Superconducting Transition Temperature for Very Strong Coupling in the Antiadiabatic Limit of Eliashberg Equations

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1. INTRODUCTION

The discovery of superconductivity [1] with critical temperature up to \( T_c = 203 \) K in pressure interval of 100–250 GPa (in diamond anvils) in H\(_3\)S system initiated numerous experimental studies of high-temperature superconductivity of hydrides in megabar region (see reviews [2, 3]). Theoretical analysis immediately confirmed that these record-breaking \( T_c \) values are ensured by traditional electron–phonon interaction in the limit of strong enough electron–phonon coupling [4, 5]. More so, the detailed calculations performed for quite a number of hydrides of transition metals under pressure [4] lead to prediction of pretty large number of such systems with record \( T_c \) values. In some cases, these predictions were almost immediately confirmed by experiment, in particular the record values \( T_c = 160–260 \) K were achieved in LaH\(_{10}\) [6, 7], ThH\(_{10}\) [8], YH\(_6\) [9], (La,Y)H\(_{6,10}\) [10]. At last, some time ago the psychological barrier was overpassed, when in [11] superconductivity was obtained with \( T_c = (287.7 \pm 1.2) \) K (i.e., near \(+15^\circ\)C) in the C–H–S system at a pressure of (267 ± 10) GPa.

The principal achievement of these works was, before everything else, the demonstration of absence of any significant limitations for \( T_c \), within the traditional picture of electron–phonon mechanism of Cooper pairing, contrary to a common opinion that \( T_c \) due to it cannot exceed 30–40 K. Correspondingly, even more demanding now is the problem of the upper limit of \( T_c \) values, which can be achieved with this mechanism of pairing.

Since BCS theory appeared, it became obvious that \( T_c \) can be increased either by an increase in the frequency of phonons responsible for Cooper pairing or by the enhancement of the effective interaction of these phonons with electrons. These problems were thoroughly studied by different authors. The most developed approach to description of superconductivity in electron–phonon system is Eliashberg–McMillan theory [5, 12, 13]. It is well known that this theory is entirely based on the applicability of adiabatic approximation and Migdal theorem [14], which allows to neglect vertex corrections while calculating the effects of electron–phonon interactions in typical metals. The actual small parameter of perturbation theory in these calculations is \( \lambda \frac{\Omega_0}{E_F} \ll 1 \), where \( \lambda \) is the dimensionless electron–phonon coupling constant, \( \Omega_0 \) is characteristic frequency of phonons and \( E_F \) is the Fermi energy of electrons. In particular, this means that vertex corrections in this theory can be neglected even in the case of \( \lambda > 1 \), as we always have an inequality \( \frac{\Omega_0}{E_F} \ll 1 \) valid for typical metals.

In [15–17], we have recently shown that in the case of strong nonadiabaticity, when \( \Omega_0 \gg E_F \), a new small parameter appears in the theory \( \lambda_D \sim \frac{\Omega_0}{E_F} \sim \lambda_D \frac{D}{\Omega_0} \ll 1 \) (\( D \) is the half-width of the electron band), so that corrections to the electronic spectrum become

\[ T_c \]
irrelevant. Vertex corrections can also be neglected, as it was shown in [18]. In general case the renormalization of the electronic spectrum (effective mass of the electron) is determined by a new dimensionless constant $\tilde{\lambda}$, which reduces to the usual $\lambda$ in the adiabatic limit, while in strong antiadiabatic limit it tends to $\lambda_D$.

At the same time, the superconducting transition temperature $T_c$ in the antiadiabatic limit is determined by Eliashberg–McMillan pairing constant $\lambda$, generalized by taking into account finite phonon frequencies.

For the case of interaction with a single optical (Einstein) phonon in [15] we have obtained the single expression for $T_c$, which is valid both in adiabatic and antiadiabatic regimes and smoothly interpolating in between:

$$T_c \sim \frac{D}{\Omega_0 + D} \exp \left( -\frac{1 + \tilde{\lambda}}{\lambda} \right),$$

where $\tilde{\lambda} = \frac{\lambda D}{\Omega_0 + D}$ is smoothly changing from $\lambda$ for $\Omega_0 \ll D \sim E_\Gamma$ to $\lambda_D$ in the limit $\Omega_0 \gg D \sim E_\Gamma$.

Besides the questions related to possible limits of $T_c$ in hydrides, where possibly some small pockets of the Fermi surface with small Fermi energies exist [5], the interest to the problem of superconductivity in strongly antiadiabatic limit is stimulated by the discovery of a number of other superconductors, where adiabatic approximation cannot be considered valid and characteristic phonon frequencies is of the order or even exceed the Fermi energy of electrons. Typical in this respect are intercalated systems with monolayers of FeSe, and monolayers of FeSe on substrates like Sr(Ba)TiO$_3$ (FeSe/STO) [19]. With respect to FeSe/STO this was first noted by Gor’kov [20, 21], while discussing the idea of the possible mechanism of increasing the superconducting transition temperature $T_c$ in FeSe/STO due to interactions with high-energy optical phonons of SrTiO$_3$ [19]. Similar situation appears also in an old problem of superconductivity in doped SrTiO$_3$ [22].

2. LIMITS FOR THE SUPERCONDUCTING TRANSITION TEMPERATURE IN THE CASE OF VERY STRONG ELECTRON–PHONON COUPLING

The general equations of the Eliashberg–McMillan theory determining the superconducting gap $\Delta(\omega_n)$ in the Matsubara representation ($\omega_n = (2n + 1)\pi T$) can be written as [5, 12, 13]

$$\Delta(\omega_n)Z(\omega_n) = T \sum_{n' < 0}^{\infty} d\xi d\alpha n x^2(\omega) F(\omega) \times D(\omega_n - \omega_n'; \omega) - \frac{\Delta(\omega_n')}{\omega_n^2 + \xi^2 + \Delta^2(\omega_n')},$$

where

$$D(\omega_n - \omega_n'; \omega) = \frac{2\omega}{(\omega_n - \omega_n')^2 + \omega^2}. \quad (4)$$

Here, $\alpha^2(\omega) F(\omega)$ is McMillan’s function, $F(\omega)$ is the phonon density of states, and for simplicity we assume here the model of half-filled band of electrons with finite width $2D (D - E_\Gamma)$ with constant density of states (two-dimensional case).

We also neglect here the effects of Coulomb repulsion leading to the appearance of Coulomb pseudopotential $\mu^*$, which is usually small and more or less irrelevant in the region of very strong electron–phonon attraction [5, 12, 13].

Then, taking into account

$$\int_{-D}^{D} d\xi \frac{1}{\omega_n^2 + \xi^2 + \Delta^2(\omega_n')} \times \frac{2}{\omega_n^2 + \Delta^2(\omega_n')} \arctan \frac{D}{\sqrt{\omega_n^2 + \Delta^2(\omega_n')}} \\rightarrow \frac{2}{|\omega_n|} \arctan \frac{D}{|\omega_n|} \quad \text{at} \quad \Delta(\omega_n') \rightarrow 0;$$

the linearized Eliashberg equations acquire the general form

$$\Delta(\omega_n)Z(\omega_n) = T \sum_{n' < 0}^{\infty} d\alpha n x^2(\omega) F(\omega) \times D(\omega_n - \omega_n'; \omega) \frac{2\Delta(\omega_n')}{|\omega_n'|} \arctan \frac{D}{|\omega_n'|}, \quad (6)$$

$$Z(\omega_n) = 1 + \frac{T}{\omega_n} \sum_{n' < 0}^{\infty} d\alpha n x^2(\omega) F(\omega) \times D(\omega_n - \omega_n'; \omega) \frac{2\Delta(\omega_n')}{|\omega_n'|} \arctan \frac{D}{|\omega_n'|}. \quad (7)$$

Consider the equation for $n = 0$ determining $\Delta(0) \equiv \Delta(\pi T) = \Delta(-\pi T)$, which follows directly from Eqs. (6), (7):

$$\Delta(0) = T \sum_{n' < 0}^{\infty} d\alpha n x^2(\omega) F(\omega) \times \frac{2\omega}{(\pi T - \omega_n')^2 + \omega^2} \arctan \frac{D}{|\omega_n'|}. \quad (8)$$
Leaving only the contribution from $n' = -1$, we immediately obtain the inequality

$$1 > \frac{2}{\pi} \int_0^\infty d\omega \alpha^2(\omega) F(\omega) \frac{2\omega}{(2\pi T)^2 + \omega^2} \arctan \frac{D}{\pi T},$$

which generalizes the similar inequality first obtained in [23] and determining the lower bound for $T_c$. For the Einstein model of the phonon spectrum, we have $F(\omega) = \delta(\omega - \Omega_0)$, so that Eq. (9) is reduced to:

$$1 > \frac{2\lambda}{\pi} \arctan \frac{\Omega_0^2}{\pi T (2\pi T)^2 + \Omega_0^2},$$

where $\lambda = 2\alpha^2(\Omega_0)/\Omega_0$ is the dimensionless pairing coupling constant. For $D \approx \pi T$, we immediately obtain the Allen–Dynes result [23]:

$$T_c > \frac{1}{2\pi} \sqrt{\lambda - \Omega_0} \approx 0.16\sqrt{\lambda}/\Omega_0 \quad \text{at} \quad \lambda \gg 1,$$

which in fact determines the asymptotic behavior of $T_c$ in the region of very strong coupling $\lambda \gg 1$. The exact numerical solution of the Eliashberg equation [23] produces for $T_c$ the result like (11) with the replacement of a numerical coefficient of 0.16 by 0.18. This asymptotic behavior rather satisfactorily describes the $T_c$ values already for $\lambda > 2$.

In the case of general phonon spectrum, it is sufficient to replace here $\Omega_0 \rightarrow \langle \Omega^2 \rangle^{1/2}$, where

$$\langle \Omega^2 \rangle = \frac{2}{\lambda_0} \int_0^\infty d\omega \alpha^2(\omega) F(\omega),$$

is the average (over the spectrum) square frequency of phonons, and the general expression for the coupling constant is [5, 12, 13]:

$$\lambda = 2 \int_0^\infty d\omega \alpha^2(\omega) F(\omega).$$

For $D \ll \pi T$ from Eq. (10), we obtain

$$T > \frac{1}{2\pi} \sqrt{\lambda^*(T) - \Omega_0}$$

where

$$\lambda^*(T) = \frac{2D}{\pi T} \lambda,$$

so that in the strongly antiadiabatic limit, we get

$$T_c > (2\pi^4)^{-1/3} (\lambda D/\Omega_0)^{2/3} \approx 0.17(\lambda D/\Omega_0)^{2/3}.$$
graphs we actually have the smooth crossover from $T_c$ behavior in the region of weak and intermediate coupling to its asymptotic behavior in the region of very strong coupling $\lambda \gg 1$. It is also seen that the increase in phonon frequencies and crossover to antiadiabatic limit does not lead, in general, to the increase in $T_c$ as compared to adiabatic case.

3. CONCLUSIONS

In this work, we have considered the case of very strong electron–phonon coupling in Eliashberg–McMillan theory, including the antiadiabatic situation with phonons of very high frequency (exceeding the Fermi energy $E_F$). The value of mass renormalization is in general determined by the coupling constant $\lambda$, [15], which is small in antiadiabatic limit. At the same time, the pairing interaction is always determined by the standard coupling constant $\lambda$ of Eliashberg–McMillan theory, appropriately generalized by taking into account the finite values of phonon frequencies [15]. However, the simplest estimates [15, 17] show, that in antiadiabatic situation this constant in general rather rapidly drops with the growth of phonon frequency $\Omega_0$ for $\Omega_0 \gg E_F$. In this sense, the asymptotic behavior of $T_c$ for very strong coupling discussed above can be possibly achieved only in some exceptional cases. Even in this case, as clear from our results, the transition into antiadiabatic region cannot increase $T_c$ as compared to the standard adiabatic situation.

While the usual expression for $T_c$ in terms of the pairing constant $\lambda$ and characteristic phonon frequency $\Omega_0 \sim \langle \Omega^2 \rangle^{1/2}$ are quite convenient and clear, it is to be taken into account that these parameters are in fact not independent. As seen from expressions like (12) and (13), these parameters are determined by the same Eliashberg–McMillan function $\alpha^2(\omega)F(\omega)$. Correspondingly, there are limitations for free changes of these parameters in estimates of optimal (maximum) values of $T_c$.

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