D(\vec{p} - \vec{p}_2, \Omega - \Omega_2) g_{mn}^2(\vec{p}, \vec{p}_1) g_{mn}^2(\vec{p}, \vec{p}_2). \]

(13)

\[ G_m(\vec{p}_1, \Omega_1) G_m(\vec{p}_1 + \vec{p}_2 - \vec{p}, \Omega_1 + \Omega_2 - \Omega) G_m(p_2, \Omega_2), \]
\[ \Sigma_m(\vec{p}\Omega) = -\frac{1}{\beta} \sum_{\vec{p}_1} \sum_{\Omega_1} \sum_{m_1} D(\vec{p} - \vec{p}_1, \Omega - \Omega_1) g_{m_1}^2(\vec{p}, \vec{p}_1) F_{m_1}(\vec{p}_1, \Omega_1) + \]
\[ + \frac{1}{\beta^2} \sum_{\vec{p}_1, \vec{p}_2} \sum_{\Omega_1, \Omega_2} D(\vec{p} - \vec{p}_1, \Omega - \Omega_1) D(p - p_2, \Omega - \Omega_2) g_{mn}^2(\vec{p}, \vec{p}_2) g_{mn}^2(\vec{p}, p_1) [G_m(\vec{p}_2, \Omega_2) \times \]
\[ \times F_m(\vec{p}_1, \Omega_1) G_m(\vec{p}_2 + \vec{p}_1 - \vec{p}, \Omega_2 + \Omega_1 - \Omega) + \]
\[ + F_m(\vec{p}_1, \Omega_1) G_m(\vec{p}_2, \Omega_2) G_m(\vec{p}_2 - \vec{p}_1 - \vec{p}, \Omega_2 - \Omega_1 - \Omega) + \]
\[ + F_m(\vec{p}_1, \Omega_1) G_m(\vec{p} - \vec{p}_1 - \vec{p}_2, \Omega - \Omega_1 - \Omega_2) G_m(-\vec{p}_2, -\Omega_2)]. \]

(14)

Here there was used the approximation over band indexes (10) and approximation for matrix elements of electron-phonon interaction that corresponds to the tunneling of electron pairs as a whole from one energy band to another (Moscalenoco model [2]):

\[ g_{mn}^2(\vec{p}, \vec{p}_1) = g^2(\vec{p}, \vec{p}_1) |\chi(m\vec{p}_F, n\vec{p}_1F)|^2, \]

(15)

where

\[ \chi(m\vec{p}_F, n\vec{p}_1F) = \int d\vec{r} U_{m\vec{p}_F}^*(\vec{r}) U_{n\vec{p}_1F}(\vec{r}) \]

(16)
$m; n = 1, 2, V_0$ is volume of the basic cell.

Assume that strong electron correlations [9],[10] can lead to low values of transferred momentum $\vec{q}$ in electron-phonon interaction. In accordance with this assumption we represent $g_{mn}(\vec{p}\vec{p'})$ in the following form:

$$g_{mn}(\vec{p},\vec{p'}) = g_{mn}^2 \eta \theta(q_c - |\vec{p} - \vec{p'}|),$$  \hspace{1cm} (17)

where $q_c$ is cut-off momentum of electron-phonon interaction, $\eta$ is determined by relation

$$\eta \ll \theta(q_c - |\vec{p} - \vec{p'}|) \gg_{FS} 1,$$  \hspace{1cm} (18)

where $\ll g_{mn}(pp') \gg_{FS} g_{mn}$. Here $\ll \ldots \gg_{FS}$ means averaging over Fermi surface.

We choose phonon Green function $D(\Omega \Omega_1)$ with simple Einstein spectrum (characteristic frequency of which is $\omega_0$):

$$D(\Omega, \Omega_1) = -\frac{\omega_0^2}{(\Omega - \Omega_1)^2 + \omega_0^2},$$  \hspace{1cm} (19)

and introduce vertex functions ($n = 1, 2$):

$$P_{Vn}(\vec{p}, \vec{p}_1, \Omega, \Omega_1) = -\frac{1}{\beta} \frac{\eta}{N_n} \sum_{\vec{p}_2} \sum_{\Omega_2} \theta(q_c - |\vec{p} - \vec{p}_2|) D(\Omega, \Omega_2) G_n(\vec{p}_2, \Omega_2) \times$$

$$\times G_n(\vec{p}_1 + \vec{p}_2 - \vec{p}, \Omega_1 + \Omega_2 - \Omega),$$

$$P_{Cn}(\vec{p}, \vec{p}_1, \Omega, \Omega_1) = -\frac{1}{\beta} \frac{\eta}{N_n} \sum_{\vec{p}_2} \sum_{\Omega_2} \theta(q_c - |\vec{p} - \vec{p}_2|) D(\Omega, \Omega_2) G_n(\vec{p}_2, \Omega_2) \times$$

$$\times G_n(\vec{p}_1 - \vec{p}_2 - \vec{p}, \Omega_1 - \Omega_2 - \Omega),$$

$$P_{Vn}'(\vec{p}, \vec{p}_1, \Omega, \Omega_1) = -\frac{1}{\beta} \frac{\eta}{N_n} \times$$

$$\times \sum_{\vec{p}_2} \sum_{\Omega_2} \theta(q_c - |\vec{p} - \vec{p}_2|) D(\Omega, \Omega_2) G_n(\vec{p}_2 - \vec{p}_1 - \vec{p}_2, \Omega - \Omega_1 - \Omega_2) G_n(-\vec{p}_2, -\Omega_2).$$  \hspace{1cm} (20)

Having used further the representation (17), (20) and performed averaging over Fermi surface in equation (13) and (14), we derive

$$\ll M_m(\vec{p}\Omega) \gg_{FS} M_m(\Omega) = -$$

$$-\frac{1}{\beta} \sum_{\vec{p}_t} \sum_{\Omega_1} g_{mn}^2 D(\Omega, \Omega_1) G_m(\vec{p}_1, \Omega_1) \left[ 1 + g_{mm}^2 P_{Vm}(Q_c, \Omega, \Omega_1) \right] -$$
\[-\frac{1}{\beta} \sum_{\vec{p}_i, \Omega_1} g_{mn}^2 D(\Omega, \Omega_1) G_n(\vec{p}_1, \Omega_1), \tag{21}\]

\[\Sigma_1(\Omega) = -\frac{1}{\beta} \sum_{\vec{p}_i, \Omega_1} D(\Omega, \Omega_1) \tilde{V}_{11}(\Omega, \Omega_1) F_1(\vec{p}_1, \Omega_1) - \frac{1}{\beta} \sum_{\vec{p}_i, \Omega_1} D(\Omega, \Omega_1) g_{12}^2 F_2(\vec{p}_1, \Omega_1),\]

\[\Sigma_2(\Omega) = -\frac{1}{\beta} \sum_{\vec{p}_i, \Omega_1} D(\Omega, \Omega_1) g_{21}^2 F_2(\vec{p}_1, \Omega_1) - \frac{1}{\beta} \sum_{\vec{p}_i, \Omega_1} D(\Omega, \Omega_1) \tilde{V}_{22}(\Omega, \Omega_1) F_2(\vec{p}_1, \Omega_1), \tag{22}\]

where

\[\tilde{V}_{11}(\Omega, \Omega_1) = g_{11}^2 + N_1 g_{11}^4 \left[ P_{V_1}(Q_c, \Omega, \Omega_1) + P_{V_1}'(Q_c, \Omega, \Omega_1) + P_{c_1}(Q_c, \Omega, \Omega_1) \right] \tag{23}\]

As it follows from (21) - (23) the vertex and “cross - intersected” functions contribute to the intraband electron - phonon interaction constants \(g_{12}^2\) and \(g_{22}^2\) without influencing the interband interaction \(g_{12}^2\). The value \(\tilde{V}_{22}\) is obtained replacing \(1 \rightarrow 2\) in the formula (23).

Expressions \(P_{V,C_n}(Q_c, \Omega, \Omega_1)\) correspond to formulas averaged over Fermi surface, \(Q_c = q_c/2p_F\).

Hereinafter, in performing calculations we use simple dispersion law of electron energy for \(n\)-th band

\[\varepsilon_n(\vec{p}) = \zeta_n + \frac{\vec{p}^2}{2m_n} - \mu. \tag{24}\]

Let’s go in definitions of function \(P_{V,C_n}\) (20) from summation over \(\vec{p}_2\) and \(\Omega_2\) to integration over energy and frequency in the standard way (as it was done at \(T = 0\)):

\[\frac{1}{\beta} \sum_{\vec{p}_2, \Omega_2} \Phi_n(\vec{p}_2, \Omega_2) = N_n \int_0^{2\pi} \frac{d\phi}{4\pi} \int_0^\pi \sin \theta d\theta \int_{\mu_n}^{W_n - \mu_n} \frac{1}{2\pi} \int \frac{d\Omega_2}{-\infty} \Phi_n(\vec{p}_2, \Omega_2) \]

where

\[N_n = \frac{m_n p_F n}{2\pi^2}, \quad \mu_n = \mu - \zeta_n. \tag{25}\]

Integration over \(\Omega_2\) with infinite limits is caused by approximation of weak coupling of electron-phonon interaction \((\omega_0/T_c \gg 1)\). Integration over angular variables is performed in accordance with lowness of transferred momentum \(q(q \ll 2p_F)\). Here we have used the
method of calculation that was developed for this case in works [12], [15], [16]. In this way we take into consideration for three-dimensional system at $\theta_c \ll \omega_0/\mu_n$ expressions

\[
P_{Vn}(Q_c, \Omega, \Omega_1) = \frac{\omega_0 A_n(\Omega, \Omega_1)}{(\Omega - \Omega_1)^2} - \frac{\omega_0 E^2}{(\Omega - \Omega_1)^4} \left[ A_n(\Omega, \Omega_1) - (\Omega - \Omega_1)^2 B_n(\Omega, \Omega_1) \right] \frac{1}{2} Q_c^4,
\]

\[
P_{Cn}(Q_c, \Omega, \Omega_1) = \frac{\omega_0 A_n(\Omega, -\Omega_1)}{(\Omega + \Omega_1)^2} - \frac{\omega_0 E^2}{(\Omega + \Omega_1)^4} \left[ A_n(\Omega, -\Omega_1) - (\Omega + \Omega_1)^2 B_n(\Omega, -\Omega_1) \right] \times
\]

\[
x \times \frac{22}{3} Q_c^4 + \frac{\omega_0 E}{(\Omega + \Omega_1)^2} C_n(\Omega, -\Omega_1) Q_c^2,
\]

(26)

where $E = 2\varepsilon_F$,

\[
A_n(\Omega, \Omega_1) = \frac{\Omega - \Omega_1}{2} \left[ 2 \arctg \frac{\Omega}{\omega_0} - \arctg \frac{\Omega}{W_n - \mu_n + \omega_0} - \arctg \frac{\Omega}{\mu_n + \omega_0} + \arctg \frac{\Omega_1}{\mu_n + \omega_0} - 2 \arctg \frac{\Omega_1}{\omega_0} + \arctg \frac{\Omega_1}{W_n - \mu_n + \omega_0} \right],
\]

\[
B_n(\Omega, \Omega_1) = -\frac{\mu_n + \omega_0}{2 ([\mu_n + \omega_0]^2 + \Omega_1^2]^2} \left[ (\mu_n + \omega_0)^2 + 2 \Omega_1^2 - \Omega \Omega_1 \right] - \frac{W_n - \mu_n + \omega_0}{2 ([W_n - \mu_n + \omega_0]^2 + \Omega_1^2]^2} \left[ (W_n - \mu_n + \omega_0)^2 + 2 \Omega_1^2 - \Omega \Omega_1 \right],
\]

\[
C_n(\Omega, \Omega_1) = \frac{1}{4} \ln \left( \frac{W_n - \mu_n + \omega_0)^2 + \Omega^2}{(\mu_n + \omega_0)^2 + \Omega^2} \right) - \frac{1}{4} \ln \left( \frac{W_n - \mu_n + \omega_0)^2 + \Omega_1^2}{(\mu_n + \omega_0)^2 + \Omega_1^2} \right) + \Omega_1(\Omega - \Omega_1) \frac{1}{2} \left[ \frac{1}{(\mu_n + \omega_0)^2 + \Omega^2} - \frac{1}{(W_n - \mu_n + \omega_0)^2 + \Omega_1^2} \right].
\]

(27)

As follows from these formulas values of vertex functions depend significantly on filling of the energy bands. At half-filling ($\mu_n = W_n/2$) all these expressions simplify significantly, the coefficient $C_n(\Omega, \Omega_1)$, for instance, is equal to zero.

4. Temperature of superconducting transition $T_c$ and coefficient of isotope effect $\alpha$. 

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Assume in formulas (26), (27) \( \Omega = 0 \) and \( \Omega_1 = \omega_0 \) while having considered one-band non-adiabatic system [12], [15]. We introduce renormalization of electron-phonon interaction couplings in accordance with their values

\[
\tilde{\lambda}_{11} = N_1 \tilde{V}_{11}(0, \omega_0) = \lambda_{11} + \lambda_{11}^2 \left[ 2P_{V_1}(Q_c, \omega_0) + P_{C_1}(Q_c, \omega_0) \right],
\]

\[
\lambda_{12} = V_{12}N_2
\]

\[
\tilde{\lambda}_{nn} = \lambda_{nn} \left[ 1 + \lambda_{nn} P_{V_n}(Q_c, \omega_0) \right].
\]

As a result of these definitions the expression for mass operators \( M_m(\Omega) \) (21) and system of equations for \( \Sigma_m(\Omega) \) has the following form:

\[
M_m(\Omega) = -\tilde{\lambda}_{mn} \frac{1}{\beta N_m} \sum_{\vec{p}_1} \sum_{\Omega_1} D(\Omega, \Omega_1)G_m(\vec{p}_1, \Omega_1) - \frac{\lambda_{mn}}{\beta N_n} \sum_{\vec{p}_1} \sum_{\Omega_1} \times
\]

\[
\times D(\Omega, \Omega_1)G_n(\vec{p}_1, \Omega_1), (m \neq n)
\]

\[
\Sigma_1(\Omega) = -\frac{\tilde{\lambda}_{11}}{\beta N_1} \sum_{\vec{p}_1} \sum_{\Omega_1} D(\Omega, \Omega_1)F_1(\vec{p}_1, \Omega_1) - \frac{\lambda_{12}}{\beta N_2} \sum_{\vec{p}_1, \Omega_1} D(\Omega, \Omega_1)F_2(\vec{p}_1, \Omega_1),
\]

\[
\Sigma_2(\Omega) = -\frac{\tilde{\lambda}_{22}}{\beta N_2} \sum_{\vec{p}_1} \sum_{\Omega_1} D(\Omega, \Omega_1)F_2(\vec{p}_1, \Omega_1) - \frac{\lambda_{21}}{\beta N_1} \sum_{\vec{p}_1} \sum_{\Omega_1} D(\Omega, \Omega_1)F_1(\vec{p}_1, \Omega_1).
\]

Introduce definitions \( \Sigma_n(\Omega) = Z_n(\Omega) \Delta_n(\Omega) \).

Having substituted in (30) definitions of Green functions (11) in linear approximation over \( \Delta_n (T \sim T_c) \) and having performed integration over energy in correspondence with (25) we obtain:

\[
\Delta_1(\Omega) = \frac{\tilde{\lambda}_{11}}{Z_1 \beta} \sum_{\Omega_1} \frac{\omega_0^2}{(\Omega - \Omega_1)^2 + \omega_0^2} \frac{\Delta_1(\Omega_1)}{|\Omega_1|} \varphi_1(\Omega_1) +
\]

\[
+ \frac{\lambda_{12}}{Z_1 \beta} \sum_{\Omega_1} \frac{\omega_0^2}{(\Omega - \Omega_1)^2 + \omega_0^2} \frac{\Delta_2(\Omega_1)}{|\Omega_1|} \varphi_2(\Omega_1),
\]

\[
\Delta_2(\Omega) = \frac{\tilde{\lambda}_{22}}{Z_2 \beta} \sum_{\Omega_1} \frac{\omega_0^2}{(\Omega - \Omega_1)^2 + \omega_0^2} \frac{\Delta_2(\Omega_1)}{|\Omega_1|} \varphi_2(\Omega_1) +
\]

\[
+ \frac{\lambda_{21}}{Z_2 \beta} \sum_{\Omega_1} \frac{\omega_0^2}{(\Omega - \Omega_1)^2 + \omega_0^2} \frac{\Delta_1(\Omega_1)}{|\Omega_1|} \varphi_1(\Omega_1),
\]

(31)

where

\[
\varphi_n(\Omega_1) = \arctan \frac{W_n - \tilde{\mu}_n}{Z_n|\Omega_1|} + \arctan \frac{\tilde{\mu}_n}{Z_n|\Omega_1|},
\]
\[
Z_n = Z_n(0) = 1 - \lim_{\Omega \to 0} \frac{1}{\Omega} \mathrm{Im} M_n(\Omega) = 1 + \lambda_n \frac{1}{2} \left[ \frac{W_n - \mu_n}{W_n - \mu_n + \omega_0 + \mu_n + \omega_0} \right] + \ddots
\]

\[
+ \lambda_n \frac{1}{2} \left[ \frac{W_m - \mu_m}{W_m - \mu_m + \omega_0 + \mu_m + \omega_0} \right], \quad \bar{\mu}_n = \mu_n - R e M_n(0), \quad (m \neq n). \quad (32)
\]

While studying the system of equation (31) we utilize approximation which was used in theory of superconductivity with taking into account the lagging effect [31]

\[
\frac{\omega^2}{(\Omega - \Omega_1)^2 + \omega^2} \rightarrow \frac{\omega^2}{\Omega^2 + \omega^2} \frac{\omega^2}{\Omega_1^2 + \omega^2}
\]

and introduce the following notation:

\[
\Delta_n(\Omega) = \frac{\omega_0^2}{\Omega^2 + \omega_0^2} \Delta_n; \quad \Phi_n(T_c) = \frac{1}{\beta_c} \sum_{\Omega_1} \frac{\omega_0^4}{(\Omega_1^2 + \omega_0^2)^2} \left| \Omega_1 \right| \varphi_n(\Omega_1), \quad (34)
\]

Having substituting (33), (34) into the system of equations (31), we represent this system of equations to the form:

\[
\Delta_1 = \frac{\lambda_{11}}{Z_1} \Delta_1 \Phi_1(T_c) + \frac{\lambda_{12}}{Z_1} \Delta_2 \Phi_2(T_c), \quad \Delta_2 = \frac{\lambda_{21}}{Z_2} \Delta_1 \Phi_1(T_c) + \frac{\lambda_{22}}{Z_2} \Delta_2 \Phi_2(T_c). \quad (35)
\]

Temperature of superconducting transition \(T_c\) is determined from the condition of consistency of the system of equations (35). Having supposed the determinant of this system to be equal to zero, we derive

\[
(\hat{\lambda}_{11} \hat{\lambda}_{22} - \hat{\lambda}_{12} \hat{\lambda}_{21}) \Phi_1(T_c) \Phi_2(T_c) - \hat{\lambda}_{11} \Phi_1(T_c) - \hat{\lambda}_{22} \Phi_2(T_c) + 1 = 0, \quad (36)
\]

were \(\hat{\lambda}_{11} = \lambda_{11}/Z_1; \quad \hat{\lambda}_{22} = \lambda_{22}/Z_2; \quad \hat{\lambda}_{12} = \lambda_{12}/Z_1; \quad \hat{\lambda}_{21} = \lambda_{21}/Z_2\).

The function \(\Phi_n(T_c)\) can be easily represented in the form:

\[
\Phi_n(T_c) = \pi T_c \sum_{\Omega_1} \frac{\omega_0^2}{\Omega_1^2 + \omega_0^2} \frac{1}{\left| \Omega_1 \right|} - T_c \sum_{\Omega_1} \frac{\omega_0^2}{\Omega_1^2 + \omega_0^2} \frac{1}{\left| \Omega_1 \right|} \left[ \arctan \frac{\left| \Omega_1 \right|}{W_n - \bar{\mu}_n} + \arctan \frac{\left| \Omega_1 \right|}{\bar{\mu}_n} \right] - T_c \sum_{\Omega_1} \frac{\omega_0^2}{\Omega_1^2 + \omega_0^2} \varphi_n(\Omega_1). \quad (37)
\]

First term of this expression contains logarithmic singularity over the quantity \(T_c\) and in the weak coupling approximation \((T_c/\omega_0 \ll 1)\) gives

\[
\pi T_c \sum_{\Omega_1} \frac{\omega_0^2}{\Omega_1^2 + \omega_0^2} \frac{1}{\left| \Omega_1 \right|} \approx ln \frac{2 \omega_0 \gamma}{\pi T_c}. \quad (38)
\]
In the same approximation we can perform integration over frequency in infinite limits (25) as in the case \( T = 0 \) in all rest terms. In this way for the function \( \Phi_n(T_c) \) we obtain:

\[
\Phi_n(T_c) = \xi_c + f_n, \quad \xi_c = \ln \left( \frac{2\omega_0\gamma}{\pi T_c} \right),
\]

where

\[
f_n = -\frac{1}{2} \left[ \ln(1 + m_n) + \ln(1 + m'_n) - \frac{1}{2} + \frac{1}{4} \left( \frac{m_n}{1 + m_n} + \frac{m'_n}{1 + m'_n} \right) \right],
\]

\[
m_n = \frac{\omega_0}{\bar{W}_n - \bar{\mu}_n}, \quad m'_n = \frac{\omega_0}{\bar{\mu}_n}, \quad \bar{W}_n = \frac{W_n}{Z_n}, \quad \bar{\mu}_n = \frac{\mu_n}{Z_n}.
\]

Having substituted (39) into the equation (36) we lead the latter one to the form:

\[
\bar{a}\xi_c^2 - \bar{b}\xi_c + \bar{c} = 0,
\]

where

\[
\bar{a} = \bar{\lambda}_{11}\bar{\lambda}_{22} - \bar{\lambda}_{12}\bar{\lambda}_{21}; \quad \bar{b} = \bar{\lambda}_{11} + \bar{\lambda}_{22} - \bar{a}(f_1 + f_2),
\]

\[
\bar{c} = 1 - \bar{\lambda}_{11}f_1 - \bar{\lambda}_{22}f_2 + \bar{a}f_1f_2.
\]

Having based on the (39) and (41) we obtain

\[
T_c = \frac{2\omega_0\gamma}{\pi} e^{-\xi_c}, \quad \xi_c = \frac{\bar{b} \pm \sqrt{\bar{b}^2 - 4\bar{a}\bar{c}}}{2\bar{a}}.
\]

This expression coincides formally with the case of usual two-band superconductors [2], [32]. But this expression differs significantly because the quantities which enter in it are renormalized by additional contributions that are determined by non-adiabaticity of system. In order to go to one-band case it is sufficient to put \( N_2 = 0 \). Having following this way we derive the temperature of superconducting transition \( T_{co} = T_c|_{N_2=0} \) [15].

\[
T_{co} = \frac{2\omega_0\gamma}{\pi \sqrt{e}} \frac{[(\bar{W}_1 - \bar{\mu}_1)\bar{\mu}_1]^{1/2}}{[(\bar{W}_1 - \bar{\mu}_1 + \omega_0)(\bar{\mu}_1 + \omega_0)]^{1/2}} \exp \left\{ -\frac{1}{\lambda_{11}} + \frac{1}{4} \left( \frac{1}{\bar{W}_1 - \bar{\mu}_1 + \omega_0} + \frac{1}{\bar{\mu}_1 + \omega_0} \right) \right\}.
\]

At half-filling of energy band \( \mu_1 = W_1/2 \) this expression goes into one which was obtained in article [12]:

\[
T_{co}^0 = \frac{2\omega_0\gamma}{\pi \sqrt{e}(1 + m)} \exp \left\{ -\frac{1}{\lambda_{11}} + \frac{1}{2} \left( \frac{m}{m + 1} \right) \right\},
\]

where \( m = \frac{2\omega_0}{W_1} \)

Therefore, the formula (43) shows the influence of overlapping of energy bands on Fermi
surface and non-adiabaticity \((\varepsilon_F \sim \omega_0)\) on the temperature of superconducting transition at arbitrary filling of energy bands.

Having based on the formula (43) the expression for the coefficient of isotope effect \(\alpha\) can be represented in the form:

\[
\alpha = -\frac{d\ln T_c}{d\ln M} = \frac{1}{2} \left[ 1 + \frac{d\ln (T_c/\omega_0)}{d\ln \omega_0} \right] = \frac{1}{2} \left[ 1 - \frac{d\xi_c}{d\ln \omega_0} \right],
\]

where

\[
\frac{d\xi_c}{d\ln \omega_0} = -\frac{\bar{b} \pm \sqrt{\bar{b}^2 - 4\bar{a}\bar{c}}}{\bar{a}} \frac{d\bar{a}}{d\ln \omega_0} + \frac{1}{2\bar{a}} \times
\]

\[
\times \left\{ \frac{\bar{b}}{d\ln \omega_0} \pm \frac{1}{\sqrt{\bar{b}^2 - 4\bar{a}\bar{c}}} \left[ \frac{\bar{d}}{d\ln \omega_0} - 2\bar{a} \frac{d\bar{c}}{d\ln \omega_0} - 2\bar{c} \frac{d\bar{a}}{d\ln \omega_0} \right] \right\},
\]

As follows from (46) and (47) the coefficient \(\alpha\) differs from \(1/2\), which characterizes the ordinary superconductors, through dependence of the quantities \(\bar{a}, \bar{b}, \bar{c}\) on \(\omega_0\). This dependence is caused by non-adiabaticity of system and by delay in the system with electron-phonon interaction.

Note that the sign in formulas (43) and (47) is chosen from the condition \(\xi_c > 0\) and maximum value of the quantity \(T_c\) as it has been done in the case of adiabatic systems.

5. Numerical calculations and discussions.

Theory of superconductivity for two-band non-adiabatic system by exceeding the bounds of Migdal theorem [7] in linear over non-adiabaticity approximation is built in this chapter. Non-adiabaticity here means that having determined the mass operators, diagonal \(M_n\) and non-diagonal \(\Sigma_n\) in electron Green function of two-band system \((n = 1, 2)\) the additional in comparison with Eliashberg-Migdal theory diagrams with intersection of two lines of electron-phonon interaction, which correspond to vertex functions \(P_{V_n}\) as well as to ”intersecting” ones \(P_{C_n}\) \((n = 1, 2)\), are taken into consideration. Applied weak coupling approximation \((T_C/\omega_0; \Delta_n/\omega_0 \ll 1)\) allows us to obtain analytical formulas for these functions and show that their behavior is determined by the value of transferred momentum \(q\) of electron-phonon interaction. At low values of cut-off momentum of electron-phonon interaction \(q_c (q_c \ll 2p_F)\) functions \(P_{V_n}\) and \(P_{C_n}\) give positive contribution and at \(q \sim 2p_F\) they give negative contribution. Lowness of the quantity \(q_c\) is provided, for instance, by presence of strong electron correlations in the system [9], [10], or by quasi-one-dimensional dispersion law of electron’s energy [13].
For numerical calculations a simplified case \( m = m_1 = m_2 (m_n = 2 \alpha_0 / W_n) \) and half filling of energy bands \( \mu_n = W_n / 2 \) were considered.

The theory parameters are: \( \lambda_{11} = 0.5; \lambda_{22} = 0.3; \lambda_{12} = 0.1; \lambda_{21} = 0.05. \)

According to the definitions (36), (28) and (32) these parameters are renormalized due to the non-adiabatic effects and strong electron correlations. The values of renormalized \( \lambda_{nm} \) at different values of Migdal parameter \( m \) are presented in the Table 1 along with the values of the functions \( P_{V_1} \) and \( P_{C_1}. \)

| \( Q_c = 0.1 \) | \( \bar{m} \) | \( P_{V_1} \) | \( P_{C_1} \) | \( \bar{\lambda}_{11} \) | \( \bar{\lambda}_{22} \) | \( \bar{\lambda}_{12} \) | \( \bar{\lambda}_{21} \) |
|-----------------|------|-------|-------|----------|----------|----------|----------|
| 0               | 0    | 0.312 | 0.24  | 0.065    | 0.038    |
| 0.1             | 0.679| 0.656 | 0.59  | 0.35     | 0.058    | 0.036    |
| 0.3             | 0.565| 0.553 | 0.584 | 0.344    | 0.064    | 0.038    |
| 0.6             | 0.426| 0.425 | 0.568 | 0.333    | 0.069    | 0.04     |
| 0.9             | 0.342| 0.342 | 0.556 | 0.32     | 0.073    | 0.042    |

| \( Q_c = 0.9 \) | \( \bar{m} \) | \( P_{V_1} \) | \( P_{C_1} \) | \( \bar{\lambda}_{11} \) | \( \bar{\lambda}_{22} \) | \( \bar{\lambda}_{12} \) | \( \bar{\lambda}_{21} \) |
|-----------------|------|-------|-------|----------|----------|----------|----------|
| 0               | 0    | 0.312 | 0.24  | 0.065    | 0.038    |
| 0.1             | -0.053 | -0.044 | 0.315 | 0.223    | 0.065    | 0.038    |
| 0.3             | -0.012 | -0.096 | 0.322 | 0.227    | 0.068    | 0.039    |
| 0.6             | -0.008 | -0.112 | 0.339 | 0.236    | 0.073    | 0.041    |
| 0.9             | 0.005 | -0.113 | 0.36  | 0.245    | 0.076    | 0.042    |

As it follows from the Table 1 the behavior of renormalized electron-phonon interaction constants is not a single-valued one and is determined in the same time both the value of cut-off momentum of electron-phonon interaction \( Q_c \) and the value of Migdal parameter \( m \). The ration \( T_c / \omega_0 \) as a function of \( m \) is presented on the Fig. 1. Here we have considered the definition (43) and the obtained results multiplied by \( \sqrt{\epsilon} \). Such correction is necessary because the approximation (33) decrease the \( T_c \) with the coefficient \( e^{-1/2} \) [34]. The curve 2 on this figure correspond to the case of two-band adiabatic system, curves 1 and 1’ correspond to the case of non-adiabatic two-band system at \( Q_c = 0.1 \) and \( Q_c = 0.9 \) respectively. The comparison of these curves shows that the non-adiabatic effects and strong electron correlations considerably increase the temperature.
of superconducting transition $T_c$ at $Q_c \ll 1$. Moreover, the biggest value of $T_c$ is reached in the area of small $m$ ($m \sim 0.1$). At $Q_c \sim 1$ the $T_c$ decreases and weakly depends on parameter $m$.

These results point on the fact that in the systems with small values of the ratio Debye energy on Fermi energy the contribution of top approximations to the superconductivity can be essential if the transmitted momentum is small.

The substances with small values of $m$ ($m \sim 0.1$) particularly are two-band superconductors $MgB_2$. The strong electron correlations presence or the peculiarities in electron energy spectrum in such systems can essentially strength the influence of non adiabatic effects on superconductivity.

The dependency of ratio $T_c/\omega_D$ on coefficient $\delta$ which determines the proportional increasing of all electron-phonon interaction constants in two-band model ($\lambda'_{nm} = \delta \lambda_{mn}$) is presented on Fig.2. The cases $m = 0, 2; Q_c = 0,1$ (curve 1) and $m = 0, 2; Q_c = 0,9$ (curve 2) are considered. Increase of $T_c$ follows from this figure with increasing the coefficient $\delta$ in both cases.

The dependency of isotopic coefficient $\alpha$ on Migdal parameter $m$ is shown on Fig. 3. At $Q_c \ll 1$ and $m < 0.1$ the coefficient $\alpha > 0.5$, then this quantity essentially decreases with the increasing of $m$ and can achieve the values $\sim 0.2$ (curve 1). At $Q_c \sim 1$ the value of $\alpha$ becomes $\approx 0.5$ (weakly decreases then increases with the increasing of $m$).

In this way, the non-adiabatic effects in two-band superconductors at small values of cut-off momentum of electron-phonon interaction $Q_c$ allow to attain high values of superconducting transition temperature $T_c$ and small values of isotopic effect. Such picture is observed in high temperature oxide metals.

The presented above numerical results are performed for the $\lambda_{11} > \lambda_{22} > \lambda_{12} > \lambda_{21}$. These results correspond qualitatively to the case of one-band superconductor [12].

In the limit case $\lambda_{11} = \lambda_{22} = 0, \lambda_{12} = 0$ and $\lambda_{21} \neq 0$ the examined non adiabatic effects do not influence the superconductivity, because in this case the interband interaction constants $\lambda_{nm}$ are not renormalized due to vertex functions consideration.

We have to emphasize that the possibility of appearance of high temperature superconductivity in the systems with strong electron correlations on the base of phonon superconducting mechanism was discussed in a chain of articles (see, for instance [35] - [37]).

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