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Antiadiabatic Phonons and Superconductivity in Eliashberg–McMillan Theory

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Abstract

The standard Eliashberg–McMillan theory of superconductivity is essentially based on the adiabatic approximation. Here we present some simple estimates of electron–phonon interaction within the Eliashberg–McMillan approach in a non–adiabatic and even antiadiabatic situation, when characteristic phonon frequency Ω_0 becomes large enough, i.e., comparable or exceeding the Fermi energy E_F. We discuss the general definition of Eliashberg–McMillan (pairing) electron–phonon coupling constant λ, taking into account the finite value of phonon frequencies. We show that the mass renormalization of electrons is in general determined by different coupling constant $\tilde{\lambda}$, which takes into account the finite width of conduction band, and describes the smooth transition from the adiabatic regime to the region of strong nonadiabaticity. In antiadiabatic limit, when $\Omega_0 \gg E_F$, the new small parameter of perturbation theory is $\lambda\frac{E_F}{\Omega_0} \sim \lambda\frac{D}{\Omega_0} \ll 1$ (D is conduction band half-width), and corrections to electronic spectrum (mass renormalization) become irrelevant. However, the temperature of superconducting transition T_c in antiadiabatic limit is still determined by Eliashberg–McMillan coupling constant λ. We consider in detail the model with discrete set of (optical) phonon frequencies. A general expression for superconducting transition temperature T_c is derived, which is valid in situation, when one (or several) of such phonons becomes antiadiabatic. We also analyze the contribution of such phonons into the Coulomb pseudopotential $\mu^\star$ and show that antiadiabatic phonons do not contribute to Tolmachev's logarithm and its value is determined by partial contributions from adiabatic phonons only.

Keywords Eliashberg–McMillan theory · Electron–phonon interaction · Antiadiabatic phonons · Coulomb pseudopotential · Critical temperature

1 Introduction

Eliashberg–McMillan superconductivity theory is currently the basis for microscopic description of Cooper pairing and all general properties of conventional superconductors [1–5]. It is essentially based on adiabatic approximation and Migdal's theorem [6], which allows to neglect the vertex corrections to electron–phonon coupling in typical metals. The actual small parameter of perturbation theory is $\lambda\frac{\Omega_0}{E_F} \ll 1$, where λ is the dimensionless Eliashberg–McMillan electron–phonon coupling constant, Ω_0 is characteristic phonon frequency, and E_F is Fermi energy of electrons. This leads to the widely accepted opinion that vertex corrections can be neglected even for the case of $\lambda > 1$, due to the fact that in common metal, $\frac{\Omega_0}{E_F} \ll 1$. The possible breaking of Migdal's theorem for the case of $\lambda \sim 1$ due to polaronic effects was widely discussed in the literature [7, 8]. In the following, we consider only the case of $\lambda < 1$ where we can safely neglect these effects [8].

Recently, a number of superconductors were discovered, where the adiabatic approximation is not necessarily valid, and characteristic frequencies of phonons are of the order or even greater than Fermi energy. In this respect, we can mention single–atomic layers of FeSe on the $SrTiO_3$ substrate (FeSe/STO) [9], as well as record–breaking hydride–based superconductors at high pressures [10]. This is also the case in the long–standing puzzle of superconductivity in doped $StTiO_3$ [11]. The role of nonadiabatic phonons was recently analyzed in important papers by Gor'kov [12, 13] within the standard BCS–like weak–coupling approach, and directly addressed to these new superconductors. Here we review

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some further estimates, derived by us in refs. [14, 15] in the framework of Eliashberg–McMillan theory.

2 Electron Self–Energy and Electron–Phonon Coupling Constant

Let us consider first a metal in normal (non-superconducting) state, which is sufficient to introduce some basic notions of Eliashberg–McMillan theory [2, 3]. The second–order (in electron–phonon coupling) diagram is shown in Fig. 1. Making all calculations in finite temperature technique, after the analytic continuation from Matsubara to real frequencies $i\omega_n \to \varepsilon \pm i\delta$ and in the limit of $T = 0$ (i.e., $E_F \gg T$), the contribution of diagram in Fig. 1 can be written [1, 2] as:

$$\Sigma(\varepsilon, \mathbf{p}) = \sum_{\mathbf{p}',\alpha} |g^{\alpha}_{\mathbf{p}\mathbf{p}'}|^2 \left\{ \frac{f_{\mathbf{p}'}}{\varepsilon - \varepsilon_{\mathbf{p}'} + \Omega^{\alpha}_{\mathbf{p}-\mathbf{p}'} - i\delta} + \frac{1 - f_{\mathbf{p}'}}{\varepsilon - \varepsilon_{\mathbf{p}'} - \Omega^{\alpha}_{\mathbf{p}-\mathbf{p}'} + i\delta} \right\} \quad (1)$$

where in notations of Fig. 1 $\mathbf{p}' = \mathbf{p} + \mathbf{q}$. Here $g^{\alpha}_{\mathbf{p},\mathbf{p}'}$ is Fröhlich electron–phonon coupling constant, $\varepsilon_{\mathbf{p}}$ is electronic spectrum with energy zero taken at the Fermi level, $\Omega^{\alpha}_{\mathbf{q}}$ represents the phonon spectrum, and $f_{\mathbf{p}}$ is Fermi distribution (step–function at $T = 0$). In these expressions index α enumerates the branches of phonon spectrum, which below is just dropped for brevity.

Now we can essentially follow the analysis, presented in Ref. [2, 3]. Eq. (1) can be identically rewritten as:

$$\Sigma(\varepsilon, \mathbf{p}) = \int d\omega \sum_{\mathbf{p}'} |g_{\mathbf{p}\mathbf{p}'}|^2 \delta(\omega - \Omega_{\mathbf{p}-\mathbf{p}'}) \times \left\{ \frac{f_{\mathbf{p}'}}{\varepsilon - \varepsilon_{\mathbf{p}'} + \omega - i\delta} + \frac{1 - f_{\mathbf{p}'}}{\varepsilon - \varepsilon_{\mathbf{p}'} - \omega + i\delta} \right\} \quad (2)$$

To simplify calculations, we can get rid of explicit momentum dependencies here by averaging the matrix element of electron–phonon interaction over surfaces of constant energies, corresponding to initial and final momenta $\mathbf{p}$ and $\mathbf{p}'$, which usually reduces to the averaging over corresponding Fermi surfaces, as phonon scattering takes place only within the narrow energy interval close to the Fermi level, with effective width of the order of double characteristic frequency of phonons $2\Omega_0$, and taking into account that in typical metals we always have $\Omega_0 \ll E_F$.

This averaging can be achieved by the following replacement in Eq. (2):

$$\begin{aligned} &|g_{\mathbf{p}\mathbf{p}'}|^2 \delta(\omega - \Omega_{\mathbf{p}-\mathbf{p}'}) \\ &\Longrightarrow \frac{1}{N(0)} \sum_{\mathbf{p}} \frac{1}{N(0)} \sum_{\mathbf{p}'} |g_{\mathbf{p}\mathbf{p}'}|^2 \delta(\omega - \Omega_{\mathbf{p}-\mathbf{p}'}) \\ &\quad \times \delta(\varepsilon_{\mathbf{p}}) \delta(\varepsilon_{\mathbf{p}'}) \\ &\equiv \frac{1}{N(0)} \alpha^2(\omega) F(\omega) \end{aligned} \quad (3)$$

where in the last expression, we have introduced the *definition* of Eliashberg function $\alpha^2(\omega)$ and $F(\omega) = \sum_{\mathbf{q}} \delta(\omega - \Omega_{\mathbf{q}})$ is the phonon density of states.

In the non–adiabatic case, when phonon energy becomes comparable with or even exceeds the Fermi energy, electron scattering is effective not only in the narrow energy layer around the Fermi surface, but in much wider energy, interval of the order of $\Omega_0 \sim E_F$. Then, for the case of initial $|\mathbf{p}| \sim p_F$, the averaging over $\mathbf{p}'$ in expression like (3) should be done over the surface of constant energy, corresponding to $E_F + \Omega_{\mathbf{p}-\mathbf{p}'}$, as is shown in Fig. 2. Now Eq. (3) is directly generalized as:

$$\begin{aligned} &|g_{\mathbf{p}\mathbf{p}'}|^2 \delta(\omega - \Omega_{\mathbf{p}-\mathbf{p}'}) \\ &\Longrightarrow \frac{1}{N(0)} \sum_{\mathbf{p}} \frac{1}{N(0)} \sum_{\mathbf{p}'} |g_{\mathbf{p}\mathbf{p}'}|^2 \\ &\quad \times \delta(\omega - \Omega_{\mathbf{p}-\mathbf{p}'}) \delta(\varepsilon_{\mathbf{p}}) \delta(\varepsilon_{\mathbf{p}'} - \Omega_{\mathbf{p}-\mathbf{p}'}) \\ &\equiv \frac{1}{N(0)} \alpha^2(\omega) F(\omega) \end{aligned} \quad (4)$$

After the replacement like (3) or (4), the explicit momentum dependence of the self–energy disappears and in fact in the following, we are dealing with Fermi surface average of self–energy $\Sigma(\varepsilon) \equiv \frac{1}{N(0)} \sum_{\mathbf{p}} \delta(\varepsilon_{\mathbf{p}}) \Sigma(\varepsilon, \mathbf{p})$, which is now written as:

$$\Sigma(\varepsilon) = \int d\varepsilon' \int d\omega \alpha^2(\omega) F(\omega) \times \left\{ \frac{f(\varepsilon')}{\varepsilon - \varepsilon' + \omega - i\delta} + \frac{1 - f(\varepsilon')}{\varepsilon - \varepsilon' - \omega + i\delta} \right\} \quad (5)$$

This expression forms the basis of Eliashberg–McMillan theory and determines the structure of Eliashberg equations for the description of superconductivity.

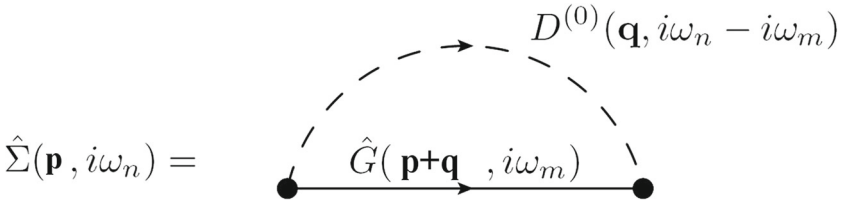

Fig. 1 Second–order diagram for self–energy. Dashed line—phonon Green's function $D^{(0)}$, continuous line—electron Green's function G in Matsubara representation

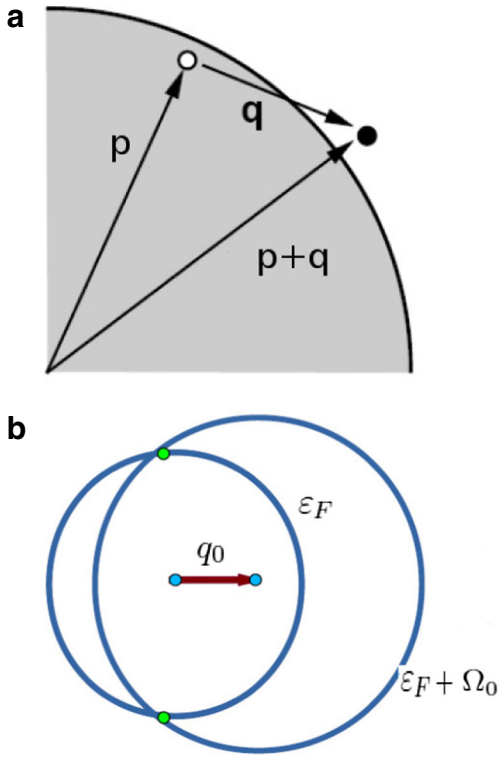

Fig. 2 **a** Elementary act of electron–phonon scattering in the vicinity of the Fermi surface. **b** Surfaces of constant energy for initial and final states of an electron scattered by an optical phonon with energy comparable with Fermi energy. Non–trivial contribution to the average of the matrix element in (11) or (13) comes here from the intersection of these surfaces

Now the self–energy is dependent only on frequency (and not on momentum) and we can use the following simple expressions, relating mass renormalization of an electron to the residue a the pole of the Green's function [16]:

$$Z^{-1} = 1 - \left.\frac{\partial \Sigma(\varepsilon)}{\partial \varepsilon}\right|_{\varepsilon=0} \tag{6}$$

$$m^\star = \frac{m}{Z} = m\left(1 - \left.\frac{\partial \Sigma(\varepsilon)}{\partial \varepsilon}\right|_{\varepsilon=0}\right) \tag{7}$$

Then from Eq. (5) by direct calculations we obtain:

$$-\left.\frac{\partial \Sigma(\varepsilon)}{\partial \varepsilon}\right|_{\varepsilon=0} = 2\int_0^\infty \frac{d\omega}{\omega}\alpha^2(\omega)F(\omega) \tag{8}$$

and introducing the dimensionless Eliashberg–McMillan electron–phonon coupling constant as:

$$\lambda = 2\int_0^\infty \frac{d\omega}{\omega}\alpha^2(\omega)F(\omega) \tag{9}$$

we immediately obtain the standard expression for electron mass renormalization due to electron–phonon interaction:

$$m^\star = m(1+\lambda) \tag{10}$$

The function $\alpha^2(\omega)F(\omega)$ in the expression for Eliashberg–McMillan electron–phonon coupling constant (9) should be calculated according to (3) or (4) depending on the relation between Fermi energy E_F and characteristic phonon frequency Ω_0 As long as $\Omega_0 \ll E_F$, we can use the standard expression (3), while in the case of $\Omega_0 \sim E_F$, we should use (4).

Using Eq. (4)m, we can rewrite (9) in the following form:

$$\lambda = \frac{2}{N(0)}\int \frac{d\omega}{\omega}\sum_{\mathbf{p}}\sum_{\mathbf{p}'}|g_{\mathbf{p}\mathbf{p}'}|^2 \times\delta(\omega - \Omega_{\mathbf{p}-\mathbf{p}'})\delta(\varepsilon_{\mathbf{p}})\delta(\varepsilon_{\mathbf{p}'} - \Omega_{\mathbf{p}-\mathbf{p}'}) \tag{11}$$

which gives the most general expression to calculate the electron–phonon constant λ, determining pairing in the Eliashberg–McMillan theory. Implicitly this result was contained already in ref. [17]. Below we shall present some simple estimates, based on this general relation.

3 Estimates of Electron–Phonon Coupling with Non–adiabatic Phonons

Let us consider the simplest possible model of electrons interacting with a single optical (Einstein–like) phonon mode with high–enough frequency Ω_0. The general qualitative picture of such scattering is shown in Fig. 2. In this case in Eq. (11) the density of phonon states is simply $F(\omega) = \delta(\omega - \Omega_0)$. Just for orientation we may take the possible momentum dependence of interaction with this optical phonon in the form proposed in Refs. [18, 19] to describe nearly "forward" scattering by optical phonons at FeSe/STO interface, as a possible mechanism of strong T_c enhancement in this system:

$$g(\mathbf{q}) = g_0 \exp(-|\mathbf{q}|/q_0), \tag{12}$$

where the typical value of $q_0 \ll p_F$ (p_F is the Fermi momentum) to ensure the nearly "forward" nature of scattering. This model allows explicit estimates, which may illustrate the general situation.

Now we can write the dimensionless pairing constant of electron–phonon interaction in Eliashberg theory as:

$$\lambda = \frac{2}{N(0)\Omega_0}\sum_{\mathbf{p}}\sum_{\mathbf{q}}|g_{\mathbf{q}}|^2\delta(\varepsilon_{\mathbf{p}})\delta(\varepsilon_{\mathbf{p}+\mathbf{q}} - \Omega_0) \tag{13}$$

As in FeSe/STO with rather shallow conduction band [18, 20, 21], where in fact we have $\Omega_0 > E_F$, the finite value of Ω_0 in the second δ-function here should be definitely taken into account.

We can make our estimates assuming the simplest linearized form of electronic spectrum near the Fermi surface (v_F is Fermi velocity): $\varepsilon_{\mathbf{p}} \approx v_F(|\mathbf{p}| - p_F)$, which allows us to perform all calculations analytically. Using (12)

in (13) and considering the two–dimensional case, after the calculation of all integrals, we obtain [21]:

$$\lambda = \frac{g_0^2 a^2}{\pi^2 v_F^2} K_1\left(\frac{2\Omega_0}{v_F q_0}\right), \tag{14}$$

where $K_1(x)$ is Bessel function of imaginary argument (McDonald function). Using the asymptotic form of $K_1(x)$ and dropping a number of irrelevant constants of the order of unity, we get:

$$\lambda \sim \lambda_0 \frac{q_0}{4\pi p_F}, \tag{15}$$

for $\frac{\Omega_0}{v_F q_0} \ll 1$, and

$$\lambda \sim \lambda_0 \frac{\Omega_0}{\pi E_F} \sqrt{\frac{v_F q_0}{\Omega_0}} \exp\left(-\frac{2\Omega_0}{v_F q_0}\right), \tag{16}$$

for $\frac{\Omega_0}{v_F q_0} \gg 1$. Here we introduced the standard dimensionless electron–phonon coupling constant:

$$\lambda_0 = \frac{2g_0^2}{\Omega_0} N(0), \tag{17}$$

where $N(0)$ is the density of electronic states at the Fermi level per single spin projection.

The result (15) is by itself rather unfavorable for significant T_c enhancement in model under discussion, where $q_0 \ll p_F$. Even worse is the situation if we take into account the large values of Ω_0, as pairing constant becomes exponentially suppressed for $\frac{\Omega_0}{v_F q_0} > 1$, which is typical for FeSe/STO interface, where $\Omega_0 > E_F \gg v_F q_0$ [9]. This makes the enhancement of T_c due to interaction of FeSe electrons with optical phonons of STO rather improbable, as was stressed in ref. [21].

However, this is not our main point here. Actually, using (12), we can also make estimates for a generally more typical case, when the optical phonon scatters electrons not only in nearly "forward" direction, but in a wider interval of transferred momenta. To do that, we have simply to use in Eq. (12) the larger values of parameter q_0. Choosing, e.g., $q_0 \sim 4\pi p_F$ and using the low frequency limit of (15) we immediately obtain $\lambda \approx \lambda_0$, i.e., the standard result. Similarly, parameter q_0 can be taken of the order of inverse lattice vector $2\pi/a$ (where a is the lattice constant). Then for $q_0 \sim 2\pi/a$ from (15) we obtain:

$$\lambda \sim \lambda_0 \frac{1}{2p_F a} \sim \lambda_0 \tag{18}$$

for the typical case of $p_F \sim 1/2a$. In general, there always remains the dependence on the value of Fermi momentum and cutoff parameter (cf. similar analysis in Ref. [16]). These particular estimates are valid for the adiabatic case.

In antiadiabatic limit of (16), assuming $q_0 \sim p_F$, we immediately obtain:

$$\lambda \sim \frac{\sqrt{2}}{\pi} \lambda_0 \sqrt{\frac{\Omega_0}{E_F}} \exp\left(-\frac{\Omega_0}{E_F}\right), \tag{19}$$

which simply signifies the effective interaction cutoff for $\Omega_0 > E_F$ in the antiadiabatic limit. This fact was already noted by Gor'kov in refs. [12, 13], where it was stressed that in antiadiabatic limit, the cutoff in the Cooper channel is determined not by the average phonon frequency, but by Fermi energy.

4 Antiadiabatic Limit and Mass Renormalization

Our discussion up to now implicitly assumed the conduction band of an infinite width. However, it is obvious that in the case of large enough characteristic phonon frequency, it may become comparable with conduction band width, which in typical metal case is of the order of Fermi energy E_F. Now we will show that in the strongly nonadiabatic (antiadiabatic) limit, when $\Omega_0 \gg E_F \sim D$ (here D is the conduction band half-width), we are in fact dealing with the situation, when there appears a new small parameter of perturbation theory $\lambda D/\Omega_0 \sim \lambda E_F/\Omega_0$.

Consider the case of conduction band of the finite width $2D$ with constant density of states (which formally corresponds to two–dimensional case). The Fermi level as always is considered as an origin of energy scale and for simplicity, we assume the case of half–filled band. Then (5) reduces to:

$$\begin{aligned}\Sigma(\varepsilon) &= \int_{-D}^{D} d\varepsilon' \int d\omega \alpha^2(\omega) F(\omega) \\ &\quad \times \left\{ \frac{f(\varepsilon')}{\varepsilon - \varepsilon' + \omega - i\delta} + \frac{1 - f(\varepsilon')}{\varepsilon - \varepsilon' - \omega + i\delta} \right\} \\ &= \int d\omega \alpha^2(\omega) F(\omega) \\ &\quad \times \left\{ \ln \frac{\varepsilon + D + \omega - i\delta}{\varepsilon - D - \omega + i\delta} - \ln \frac{\varepsilon + \omega - i\delta}{\varepsilon - \omega + i\delta} \right\}\end{aligned} \tag{20}$$

For the model of a single optical phonon, $F(\omega) = \delta(\omega - \Omega_0)$ and we immediately obtain:

$$\begin{aligned}\Sigma(\varepsilon) = \alpha^2(\Omega_0) F(\Omega_0) \Bigg\{ &\ln \frac{\varepsilon + D + \Omega_0 - i\delta}{\varepsilon - D - \Omega_0 + i\delta} \\ &- \ln \frac{\varepsilon + \Omega_0 - i\delta}{\varepsilon - \Omega_0 + i\delta} \Bigg\}\end{aligned} \tag{21}$$

Correspondingly, from (20), we get:

$$-\left.\frac{\partial\Sigma(\varepsilon)}{\partial\varepsilon}\right|_{\varepsilon=0}=2\int_0^\infty d\omega\alpha^2(\omega)F(\omega)\frac{D}{\omega(\omega+D)} \tag{22}$$

and we can define the *new* generalized coupling constant as:

$$\tilde{\lambda}=2\int_0^\infty\frac{d\omega}{\omega}\alpha^2(\omega)F(\omega)\frac{D}{\omega+D} \tag{23}$$

which for $D\to\infty$ reduces to the usual Eliashberg–McMillan constant (9), while for $D\to 0$ ($D\ll\Omega_0$), it gives the "antiadiabatic" coupling constant:

$$\lambda_D=2D\int\frac{d\omega}{\omega^2}\alpha^2(\omega)F(\omega) \tag{24}$$

Equation (23) describes the smooth transition between the limits of wide and narrow conduction bands. Mass renormalization in general case is determined by $\tilde{\lambda}$:

$$m^\star=m(1+\tilde{\lambda}) \tag{25}$$

For the model of a single optical phonon with frequency Ω_0, we have:

$$\tilde{\lambda}=\frac{2}{\Omega_0}\alpha^2(\Omega_0)\frac{D}{\Omega_0+D}=\lambda\frac{D}{\Omega_0+D}=\lambda_D\frac{\Omega_0}{\Omega_0+D} \tag{26}$$

where Eliashberg–McMillan constant is:

$$\lambda=2\int_0^\infty\frac{d\omega}{\omega}\alpha^2(\omega)F(\omega)=\alpha^2(\Omega_0)\frac{2}{\Omega_0} \tag{27}$$

and λ_D reduces to:

$$\lambda_D=2\alpha^2(\Omega_0)\frac{D}{\Omega_0^2}=2\alpha^2(\Omega_0)\frac{1}{\Omega_0}\frac{D}{\Omega_0}=\lambda\frac{D}{\Omega_0} \tag{28}$$

where in the last expression, we explicitly introduced the new small parameter $D/\Omega_0\ll 1$, appearing in strong antiadiabatic limit. Correspondingly, in this limit, we always have:

$$\lambda_D=\lambda\frac{D}{\Omega_0}\sim\lambda\frac{E_F}{\Omega_0}\ll\lambda \tag{29}$$

so that for reasonable values of λ (even up to a strong coupling region of $\lambda\sim 1$), "antiadiabatic" coupling constant remains small. Obviously, all vertex corrections here are also small, as was shown rather long ago by direct calculations in ref. [22]. Thus, we come to an unexpected conclusion—in the limit of strong nonadiabaticity, the electron–phonon coupling becomes weak and we obtain a kind of "anti–Migdal" theorem.

Physically, the weakness of electron–phonon coupling in strong nonadiabatic limit is more or less clear—when ions move much faster than electrons, these rapid oscillation are just averaged in time as electrons cannot follow the very rapidly changing configuration of ions.

5 Eliashberg Equations and the Temperature of Superconducting Transition

All analyses above were performed for the normal state of a metal. Now let us turn to the superconducting phase. The problem arises, to what extent the results obtained can be generalized for the case of a metal in superconducting state? In particular, what coupling constant (λ or $\tilde{\lambda}$) determines the temperature of superconducting transition T_c in antiadiabatic limit? Let us analyze this situation within appropriate generalization of Eliashberg equations.

Taking into account that in antiadiabatic approximation, vertex corrections are again irrelevant and neglecting the direct Coulomb repulsion, Eliashberg equations can be derived in the usual way by calculating the diagram of Fig. 1, where electronic Green's function in superconducting state is taken in Nambu's matrix representation. For real frequencies, this Green's function is written in the following standard form [3, 4]:

$$G(\varepsilon,\mathbf{p})=\frac{Z(\varepsilon)\varepsilon\tau_0+\varepsilon_{\mathbf{p}}\tau_3+Z(\varepsilon)\Delta(\varepsilon)\tau_1}{Z^2(\varepsilon)\varepsilon^2-Z^2(\varepsilon)\Delta^2(\varepsilon)-\varepsilon_{\mathbf{p}}^2} \tag{30}$$

which corresponds to the matrix of self–energy:

$$\Sigma(\varepsilon)=[1-Z(\varepsilon)]\varepsilon\tau_0+Z(\varepsilon)\Delta(\varepsilon)\tau_1 \tag{31}$$

where τ_i are standard Pauli matrices, while functions of mass renormalization $Z(\varepsilon)$ and energy gap $\Delta(\varepsilon)$ are determined from solution of integral Eliashberg equations [3, 4]. For us now, it is sufficient to consider only the linearized Eliashberg equations, determining superconducting transition temperature T_c, which for the case of real frequencies are written as [3, 4]:

$$[1-Z(\varepsilon)]\varepsilon=\int_0^D d\varepsilon'\int_0^\infty d\omega\alpha^2(\omega)F(\omega)f(-\varepsilon')\times\left(\frac{1}{\varepsilon'+\varepsilon+\omega+i\delta}-\frac{1}{\varepsilon'-\varepsilon+\omega-i\delta}\right) \tag{32}$$

$$Z(\varepsilon)\Delta(\varepsilon)=\int_0^D\frac{d\varepsilon'}{\varepsilon'}th\frac{\varepsilon'}{2T_c}Re\Delta(\varepsilon')\times\int_0^\infty d\omega\alpha^2(\omega)F(\omega)\times\left(\frac{1}{\varepsilon'+\varepsilon+\omega+i\delta}+\frac{1}{\varepsilon'-\varepsilon+\omega-i\delta}\right) \tag{33}$$

In difference with the standard approach [4], we have introduced the finite integration limits, determined by the (half)bandwidth D. To simplify the analysis, we again assume the half–filled band of degenerate electrons in two dimensions, so that $D=E_F\gg T_c$, with constant density of states.

The situation is considerably simplified [14, 15], if we consider these equations in the limit of $\varepsilon\to 0$ and look for

the solutions[1] $Z(0) = Z$ and $\Delta(0) = \Delta$. Then from (32), we obtain:

$$[1 - Z]\varepsilon = -2\varepsilon \int_0^\infty d\omega \alpha^2(\omega) F(\omega) \frac{D}{\omega(\omega + D)} \tag{34}$$

and we get the mass renormalization factor as:

$$Z = 1 + \tilde{\lambda} \tag{35}$$

where constant $\tilde{\lambda}$ was defined above in Eq. (23), which for $D \to \infty$ reduces to the usual Eliasberg–McMillan constant (9), while for D significantly smaller than characteristic phonon frequencies, it gives the "antiadiabatic" coupling constant (24). Mass renormalization is again determined by this generalized coupling constant $\tilde{\lambda}$ as in Eq. (25). In particular, in the strong antiadiabatic limit, this renormalization is quite small and determined by the limiting expression λ_D given by Eq. (24).

The situation is quite different in Eq. (33). In the limit of $\varepsilon \to 0$, using (35), we immediately obtain from (33) the following equation for T_c:

$$1 + \tilde{\lambda} = 2 \int_0^\infty d\omega \alpha^2(\omega) F(\omega) \int_0^D \frac{d\varepsilon'}{\varepsilon'(\varepsilon' + \omega)} th \frac{\varepsilon'}{2T_c} \tag{36}$$

where λ is the *standard* Eliashberg–McMillan coupling constant as defined above in Eq. (9). Thus, in general case, *different* coupling constants determine mass renormalization and T_c.

Let us consider rather a general model with discrete set of dispersionless phonon modes (Einstein phonons). In this case, the phonon density of states is written as:

$$F(\omega) = \sum_i \delta(\omega - \Omega_i) \tag{37}$$

where Ω_i are discrete frequencies modeling the optical branches of the phonon spectrum. Then from Eqs. (9) and (23), we get:

$$\lambda = 2 \sum_i \frac{\alpha^2(\Omega_i)}{\Omega_i} \equiv \sum_i \lambda_i \tag{38}$$

$$\tilde{\lambda} = 2 \sum_i \frac{\alpha^2(\Omega_i) D}{\Omega_i(\Omega_i + D)} = \sum_i \lambda_i \frac{D}{\Omega_i + D} \equiv \sum_i \tilde{\lambda}_i \tag{39}$$

Correspondingly, in this case:

$$\begin{aligned} \alpha^2(\omega) F(\omega) &= \sum_i \alpha^2(\Omega_i) \delta(\omega - \Omega_i) \\ &= \sum_i \frac{\lambda_i}{2} \Omega_i \delta(\omega - \Omega_i) \end{aligned} \tag{40}$$

The standard Eliashberg equation (in adiabatic limit) for such model was consistently solved in Ref. [23]. For our purposes, it is sufficient to analyze only Eq. (36), which takes now the following form:

$$1 + \tilde{\lambda} = 2 \sum_i \alpha^2(\Omega_i) \int_0^D \frac{d\varepsilon'}{\varepsilon'(\varepsilon' + \Omega_i)} th \frac{\varepsilon'}{2T_c} \tag{41}$$

This equation is easily solved to obtain:

$$T_c \sim \prod_i \left(\frac{D}{1 + \frac{D}{\Omega_i}} \right)^{\frac{\lambda_i}{\lambda}} \exp\left(-\frac{1 + \tilde{\lambda}}{\lambda} \right) \tag{42}$$

In the simple case of two optical phonons with frequencies Ω_1 and Ω_2, we have:

$$T_c \sim \left(\frac{D}{1 + \frac{D}{\Omega_1}} \right)^{\frac{\lambda_1}{\lambda}} \left(\frac{D}{1 + \frac{D}{\Omega_2}} \right)^{\frac{\lambda_2}{\lambda}} \exp\left(-\frac{1 + \tilde{\lambda}}{\lambda} \right) \tag{43}$$

where $\tilde{\lambda} = \tilde{\lambda}_1 + \tilde{\lambda}_2$ and $\lambda = \lambda_1 + \lambda_2$. For the case of $\Omega_1 \ll D$ (adiabatic phonon) and $\Omega_2 \gg D$ (antiadiabatic phonon), Eq. (43) is immediately reduced to:

$$T_c \sim (\Omega_1)^{\frac{\lambda_1}{\lambda}} (D)^{\frac{\lambda_2}{\lambda}} \exp\left(-\frac{1 + \tilde{\lambda}}{\lambda} \right) \tag{44}$$

Now we can see that in the preexponential factor, the frequency of antiadiabatic phonon is replaced by band half–width (Fermi energy), which plays a role of the cutoff for logarithmic divergence in Cooper channel in antiadiabatic limit [12–14].

Our general result (42) gives the general expression for T_c for the model with discrete set of optical phonons, valid both in adiabatic and antiadiabatic regimes and interpolating between these limits in intermediate region. Actually, Eq. (42) can be easily rewritten as:

$$T_c \sim \langle \Omega \rangle \exp\left(-\frac{1 + \tilde{\lambda}}{\lambda} \right) \tag{45}$$

where we have introduced the average logarithmic frequency $\langle \Omega \rangle$ as:

$$\ln\langle \Omega \rangle = \ln \prod_i \left(\frac{D}{1 + \frac{D}{\Omega_i}} \right)^{\frac{\lambda_i}{\lambda}} = \sum_i \frac{\lambda_i}{\lambda} \ln \frac{D}{1 + \frac{D}{\Omega_i}} \tag{46}$$

In the limit of continuous distribution of phonon frequencies, this last expression reduces to:

$$\ln\langle \Omega \rangle = \frac{2}{\lambda} \int \frac{d\omega}{\omega} \alpha^2(\omega) F(\omega) \ln \frac{D}{1 + \frac{D}{\omega}} \tag{47}$$

where λ is given by the usual expression (9). Equation (47) generalizes the standard definition of average logarithmic frequency of Eliasberg–McMillan theory [4] for the case of finite bandwidth. Obviously, it reduces to the standard expression in adiabatic limit of phonon frequencies much lower than D, and gives $\langle \Omega \rangle \sim D$ in extreme antiadiabatic limit, when all phonon frequencies are much larger than D.

[1] To avoid confusion, note that according to standard notations of Eliashberg–McMillan theory, the renormalization factor Z as defined here is just the inverse of a similar factor defined in Eq. (6) for the normal state

6 Coulomb Pseudopotential

Up to now we have neglected the direct Coulomb repulsion of electrons, which in the standard approach [1–5] is described by Coulomb pseudopotential $\mu^\star$, which is effectively suppressed by large Tolmachev's logarithm. As we noted in ref. [14], antiadiabatic phonons actually suppress Tolmachev's logarithm, which can probably lead to rather strong suppression of the temperature of superconducting transition. To clarify this situation, we consider the simplified version of integral equation for the gap (33), writing it in the standard form:

$$Z(\varepsilon)\Delta(\varepsilon) = \int_0^D d\varepsilon' K(\varepsilon,\varepsilon')\frac{1}{\varepsilon'} th\frac{\varepsilon'}{2T_c}\Delta(\varepsilon') \tag{48}$$

where the integral kernel is a combination of two step–functions:

$$K(\varepsilon,\varepsilon') = \lambda\theta(\langle\Omega\rangle - |\varepsilon|)\theta(\langle\Omega\rangle - |\varepsilon'|) - \mu\theta(D - |\varepsilon|)\theta(D - |\varepsilon'|) \tag{49}$$

where μ is the dimensionless (repulsive) Coulomb potential, while the parameter $\langle\Omega\rangle$, determining the energy width of attraction region due to phonons, is determined by preexponential factor (average logarithmic frequency) of Eqs. (42) and (45).

$$\langle\Omega\rangle = \prod_i \left(\frac{D}{1+\frac{D}{\Omega_i}}\right)^{\frac{\lambda_i}{\lambda}} \tag{50}$$

It is important that we always have $\langle\Omega\rangle < D$. Equation (48) is now rewritten as:

$$Z(\varepsilon)\Delta(\varepsilon) = (\lambda-\mu)\int_0^{\langle\Omega\rangle}\frac{d\varepsilon'}{\varepsilon'} th\frac{\varepsilon'}{2T_c}\Delta(\varepsilon') - \mu\int_{\langle\Omega\rangle}^D \frac{d\varepsilon'}{\varepsilon'}\Delta(\varepsilon') \tag{51}$$

Writing the mass renormalization due to phonons as:

$$Z(\varepsilon) = \begin{cases} 1+\tilde{\lambda} & \text{for} \quad \varepsilon < \langle\Omega\rangle \\ 1 & \text{for} \quad \varepsilon > \langle\Omega\rangle \end{cases} \tag{52}$$

we look for the solution of Eq. (48) for $\Delta(\varepsilon)$, as usual, in the following form [2, 4, 5]:

$$\Delta(\varepsilon) = \begin{cases} \Delta_1 & \text{for} \quad \varepsilon < \langle\Omega\rangle \\ \Delta_2 & \text{for} \quad \varepsilon > \langle\Omega\rangle \end{cases} \tag{53}$$

Then Eq. (51) is transformed into the system of two homogeneous linear equations for constants Δ_1 and Δ_2:

$$\begin{aligned} (1+\tilde{\lambda})\Delta_1 &= (\lambda-\mu)\ln\frac{\langle\Omega\rangle}{T_c}\Delta_1 - \mu\ln\frac{D}{\langle\Omega\rangle}\Delta_2 \\ \Delta_2 &= -\mu\ln\frac{\langle\Omega\rangle}{T_c}\Delta_1 - \mu\ln\frac{D}{\langle\Omega\rangle}\Delta_2 \end{aligned} \tag{54}$$

The condition of the existence of nontrivial solution here is:

$$1+\tilde{\lambda} = \left(\lambda - \frac{\mu}{1+\mu\ln\frac{D}{\langle\Omega\rangle}}\right)\ln\frac{\langle\Omega\rangle}{T_c} \tag{55}$$

Then the transition temperature is given by:

$$T_c = \langle\Omega\rangle\exp\left(-\frac{1+\tilde{\lambda}}{\lambda-\mu^\star}\right) \tag{56}$$

where the Coulomb pseudopotential is determined as:

$$\mu^\star = \frac{\mu}{1+\mu\ln\frac{D}{\langle\Omega\rangle}} = \frac{\mu}{1+\mu\ln\prod_i\left(1+\frac{D}{\Omega_i}\right)^{\frac{\lambda_i}{\lambda}}} \tag{57}$$

Now the phonon frequencies enter Tolmachev's logarithm as the product of partial contributions, with its values determined also by corresponding coupling constants. A similar structure of Tolmachev's logarithm was first obtained (in somehow different model) in ref. [24], where the case of frequencies going outside the limits of adiabatic approximation was not considered. In this sense, Eq. (57) has a wider region of applicability. In particular, for the model of two optical phonons with frequencies $\Omega_1 \ll D$ (adiabatic phonon) and $\Omega_2 \gg D$, from Eq. (57), we get:

$$\mu^\star = \frac{\mu}{1+\mu\ln\left(\frac{D}{\Omega_1}\right)^{\frac{\lambda_1}{\lambda}}} = \frac{\mu}{1+\mu\frac{\lambda_1}{\lambda}\ln\frac{D}{\Omega_1}} \tag{58}$$

We can see that the contribution of antiadiabatic phonon drops out of Tolmachev's logarithm, while the logarithm itself persists, with its value determined by the ratio of the band half-width (Fermi energy) to the frequency of adiabatic (low frequency) phonon. The general effect of suppression of Coulomb repulsion also persists, though it becomes somehow weaker due to the partial interaction of electrons with corresponding phonon. This situation is conserved also in the general case—the value of Tolmachev's logarithm and corresponding Coulomb pseudopotential is determined by contributions of adiabatic phonons, while antiadiabatic phonons drop out. Thus, in general case, the situation becomes more favorable for superconductivity, as compared with the case of a single antiadiabatic phonon, considered in ref. [14].

7 Conclusions

In the present paper, we have considered the electron–phonon coupling in Eliashberg–McMillan theory, taking into account antiadiabatic phonons with high enough frequency (comparable or exceeding the Fermi energy E_F). The value of mass renormalization, in general case, was shown to be determined by the new coupling constant $\tilde{\lambda}$, while the value of the pairing interaction is always determined by the standard coupling constant λ of

Eliashberg–McMillan theory, appropriately generalized by taking into account the finite value of phonon frequency [14]. Mass renormalization due to strongly antiadiabatic phonons is in general small and determined by the coupling constant $\lambda_D \ll \lambda$. In this sense, in the limit of strong antiadiabaticity, the coupling of such phonons with electrons becomes weak and corresponding vertex correction again becomes irrelevant [14, 22], creating a kind of "anti–Migdal" situation. This fact allows us to use the Eliashberg–McMillan approach in the limit of strong antiadiabaticity. In the intermediate region, all our expressions just produce a smooth interpolation between adiabatic and antiadiabatic limits.

The cutoff of pairing interaction in Cooper channel in antiadiabatic limit becomes effective at energies $\sim E_F \sim D$, as was previously noted in refs. [12–14]), so that corresponding phonons do not contribute to Tolmachev's logarithm in Coulomb pseudopotential. However, the large enough values of this logarithm (and corresponding smallness of $\mu^\star$) can be guaranteed due to contributions from adiabatic phonons [15].

Note that above, we have used a rather simplified analysis of Eliashberg equations. However, in our opinion, a more elaborate approach, e.g., along the lines of ref. [23], will not lead to qualitative change of our results. Some simple estimates for FeSe/STO system, based on these results, can be found in refs. [14, 15].

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References

1. Schrieffer, J.R.: Theory of Superconductivity. WA Benjamin, NY (1964)
2. Scalapino, D.J.: In: Parks, R.D. (ed.) Superconductivity, p. 449. Marcel Dekker, NY (1969)
3. White, R.M., Geballe, T.H.: Long Range Order in Solids. Academic Press, New York (1979)
4. Vonsovsky, S.V., Izyumov, Yu.A., Kurmaev, E.Z.: Superconductivity of Transition Metals, Their Alloys and Compounds. Springer, Berlin (1982)
5. Allen, P.B., Mitrović, B. In: Seitz, F., Turnbull, D., Ehrenreich, H. (eds.): Solid State Physics, vol. 37, p. 1. Academic Press, NY (1982)
6. Migdal, A.B.: Zh. Eksp. Teor. Fiz. **34**, 1438 (1958). [Sov. Phys. JETP 7, 996 (1958)]
7. Alexandrov, A.S., Krebs, A.B.: Usp. Fiz. Nauk **162**, 1 (1992). [Physics Uspekhi 35, 345 (1992)]
8. Esterlis, I., Nosarzewski, B., Huang, E.W., Moritz, D., Devereux, T.P., Scalapino, D.J., Kivelson, S.A.: Phys. Rev. B **97**, 140501(R) (2018)
9. Sadovskii, M.V.: Usp. Fiz. Nauk **178**, 1243 (2008). [Physics Uspekhi 51, 1243 (2008)]
10. Gor'kov, L.P., Kresin, V.Z.: Rev. Mod. Phys. **90**, 011001 (2018)
11. Gor'kov, L.P.: PNAS **113**, 4646 (2018)
12. Gor'kov, L.P.: Phys. Rev. B **93**, 054517 (2016)
13. Gor'kov, L.P.: Phys. Rev. B **93**, 060507 (2016)
14. Sadovskii, M.V.: Zh. Eksp. Teor. Fiz. **155**, 527 (2019). [JETP 128, 455 (2019)]
15. Sadovskii, M.V.: Pis'ma Zh. Eksp. Teor. Fiz. **109**, 165 (2010). [JETP Letters 109, 166 (2019)]
16. Sadovskii, M.V.: Diagrammatics. World Scientific, Singapore (2006)
17. Allen, P.B.: Phys. Rev. B **6**, 2577 (1972)
18. Lee, J.J., Schmitt, F.T., Moore, R.G., Johnston, S., Cui, Y.T., Li, W., Liu, Z.K., Hashimoto, M., Zhang, Y., Lu, D.H., Devereaux, T.P., Lee, D.H., Shen, Z.X.: Nature **515**, 245 (2014)
19. Kulić, M.L., Dolgov, O.V.: New J. Phys. **19**, 013020 (2017)
20. Nekrasov, I.A., Pavlov, N.S., Sadovskii, V.V.: Pis'ma Zh. Eksp. Teor. Fiz. **105**, 354 (2017). [JETP Letters 105, 370 (2017)]
21. Nekrasov, I.A., Pavlov, N.S., Sadovskii, M.V.: Zh. Eksp. Teor. Fiz. **153**, 590 (2016). [JETP 126, 485 (2018)] Phys. Rev. B 93, 134513
22. Ikeda, M.A., Ogasawara, A., Sugihara, M.: Phys. Lett. A **170**, 319 (1992)
23. Karakozov, A.E., Maksimov, A.E., Mashkov, S.A.: Zh. Eksp. Teor. Fiz. **68**, 1937 (1975). [JETP 41, 971 (1975)]
24. Kirzhnits, D.A., Maksimov, E.G., Khomskii, D.I.: J. Low. Temp. Phys. **10**, 79 (1973)