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Limits of Eliashberg theory and bounds for superconducting transition temperature

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Contents

Abstract. The discovery of record-breaking values of superconducting transition temperature T_c in quite a number of hydrides under high pressure was an impressive demonstration of the capabilities of the electron–phonon mechanism of Cooper pairing. This led to increased interest in the foundations and limitations of the Eliashberg–McMillan theory as the main theory describing superconductivity in a system of electrons and phonons. Below, we shall consider both the elementary basics of this theory and a number of new results derived only recently. We shall discuss limitations on the value of the coupling constant related to lattice instability and a phase transition to another phase (CDW, bipolarons). Within the stable metallic phase, the effective pairing constant may acquire arbitrary values. We consider extensions beyond the traditional adiabatic approximation. It is shown that the Eliashberg–McMillan theory is also applicable in the strong antiadiabatic limit. The limit of very strong coupling, being the most relevant one for the physics of hydrides, is analyzed in detail. We also discuss the bounds for T_c appearing in this limit.

Keywords: Eliashberg equations, superconducting transition temperature, strong coupling, adiabatic and antiadiabatic approximation, superhydrides

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1. Introduction

The discovery [1] of superconductivity with the critical temperature approaching $T_c = 203$ K under pressure in the interval of 100–250 GPa (in diamond anvils) in an H_3S system led to a stream of papers devoted to experimental studies of high-temperature superconductivity in hydrides in the megabar region (cf. reviews [2–4]). Theoretical analyses immediately confirmed that these record-breaking values of T_c are ensured by traditional electron–phonon interaction in the limit of quite strong electron–phonon coupling [5, 6]. Moreover, detailed calculations for a number of rare earth hydrides under pressure [6] led to the prediction of a fairly large number of such systems with record values of T_c. In some cases, these predictions were spectacularly confirmed. In particular, experimentally, values of $T_c = 220-260$ K were obtained in systems like LaH_{10} [7, 8], YH_6 [9], $(La,Y)H_{6,10}$ [10], and YH_9 [11]. Finally, quite recently a psychological border was crossed when, in Ref. [12], superconductivity with $T_c = 287.7 \pm 1.2$ K (i.e., about 15 °C) was obtained in C–H–S systems at pressures of 267 ± 10 GPa.

The matter of principle here is that these studies explicitly demonstrated the absence of any significant limitations for T_c within the electron–phonon mechanism of Cooper pairing, where it was traditionally believed that T_c can not exceed 30–40 K. Correspondingly, the question of the upper limit of T_c which can be achieved due to this pairing mechanism now became the most pressing issue.

Since the appearance of the Bardeen–Cooper–Schrieffer (BCS) theory it became obvious that an increase in T_c in superconductors can be realized by increasing the frequency of phonons responsible for Cooper pairing, as well as by an increase in the effective interaction of these phonons with electrons. These questions have been studied by numerous authors. The most developed approach for describing super-

conductivity in a system of electrons of phonons remains the Eliashberg–McMillan theory [5, 13–16]. It is well known that this theory is entirely based upon the adiabatic approximation and Migdal theorem [17–20], which allows us to neglect vertex corrections while calculating the effects of electron–phonon interaction in typical metals. The real small parameter of the perturbation theory here is $\lambda\Omega_0/E_F \ll 1$, where λ is a dimensionless constant of electron–phonon interaction, Ω_0 is the characteristic phonon frequency, and E_F is the Fermi energy of electrons. In particular, this leads to the conclusion that vertex corrections in this theory can be neglected even in the case of $\lambda > 1$, because the inequality $\Omega_0/E_F \ll 1$ is valid in typical metals. Recently, a number of papers have appeared [21–23] where some doubts were expressed about these conclusions and some revisions were proposed based on the results of quantum Monte Carlo calculations for electron–phonon systems.

In Refs [24–26], we have shown that, under conditions of strong nonadiabaticity, when $\Omega_0 \gg E_F$, the theory acquires a new small parameter $\lambda_D \sim \lambda E_F/\Omega_0 \sim \lambda D/\Omega_0 \ll 1$ (D is the half-width of electron band), so that corrections to the electronic spectrum become insignificant. Vertex corrections can also be neglected in this case, as was earlier shown in Ref. [27]. In the general case, the renormalization of the electron spectrum (effective mass of an electron) is determined by the new dimensionless coupling constant $\tilde{\lambda}$, which tends to the usual λ in the adiabatic limit, while in the strong antiadiabatic limit it tends to λ_D. At the same time, the temperature of superconducting transition T_c in the antiadiabatic limit is determined by the usual pairing constant of the Eliashberg–McMillan theory λ, generalized to take into account the finiteness of the phonon frequency. Thus, the Eliashberg–McMillan approach also remains valid in the strong antiadiabatic limit.

In general, interest in the problem of superconductivity in the strong antiadiabatic limit is stimulated by the discovery of a number of other superconductors, where the adiabatic approximation becomes invalid and characteristic phonon frequencies are of the order of or even higher than the electron Fermi energy. Typical in this respect are intercalated systems with FeSe monolayers, as are single-layer films of FeSe on Sr(Ba)TiO_3 (FeSe/STO) substrates [28].

The nonadiabatic nature of superconductivity in an FeSe/STO system was first noted by Gor'kov [29, 30] while discussing a possible mechanism of superconducting T_c enhancement in FeSe/STO due to interaction with high-energy optical phonons of $SrTiO_3$ [28]. A similar situation, in fact, also appears in an old problem of superconductivity in doped $SrTiO_3$ [31], as well as in twisted bi(tri)layers of graphene [32]. In hydrides, there is also the possibility of the existence of some small 'pockets' of the Fermi surface with small values of Fermi energy [5].

This paper is devoted to a critical review of these problems on a rather elementary level. Our presentation does not purport to be exhaustive or to give a complete review of multiple papers devoted to studies of Eliashberg equations in recent decades. However, the author hopes that this presentation can be useful both to young theorists and to some experts in this field.

2. Eliashberg–McMillan approximation

The Fröhlich Hamiltonian, which is usually used to describe electron–phonon interaction, can be written as [13, 19]

$$H = \sum_{\mathbf{p}} \varepsilon_{\mathbf{p}} a_{\mathbf{p}}^{+} a_{\mathbf{p}} + \sum_{\mathbf{k}} \Omega_{0\mathbf{k}} b_{\mathbf{k}}^{+} b_{\mathbf{k}} + \frac{1}{\sqrt{N}} \sum_{\mathbf{pk}} g_{\mathbf{k}} a_{\mathbf{p}+\mathbf{k}}^{+} a_{\mathbf{p}} (b_{\mathbf{k}} + b_{-\mathbf{k}}^{+}) , \quad (1)$$

where $\varepsilon_{\mathbf{p}}$ is the electron spectrum counted from the Fermi level, $\Omega_{0\mathbf{k}}$ is the phonon spectrum,[1] we have introduced the standard notations for creation $a_{\mathbf{p}}^{+}$ and annihilation $a_{\mathbf{p}}$ operators of electrons and phonons $b_{\mathbf{k}}^{+}$ and $b_{\mathbf{k}}$, and N is the number of atoms in the crystal.

The matrix element of electron–phonon interaction has the following form [13, 19]:

$$g_{\mathbf{k}} = -\frac{1}{\sqrt{2M\Omega_{0\mathbf{k}}}} \langle \mathbf{p} | \mathbf{e}(\mathbf{q}) \nabla V_{ei}(\mathbf{r}) | \mathbf{p} + \mathbf{q} \rangle \equiv -\frac{1}{\sqrt{2M\Omega_{0\mathbf{k}}}} I(\mathbf{k}) , \quad (2)$$

where V_{ei} is the electron–ion interaction potential, M is the ion mass, and $\mathbf{e}(\mathbf{q})$ is the polarization vector of a phonon with frequency $\Omega_{0\mathbf{q}}$.

To describe the phonon spectrum, we often use simplified Debye and Einstein models. In the Debye model, the phonon spectrum is assumed to be $\Omega_{0\mathbf{k}} = ck$ (c is the speed of sound) for all $k < k_D$, which gives an elementary model of acoustic phonons. In this case, Debye frequency $\Omega_D = ck_D$ defines the upper limit of phonon frequencies. In the Einstein model, the phonon frequency is assumed to be independent of the wave vector: $\Omega_{0\mathbf{k}} = \Omega_0$ for all k within the Brillouin zone, which gives the simplified model of optical phonons.

To describe the interaction of electrons with optical (Einstein) phonons, the so-called Holstein model is also often used. Its Hamiltonian is commonly written in a coordinate (site) representation in the lattice, and electron–phonon interaction is assumed to be local (single-site):

$$H = -t \sum_{ij\sigma} (t_{ij} a_{i\sigma}^{+} a_{j\sigma} + \text{h.c.}) + \Omega_0 \sum_i b_i^{+} b_i - \mu \sum_{i\sigma} n_{i\sigma} + g \sum_i (b_i + b_i^{+}) \sum_\sigma n_{i\sigma} , \quad (3)$$

where $a_{i\sigma}^{+}$ and $a_{i\sigma}$ are creation and annihilation operators of an electron with spin σ on lattice site i, $n_i = a_{i\sigma}^{+} a_{i\sigma}$ is the electron density operator on the site, t_{ij} are transfer integrals of electrons between lattice sites determining their spectrum (bandwidth) in the tight-binding approximation, and b_i^{+} and b_i are corresponding operators for phonons with frequency Ω_0. The strength of electron–phonon interaction is determined by interaction constant g. Obviously, this interaction describes the local interaction of an Einstein phonon with the electron density at a lattice site. Chemical potential μ is determined by conduction band filling and defines the origin of the energy scale for electrons.

Consider the simplest second-order diagram of electron–phonon interaction, shown in Fig. 1. Let us perform calculations using the Matsubara technique (i.e., at finite temperatures $T > 0$). The analytical expression correspond-

[1] Note that here we have introduced the 'bare' phonon spectrum *in the absence* of electron–phonon interaction, which has no obvious definition in a real metal.

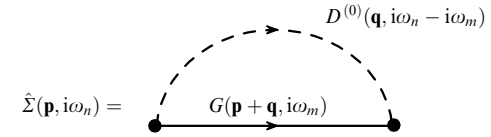

Figure 1. Second-order diagram for electronic self-energy.

ing to this diagram has the form

$$\Sigma(\mathrm{i}\omega_n, \mathbf{p}) = -T \sum_{n'=-\infty}^{\infty} \sum_{\mathbf{p}'} |g_{\mathbf{p}\mathbf{p}'}|^2 G_0(\mathrm{i}\omega_{n'}, \mathbf{p}') \times D_0(\mathrm{i}\omega_n - \mathrm{i}\omega_{n'}, \mathbf{p} - \mathbf{p}') \,. \tag{4}$$

The subscript 0 on Green's functions of the electron $G_0(\mathrm{i}\omega_{n'}, \mathbf{p}')$ and phonon $D_0(\mathrm{i}\omega_n - \mathrm{i}\omega_{n'}, \mathbf{p} - \mathbf{p}')$ in (4) indicates that these are Green's functions of free particles.

Summation over Matsubara frequencies is performed in a standard way [19, 20], so that

$$\Sigma(\mathrm{i}\omega_n, \mathbf{p}) = \sum_{\mathbf{p}'} |g_{\mathbf{p}\mathbf{p}'}|^2 \left(\frac{f_{\mathbf{p}'} + n_{\mathbf{p}-\mathbf{p}'}}{\mathrm{i}\omega_n - \varepsilon_{\mathbf{p}'} + \Omega_{0\mathbf{p}-\mathbf{p}'}} + \frac{1 - f_{\mathbf{p}'} + n_{\mathbf{p}-\mathbf{p}'}}{\mathrm{i}\omega_n - \varepsilon_{\mathbf{p}'} - \Omega_{0\mathbf{p}-\mathbf{p}'}} \right), \tag{5}$$

where $f(\mathbf{p}) = 1/[\exp(\varepsilon_{\mathbf{p}}/T) + 1]$ is the Fermi distribution of electrons, while $n_q = 1/[\exp(\Omega_{0q}/T) - 1]$ is the Planckian (Bose) distribution of phonons. For temperatures $T \to 0$, the Fermi distribution of electrons transforms into a step function, while the Planckian function of phonons tends to zero, so that the first term on the right-hand side of (5) in parentheses is different from zero only for $\varepsilon_{\mathbf{p}'} < 0$, while the second one, for $\varepsilon_{\mathbf{p}'} > 0$. Correspondingly, in the limit of $T = 0$, after the substitution $\mathrm{i}\omega_n \to \varepsilon + \mathrm{i}\delta \operatorname{sign} \varepsilon_{\mathbf{p}'}$, the contribution of the diagram of Fig. 1 can be written as [13]

$$\Sigma(\varepsilon, \mathbf{p}) = \sum_{\mathbf{p}'} |g_{\mathbf{p}\mathbf{p}'}|^2 \left(\frac{f_{\mathbf{p}'}}{\varepsilon - \varepsilon_{\mathbf{p}'} + \Omega_{0\mathbf{p}-\mathbf{p}'} - \mathrm{i}\delta} + \frac{1 - f_{\mathbf{p}'}}{\varepsilon - \varepsilon_{\mathbf{p}'} - \Omega_{0\mathbf{p}-\mathbf{p}'} + \mathrm{i}\delta} \right). \tag{6}$$

Equation (6) can be identically rewritten as

$$\Sigma(\varepsilon, \mathbf{p}) = \int \mathrm{d}\omega \sum_{\mathbf{p}'} |g_{\mathbf{p}\mathbf{p}'}|^2 \delta(\omega - \Omega_{0\mathbf{p}-\mathbf{p}'}) \times \left(\frac{f_{\mathbf{p}'}}{\varepsilon - \varepsilon_{\mathbf{p}'} + \omega - \mathrm{i}\delta} + \frac{1 - f_{\mathbf{p}'}}{\varepsilon - \varepsilon_{\mathbf{p}'} - \omega + \mathrm{i}\delta} \right). \tag{7}$$

Scattering of electrons by phonons in fact takes place in some narrow energy layer close to the Fermi level with a width of the order of double Debye frequency $2\Omega_{\mathrm{D}}$, and in typical metals we always have $\Omega_{\mathrm{D}} \ll E_{\mathrm{F}}$. In this situation, with high accuracy we can assume that both initial and final momenta of electrons $\mathbf{p}$ and $\mathbf{p}'$ are on the Fermi surface. The main idea of the Eliashberg–McMillan approach is that we can avoid explicit dependence on momenta, performing the averaging of the matrix element of electron–phonon interaction over surfaces of constant energy corresponding to initial and final momenta $\mathbf{p}$ and $\mathbf{p}'$, which is practically the same as averaging over corresponding real Fermi surfaces of a metal, which are defined by equations $\varepsilon(\mathbf{p}) = 0$ and $\varepsilon(\mathbf{p}') = 0$. This is achieved by the following substitution ($N(0)$ is the density of states at the Fermi level):

$$|g_{\mathbf{p}\mathbf{p}'}|^2 \delta(\omega - \Omega_{0\mathbf{p}-\mathbf{p}'}) \Longrightarrow \frac{1}{N(0)} \sum_{\mathbf{p}} \frac{1}{N(0)} \sum_{\mathbf{p}'} |g_{\mathbf{p}\mathbf{p}'}|^2 \delta(\omega - \Omega_{0\mathbf{p}-\mathbf{p}'}) \delta(\varepsilon_{\mathbf{p}}) \delta(\varepsilon_{\mathbf{p}'}) \equiv \frac{1}{N(0)} \alpha^2(\omega) F(\omega) \,, \tag{8}$$

where in the final line we have introduced the standard *definition* of Eliashberg function $\alpha^2(\omega)$, which reflects the strength of electron–phonon interaction, while $F(\omega) = \sum_{\mathbf{q}} \delta(\omega - \Omega_{0\mathbf{q}})$ is the phonon density of states. In principle, these functions can be directly determined from experiments.

When the phonon energy becomes comparable to or even exceeds the Fermi energy, electron scattering takes place not in a narrow layer close to the Fermi surface but in a much wider energy interval. Then, for an initial $|\mathbf{p}| \sim p_{\mathrm{F}}$, the averaging over $\mathbf{p}'$ in expressions like (8) should be made over a surface of constant energy, corresponding to $E_{\mathrm{F}} + \Omega_{0\mathbf{p}-\mathbf{p}'}$ [24, 26]. Correspondingly, Eqn (8) is obviously generalized as

$$|g_{\mathbf{p}\mathbf{p}'}|^2 \delta(\omega - \Omega_{0\mathbf{p}-\mathbf{p}'}) \Longrightarrow \frac{1}{N(0)} \sum_{\mathbf{p}} \frac{1}{N(0)} \times \sum_{\mathbf{p}'} |g_{\mathbf{p}\mathbf{p}'}|^2 \delta(\omega - \Omega_{0\mathbf{p}-\mathbf{p}'}) \delta(\varepsilon_{\mathbf{p}}) \delta(\varepsilon_{\mathbf{p}'} - \Omega_{0\mathbf{p}-\mathbf{p}'}) \equiv \frac{1}{N(0)} \alpha^2(\omega) F(\omega) \,, \tag{9}$$

which in the last δ-function simply corresponds to a transition from chemical potential μ to $\mu + \Omega_{\mathbf{p}-\mathbf{p}'}$. Remember that we always put the origin of an energy scale at $\mu = 0$.

After replacement (8), the explicit dependence on momenta in self-energy vanishes, and in the following we are dealing with the average over the Fermi surface,

$$\Sigma(\varepsilon) \equiv \frac{1}{N(0)} \sum_{\mathbf{p}} \delta(\varepsilon_{\mathbf{p}}) \Sigma(\varepsilon, \mathbf{p}) \,,$$

which is now written as

$$\Sigma(\varepsilon) = \int \mathrm{d}\varepsilon' \int \mathrm{d}\omega \, \alpha^2(\omega) F(\omega) \left(\frac{f(\varepsilon')}{\varepsilon - \varepsilon' + \omega - \mathrm{i}\delta} + \frac{1 - f(\varepsilon')}{\varepsilon - \varepsilon' - \omega + \mathrm{i}\delta} \right). \tag{10}$$

In the case of self-energy depending only on the frequency (and not on momentum), we can use the usual expressions for the (inverse) residue at the pole of the Green's function and electron mass renormalization [20][2]

$$Z = 1 - \left. \frac{\partial \Sigma(\varepsilon)}{\partial \varepsilon} \right|_{\varepsilon = 0} , \tag{11}$$

$$m^* = Zm = m \left(1 - \left. \frac{\partial \Sigma(\varepsilon)}{\partial \varepsilon} \right|_{\varepsilon = 0} \right). \tag{12}$$

[2] Here, we use the notation inverse to that used in the theory of normal metals [20] to make it consistent with notations usually used in Eliashberg equations of the superconductivity theory. Correspondingly, we have $Z \geqslant 1$, so that the residue at the pole of the Green's function is given by $Z^{-1} \leqslant 1$.

Defining the dimensionless electron–phonon coupling constant of the Eliashberg–McMillan theory as

$$\lambda = 2\int_0^\infty \frac{\mathrm{d}\omega}{\omega}\,\alpha^2(\omega)F(\omega)\,, \tag{13}$$

by direct calculations, we immediately obtain from (10) the standard expression for electron mass renormalization due to interaction with phonons as

$$m^\star = m(1+\lambda)\,. \tag{14}$$

The function $\alpha^2(\omega)F(\omega)$ in the expression for the Eliashberg constant of electron–phonon interaction (13) is to be calculated via (8) or is to be determined from experiments.

Using Eqn (8), we can rewrite (13) as

$$\lambda = \frac{2}{N(0)}\int_0^\infty \frac{\mathrm{d}\omega}{\omega}\sum_{\mathbf{p}}\sum_{\mathbf{p}'}|g_{\mathbf{p}\mathbf{p}'}|^2\delta(\omega-\Omega_{0\mathbf{p}-\mathbf{p}'})\delta(\varepsilon_{\mathbf{p}})\delta(\varepsilon_{\mathbf{p}'})\,, \tag{15}$$

which gives the standard way to calculate electron–phonon coupling constant λ, which determines, in particular, the Cooper pairing in the Eliashberg–McMillan theory.

In the model of Einstein phonons, $\Omega_{0k}\to\Omega_0$ and $g_k\to g_0$, so that dimensionless electron–phonon coupling constant (15) immediately reduces to the standard form [20]:

$$\lambda_0 = \frac{2g_0^2N(0)}{\Omega_0}\,. \tag{16}$$

However, we must remember that, in the general case, the function $\alpha^2(\omega)F(\omega)$ in the expression for the Eliashberg electron–phonon coupling constant (13) is to be calculated either via (8) or from (9), depending on the ratio of Fermi energy E_F and characteristic phonon frequency Ω_0. Until $\Omega_0 \ll E_\mathrm{F}$, we can use the standard expression (8), while in the case of $\Omega) \sim E_\mathrm{F}$ we have to use (9). Using Eqn (9), we can rewrite (13) in the following form:

$$\lambda = \frac{2}{N(0)}\int_0^\infty \frac{\mathrm{d}\omega}{\omega}\sum_{\mathbf{p}}\sum_{\mathbf{p}'}|g_{\mathbf{p}\mathbf{p}'}|^2 \times\delta(\omega-\Omega_{0\mathbf{p}-\mathbf{p}'})\delta(\varepsilon_{\mathbf{p}})\delta(\varepsilon_{\mathbf{p}'}-\Omega_{0\mathbf{p}-\mathbf{p}'})\,, \tag{17}$$

which gives the most general way to calculate electron–phonon constant λ, determining the Cooper pairing in the Eliashberg–McMillan theory.

3. Migdal theorem

In Section 2, while calculating electron self-energy due to electron–phonon interaction, we limited ourselves to the simplest contribution shown in Fig. 1. It may seem that we must also take into account other graphs related to corrections to one of the vertices in this diagram. In fact, this is unnecessary, as these corrections to the vertex part are small over the adiabatic parameter $\Omega_0/E_\mathrm{F}\sim\sqrt{m/M}\ll 1$ (Migdal theorem) [17] (cf. also Refs [13, 18–20]). Here, Ω_0 is the characteristic phonon frequency of the order of the Debye frequency.

Let us show this by estimating the simplest vertex correction determined by the graph shown in Fig. 2. We shall limit our analysis to a model with an Einstein spectrum of phonons. The analytic expression corresponding to the diagram in Fig. 2 is

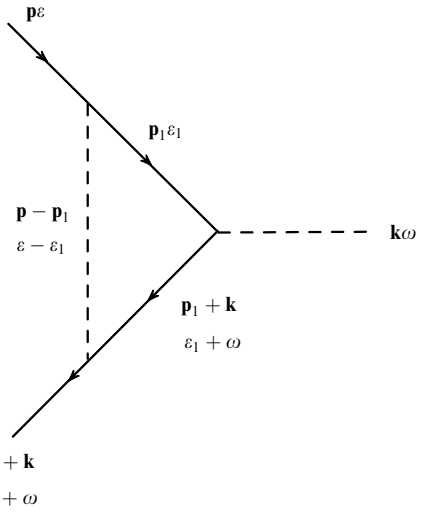

Figure 2. Simplest vertex correction due to electron–phonon interaction.

$$\Gamma^{(1)} = -g_0^3\int G_0(\mathbf{p}_1\varepsilon_1)G_0(\mathbf{p}_1+\mathbf{k},\varepsilon_1+\omega) \times D_0(\varepsilon-\varepsilon_1,\mathbf{p}-\mathbf{p}_1)\,\frac{\mathrm{d}^3p_1\,\mathrm{d}\varepsilon_1}{(2\pi)^4}\,. \tag{18}$$

Let us make a rough estimate of this expression. Consider first the integral over ε_1. Assuming that the characteristic momentum transfer due to phonon exchange is of the order of $k_\mathrm{D}\sim p_\mathrm{F}$, and taking into account that $D_0(\varepsilon-\varepsilon_1)$ drops quadratically in the region of $|\varepsilon-\varepsilon_1|\gg\Omega_0$, we obtain the main contribution to this integral from the region of $|\varepsilon-\varepsilon_1|\sim\Omega_0$. Then, the integral over ε_1 is of the order of 1, and we can write

$$\Gamma^{(1)}\sim g_0^3\int \mathrm{d}^3p_1 \times\frac{1}{(\varepsilon_1-\varepsilon_{\mathbf{p}_1}+\mathrm{i}\delta\,\mathrm{sign}\,\varepsilon_{\mathbf{p}_1})(\varepsilon_1+\omega-\varepsilon_{\mathbf{p}_1+\mathbf{k}}+\mathrm{i}\delta\,\mathrm{sign}\,\varepsilon_{\mathbf{p}_1+\mathbf{k}})}\,. \tag{19}$$

Consider now the remaining integral over p_1. Characteristic momentum transfer here is of the order of $k_\mathrm{D}\sim p_\mathrm{F}$. We can then estimate all denominators to be $\sim E_\mathrm{F}$, and $\int \mathrm{d}^3p_1\sim N(0)E_\mathrm{F}$. Then, we obtain

$$\Gamma^{(1)}\sim g_0^3N(0)\,\frac{E_\mathrm{F}}{E_\mathrm{F}^2}\sim g_0^3\,\frac{N(0)}{\Omega_0}\,\frac{\Omega_0}{E_\mathrm{F}}\sim g_0\lambda_0\,\frac{\Omega_0}{E_\mathrm{F}}\,. \tag{20}$$

Thus, the relative size of this correction is

$$\frac{\Gamma^{(1)}}{g_0}\sim\lambda_0\,\frac{\Omega_0}{E_\mathrm{F}}\sim\lambda_0\sqrt{\frac{m}{M}}\,, \tag{21}$$

where we have used $\Omega_0/E_\mathrm{F}\sim\omega_\mathrm{D}/E_\mathrm{F}\sim\sqrt{m/M}$, where m is the electron mass, and M is the ion mass. Electrons are much lighter than ions (nuclei), and this correction to the vertex part is negligible. More accurate analysis confirms this conclusion [13, 18], which is the essence of the Migdal theorem.

Migdal's theorem allows us to neglect vertex corrections in calculations related to electron–phonon interaction in

typical metals. The actual small parameter of the perturbation theory is $\lambda_0\Omega_0/E_F \ll 1$, where λ_0 is the dimensionless constant of electron–phonon interaction, Ω_0 is the characteristic phonon frequency, while E_F is the Fermi energy of electrons, which in typical metals is of the order of the conduction band width and determines the maximal energy scale. Notably, this leads to the common belief that vertex corrections in this theory can be neglected, even for $\lambda_0 > 1$, until inequality $\Omega_0/E_F \ll 1$ is valid, which is characteristic of typical metals. In fact, this means that taking into account the diagram in Fig. 1 only is sufficient even in the case of quite strong coupling between electrons and phonons.

Previous analysis implicitly assumed a conduction band of infinite width. In the case of a sufficiently large characteristic frequency of phonons, it may become comparable not only to the Fermi energy but also to the conduction band width. Curiously enough, in the limit of very strong nonadiabaticity, when $\Omega_0 \gg E_F \sim D$ (D is the conduction band half-width), a new small parameter of perturbation theory $\lambda D/\Omega_0 \sim \lambda E_F/\Omega_0$ appears [24, 26]. Naturally, λ in this case should be calculated using Eqn (17).

Consider the case of a conduction band of finite width $2D$ with a constant density of states (two-dimensional case). The Fermi level as above is assumed to be at zero of the energy scale, and we assume the typical case of a half-filled band, so that $E_F = D$. Then, Eqn (10) reduces to

$$\Sigma(\varepsilon) = \int_{-D}^{D} d\varepsilon' \int_0^\infty d\omega\, \alpha^2(\omega)F(\omega)\left(\frac{f(\varepsilon')}{\varepsilon - \varepsilon' + \omega - i\delta} + \frac{1 - f(\varepsilon')}{\varepsilon - \varepsilon' - \omega + i\delta}\right)$$
$$= \int_0^\infty d\omega\, \alpha^2(\omega)F(\omega)\left(\ln\frac{\varepsilon + D + \omega - i\delta}{\varepsilon - D - \omega + i\delta} - \ln\frac{\varepsilon + \omega - i\delta}{\varepsilon - \omega + i\delta}\right). \quad (22)$$

Correspondingly, from Eqn (22) we get

$$-\left.\frac{\partial\Sigma(\varepsilon)}{\partial\varepsilon}\right|_{\varepsilon=0} = 2\int_0^D d\varepsilon' \int_0^\infty d\omega\, \alpha^2(\omega)F(\omega)\,\frac{1}{(\omega + \varepsilon')^2}$$
$$= 2\int_0^\infty d\omega\, \alpha^2(\omega)F(\omega)\,\frac{D}{\omega(\omega + D)}, \quad (23)$$

so that we can define the generalized coupling constant as

$$\tilde{\lambda} = 2\int_0^\infty \frac{d\omega}{\omega}\,\alpha^2(\omega)F(\omega)\,\frac{D}{\omega + D}, \quad (24)$$

which for $D \to \infty$ reduces to the usual Eliashberg–McMillan constant (13), while for $D \to 0$ it gives the 'antiadiabatic' coupling constant:

$$\lambda_D = 2D\int\frac{d\omega}{\omega^2}\,\alpha^2(\omega)F(\omega). \quad (25)$$

Equation (24) describes a smooth crossover between the limits of wide and narrow conduction bands. Mass renormalization, in general, is determined by constant $\tilde{\lambda}$:

$$m^\star = m(1 + \tilde{\lambda}). \quad (26)$$

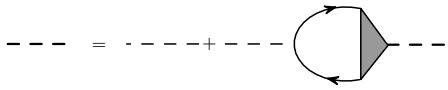

Figure 3. Dyson equation for the full ('dressed') phonon Green's function.

For the model of one Einstein phonon with frequency Ω_0, we have $F(\omega) = \delta(\omega - \Omega_0)$, so that

$$\tilde{\lambda} = \frac{2}{\Omega_0}\,\alpha^2(\Omega_0)\,\frac{D}{\Omega_0 + D} = \lambda\,\frac{D}{\Omega_0 + D} = \lambda_D\,\frac{\Omega_0}{\Omega_0 + D}, \quad (27)$$

where the Eliashberg–McMillan coupling constant

$$\lambda = 2\int_0^\infty \frac{d\omega}{\omega}\,\alpha^2(\omega)F(\omega) = \alpha^2(\Omega_0)\,\frac{2}{\Omega_0}. \quad (28)$$

A comparison with Eqn (16) gives $\alpha^2(\Omega_0) = g_0^2 N(0)$, and λ_D reduces to

$$\lambda_D = 2\alpha^2(\Omega_0)\,\frac{D}{\Omega_0^2} = 2\alpha^2(\Omega_0)\,\frac{1}{\Omega_0}\,\frac{D}{\Omega_0}, \quad (29)$$

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

$$\lambda_D = \lambda\,\frac{D}{\Omega_0} \sim \lambda\,\frac{E_F}{\Omega_0} \ll \lambda, \quad (30)$$

so that for reasonable values of λ (up to the strong coupling region of $\lambda \sim 1$) the 'antiadiabatic' coupling constant remains small. It is obvious that vertex corrections also become small in this limit, as was shown by direct calculations in Ref. [27].

Thus, we came to an unexpected conclusion: in the strong antiadiabatic limit, electron–phonon coupling becomes weak again! In this sense, we can again speak of the validity of the Migdal theorem also in the antiadiabatic limit. The physics here is simple: in the strong nonadiabatic limit, ions move much faster than electrons, so that electrons can not 'adjust' to rapidly changing ion configurations and, in this sense, only weakly react to ion movements.

4. Strong coupling and lattice instability

The general expression for the phonon Green's function, taking into account the interaction with electrons, is given by the Dyson equation shown in Fig. 3. In the analytic form, we have

$$D^{-1}(\mathbf{k}, i\omega_m) = D_0^{-1}(\mathbf{k}, i\omega_m) - |g_\mathbf{k}|^2\Pi(\mathbf{k}, i\omega_m). \quad (31)$$

We then obtain

$$D(\mathbf{k}, i\omega_m) = \frac{2\Omega_{0\mathbf{k}}}{(i\omega_m)^2 - \Omega_{0\mathbf{k}}^2 - 2\Omega_{0\mathbf{k}}|g_\mathbf{k}|^2\Pi(\mathbf{k}, i\omega_m)}. \quad (32)$$

After the usual transition to real frequencies, the phonon spectrum (renormalized by interaction) is determined from the equation

$$\Omega_\mathbf{k}^2 = \Omega_{0\mathbf{k}}^2\left(1 + \frac{2|g_\mathbf{k}|^2}{\Omega_{0\mathbf{k}}}\,\Pi(\mathbf{k}, \Omega_\mathbf{k})\right). \quad (33)$$

In the adiabatic approximation, taking into account the Migdal theorem, the polarization operator here can be taken as a simple loop. In the simplest case of free electrons, we have [20]

$$\Pi(\mathbf{k}, \mathrm{i}\omega_m) = -2N(0)\left(1 + \frac{\mathrm{i}\omega_m}{2v_\mathrm{F}k}\ln\frac{\mathrm{i}\omega_m - v_\mathrm{F}k}{\mathrm{i}\omega_m + v_\mathrm{F}k}\right), \quad (34)$$

or, after $\mathrm{i}\omega_m \to \omega + \mathrm{i}\delta$,

$$\Pi(\mathbf{k}, \omega + \mathrm{i}\delta) = -2N(0)\left(1 + \frac{\omega}{2v_\mathrm{F}k}\ln\frac{\omega - v_\mathrm{F}k + \mathrm{i}\delta}{\omega + v_\mathrm{F}k + \mathrm{i}\delta}\right), \quad (35)$$

where v_F is the electron velocity on the Fermi surface, which greatly exceeds the sound velocity, so that the values of $v_\mathrm{F}k$ are much higher than the frequencies of acoustical phonons, and for typical $k \sim p_\mathrm{F}$, also those of optical phonons. This again demonstrates the importance of the adiabatic approximation in metals. Thus, in calculations of the phonon spectrum using (33), we can, with high accuracy, immediately put $\omega = 0$ in the polarization operator. In this case, the imaginary part of the polarization operator becomes zero, and we simply have $\Pi(0,0) = -2N(0)$. Then, the phonon spectrum, renormalized by interaction with electrons, is determined from

$$\Omega_\mathbf{k}^2 = \Omega_{0\mathbf{k}}^2\left[1 + \frac{2|g_\mathbf{k}|^2}{\Omega_{0\mathbf{k}}}\Pi(0,0)\right] = \Omega_{0\mathbf{k}}^2\left[1 + \frac{\lambda_0^k}{N(0)}\Pi(0,0)\right] \quad (36)$$

and takes the form

$$\Omega_\mathbf{k}^2 = \Omega_{0\mathbf{k}}^2[1 - 2\lambda_0^k], \quad (37)$$

where we have introduced the usual definition of the dimensionless coupling constant of electron–phonon interaction [20]:

$$\lambda_0^k = \frac{2|g_\mathbf{k}|^2 N(0)}{\Omega_{0\mathbf{k}}}. \quad (38)$$

In this (fairly rough) approximation, the relatively small damping of phonons due to electron–phonon interaction just vanishes. It can be obtained with a more accurate treatment of the imaginary part of the polarization operator [20].

The 'bare' Green's function of phonons at real frequencies ($T = 0$)

$$D_0(\mathbf{k}, \omega) = \frac{1}{\omega - \Omega_{0\mathbf{k}} + \mathrm{i}\delta} - \frac{1}{\omega + \Omega_{0\mathbf{k}} - \mathrm{i}\delta} = \frac{2\Omega_{0\mathbf{k}}}{\omega^2 - \Omega_{0\mathbf{k}}^2 + \mathrm{i}\delta} \quad (39)$$

after such 'dressing' by interaction with electrons, transforms into [20]

$$D(\mathbf{k}, \omega) = \frac{2\Omega_{0\mathbf{k}}}{\omega^2 - \Omega_\mathbf{k}^2 + \mathrm{i}\delta}, \quad (40)$$

where the renormalized phonon spectrum is given by (37).

The spectrum given by Eqn (37) signifies the lattice instability for $\lambda_0^k > 1/2$. This instability is often considered to be unphysical, as was noted already in an early paper by Fröhlich [33], where it was obtained for the first time. This point can be explained as follows. Let us rewrite the 'dressed' Green's function (40) identically as

$$D(\mathbf{k}, \omega) = \frac{2\Omega_\mathbf{k}}{\omega^2 - \Omega_\mathbf{k}^2 + \mathrm{i}\delta}\frac{\Omega_{0\mathbf{k}}}{\Omega_\mathbf{k}}. \quad (41)$$

Then, it becomes clear that, during diagram calculations, and Fig. 1 in particular for electron self-energy using from the very beginning this renormalized Green's function of phonons, the physical coupling constant of electron–phonon coupling takes the form (instead of (38))

$$\lambda^k = \frac{2|g_\mathbf{k}|^2 N(0)}{\Omega_\mathbf{k}}\frac{\Omega_{0\mathbf{k}}}{\Omega_\mathbf{k}} = \frac{2|g_\mathbf{k}|^2 N(0)}{\Omega_{0\mathbf{k}}}\frac{\Omega_{0\mathbf{k}}^2}{\Omega_\mathbf{k}^2} = \lambda_0^k\frac{\Omega_{0\mathbf{k}}^2}{\Omega_\mathbf{k}^2}, \quad (42)$$

or, using (37),

$$\lambda^k = \frac{\lambda_0^k}{1 - 2\lambda_0^k}. \quad (43)$$

We see that for $\lambda_0^k \to 1/2$ the *renormalized* coupling constant λ^k monotonously grows and finally diverges. It is this constant that determines the 'true' value of electron–phonon interaction (with 'dressed' phonons), and there are no limitations on its value at all. This physical picture was discussed in detail, e.g., in the famous book [34].

In a model with a single Einstein phonon, which is a reasonable approximation for an optical phonon, we have $\Omega_\mathbf{k} = \Omega_0$ and can forget about the dependence of the coupling constant on the phonon momentum, so that

$$\lambda_0 = \frac{2g_0^2 N(0)}{\Omega_0}, \quad (44)$$

$$\Omega^2 = \Omega_0^2[1 - 2\lambda_0], \quad (45)$$

$$\lambda = \frac{2g_0^2 N(0)}{\Omega_0}\left(\frac{\Omega_0}{\Omega}\right)^2 = \frac{\lambda_0}{1 - 2\lambda_0}. \quad (46)$$

Equation (43) can be reversed, and we can write

$$\lambda_0^k = \frac{\lambda^k}{1 + 2\lambda^k}, \quad (47)$$

expressing the nonphysical 'bare' constant of electron–phonon coupling λ_0^k via the 'true' physical coupling constant λ^k. Using this relation in the equation for the renormalized phonon spectrum (37), we can write it as

$$\Omega_\mathbf{k}^2 = \Omega_{0\mathbf{k}}^2\left(1 - \frac{2\lambda^k}{1 + 2\lambda^k}\right) = \Omega_{0\mathbf{k}}^2\frac{1}{1 + 2\lambda^k}, \quad (48)$$

so that, in this representation, there is no instability of the spectrum (lattice), and the growth of λ^k just leads to continuous 'softening' of the spectrum due to the growth of electron–phonon coupling.

In a model of the Einstein phonon, all relations simplify, and we get

$$\lambda_0 = \frac{\lambda}{1 + 2\lambda}, \quad (49)$$

$$\Omega = \frac{\Omega_0}{\sqrt{1 + 2\lambda}}. \quad (50)$$

In the Eliashberg–McMillan formalism, where we perform averaging over the momenta of electrons on the (arbitrary) Fermi surface, McMillan function $\alpha^2(\omega)F(\omega)$ should naturally be determined by the physical (renormalized) spectrum of phonons:

$$\alpha^2(\omega)F(\omega) = \frac{1}{N(0)}\sum_{\mathbf{pp}'} |g_{\mathbf{pp}'}|^2 \delta(\omega - \Omega_{\mathbf{p}-\mathbf{p}'})\delta(\varepsilon_{\mathbf{p}})\delta(\varepsilon_{\mathbf{p}'})\,. \quad (51)$$

In the particular case of the Einstein phonon, it immediately reduces to (46) and there are no limitations on the value of λ.

In a self-consistent derivation of the Eliashberg equations, we have to use the diagram in Fig. 1, where the phonon Green's function is taken in a 'dressed' form, (40) or (41), and describes the physical (renormalized) phonon spectrum. In this case, we *do not have* to include corrections to this function due to electron–phonon interaction, as they are already taken into account in the phonon spectrum (37).

It should be noted that the value of the critical coupling constant obtained above, at which the Fröhlich instability of the phonon spectrum appears, is obviously directly related to the use of the simplest expression for the polarization operator of the gas of free electrons (34), (35), which was calculated neglecting vertex corrections and self-consistent 'dressing' of electron Green's functions entering the loop. Naturally, even the simplest cases, like the problem with the Einstein spectrum accounting for these higher corrections, as well as the more realistic structure of an electron spectrum in a lattice, can somehow change the value of λ_0, corresponding to instability of the 'bare' phonon spectrum, so that it will differ from 1/2. In this sense, it is better to speak about instability at some 'critical' value $\lambda_0^{\mathrm{c}} \sim 1/2$.

In general, the inverse influence of electrons on phonons can be taken into account by generalizing Eqn (51) in the following way:

$$\begin{aligned}\alpha^2(\omega)F(\omega) &= \frac{1}{N(0)}\sum_{\mathbf{pp}'} |g_{\mathbf{pp}'}|^2 \left(-\frac{1}{\pi}\,\mathrm{Im}\,D(\omega,\mathbf{p}-\mathbf{p}')\right) \\ &\quad\times \delta(\varepsilon_{\mathbf{p}})\delta(\varepsilon_{\mathbf{p}'}) \\ &= \frac{1}{N(0)}\sum_{\mathbf{pp}'} |g_{\mathbf{pp}'}|^2 B(\mathbf{p}-\mathbf{p}',\omega)\delta(\varepsilon_{\mathbf{p}})\delta(\varepsilon_{\mathbf{p}'})\,, \quad (52)\end{aligned}$$

where we have introduced phonon spectral density $B(\mathbf{q},\omega)$, which determines the phonon Green's function (in the Matsubara representation) via the spectral relation

$$D(\mathbf{q},\mathrm{i}\omega_m) = \int_0^\infty B(\mathbf{q},\omega)\,\frac{2\omega}{(\mathrm{i}\omega_m^2) - \omega^2}\,\mathrm{d}\omega\,. \quad (53)$$

In particular, from here we get

$$D(\mathbf{q},0) = -2\int_0^\infty \frac{\mathrm{d}\omega}{\omega}\,B(\mathbf{q},\omega)\,. \quad (54)$$

We can then write the following general relation for Eliashberg–McMillan constant λ:

$$\begin{aligned}\lambda &= 2\int_0^\infty \frac{\mathrm{d}\omega}{\omega}\,\alpha^2(\omega)F(\omega) \\ &= \frac{2}{N(0)}\int_0^\infty \frac{\mathrm{d}\omega}{\omega}\sum_{\mathbf{pp}'} |g_{\mathbf{pp}'}|^2 B(\mathbf{p}-\mathbf{p}',\omega)\delta(\varepsilon_{\mathbf{p}})\delta(\varepsilon_{\mathbf{p}'}) \\ &= -\frac{1}{N(0)}\sum_{\mathbf{pp}'} |g_{\mathbf{pp}'}|^2 D(\mathbf{p}-\mathbf{p}',0)\delta(\varepsilon_{\mathbf{p}})\delta(\varepsilon_{\mathbf{p}'})\,. \quad (55)\end{aligned}$$

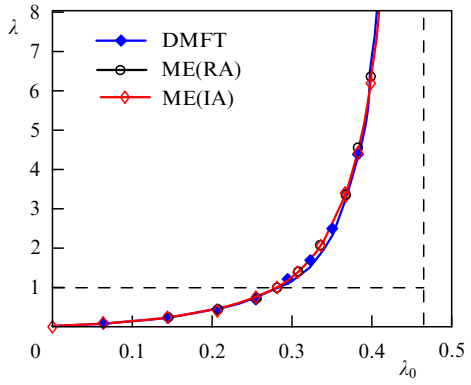

Figure 4. Dependence of renormalized coupling constant λ, calculated from (56), on the 'bare' λ_0, obtained within the self-consistent Eliashberg theory (ME(RA) — real frequency technique, ME(IA) — Matsubara technique) and in the DMFT(QMC) [39]. Vertical dashed line corresponds to $\lambda_0^{\mathrm{c}} \approx 0.464$.

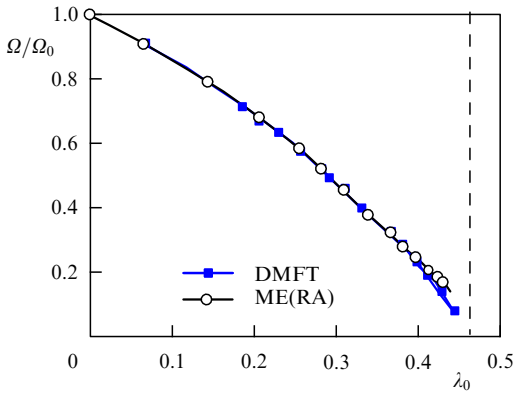

Figure 5. Dependence of renormalized Einstein phonon frequency Ω on 'bare' λ_0, obtained within the self-consistent Eliashberg theory (ME(RA) — real frequency technique) and in the DMFT(QMC) [39]. Vertical dashed line corresponds to $\lambda_0^{\mathrm{c}} \approx 0.464$.

For the model of an optical phonon with frequency Ω_0, this immediately reduces to

$$\lambda = -g_0^2 N(0)\langle D(\mathbf{p}-\mathbf{p}',0)\rangle_{\mathrm{FS}} = -\frac{\lambda_0\Omega_0}{2}\langle D(\mathbf{p}-\mathbf{p}',0)\rangle_{\mathrm{FS}}\,, \quad (56)$$

where we have introduced the usual notation for momentum averaging over the Fermi surface, $\langle\ldots\rangle_{\mathrm{FS}}$.

The previous analysis can be significantly improved within the simplified Holstein model (3), where the local (single site) nature of interaction allows solving it using the dynamical mean-field theory (DMFT) [35–38], which becomes (numerically) exact in the limit of the lattice of infinite dimensions (infinite number of nearest neighbors). Such an analysis was performed, for example, in Ref. [39], using the quantum Monte Carlo (QMC) method as the impurity solver in the DMFT. The main results are shown in Figs 4 and 5.

In particular, in Fig. 4, we show the dependence of renormalized λ on 'bare' λ_0. It can be seen that the usual behavior of the Fröhlich theory is nicely reproduced with slightly changed $\lambda_0^{\mathrm{c}} = 0.464$. Similar behavior is observed for renormalized phonon frequency Ω, as seen in Fig. 5. Rather insignificant deviations from predictions of the Eliashberg

theory are observed only in the immediate vicinity of λ_0^c, especially for $\lambda_0 > 0.4$.

The instability appearing at $\lambda_0 = \lambda_0^c$ in the Holstein model (in the DMFT approximation) with a half-filled bare band was convincingly interpreted in Ref. [40] as a transition into the state of a *bipolaron insulator*. Until this transition, the system remains metallic and is nicely described by the Eliashberg theory (with insignificant numerical corrections).

In a series of papers [21–23], direct calculations by the dynamical quantum Monte Carlo (DQMC) method were performed for a number of characteristics of the Holstein model on a two-dimensional (square) lattice. The results obtained were in some respects similar to the conclusions of Refs [39, 40] — up to the values of the 'bare' constant $\lambda_0 < 0.4$ there is good agreement with predictions of the Eliashberg theory, but, in the interval of λ_0 from 0.4 to 0.5, certain deviations are observed. This interval of λ_0 values, according to the same calculations, corresponds to the interval of renormalized λ from 1.7 to 4.6. For $\lambda_0 \approx 0.5$, the system undergoes a transition into the state of bipolaron insulator with a commensurate charge density wave (CDW).

It is quite clear that the critical value of the electron–phonon coupling constant obtained above, corresponding to Fröhlich instability of the phonon spectrum at $\lambda_0 = 1/2$, was the direct result of our use of the simplest expression for the polarization operator of free electron gas (34), (35), where there was no significant dependence on the wave vector $\mathbf{k}$. Naturally, this dependence is also absent in the DMFT approximation. If we go to some more realistic model of the electron spectrum, like the tight-binding approximation in some definite crystal lattice (not in infinite dimensions!), we can obtain the instability of the phonon spectrum at some finite value of phonon wave vector $\mathbf{k}$ [21–23, 41]. The appearance of such instabilities, as is well known, usually corresponds to the formation in the system of charge density waves [20]. In the case of the 'nesting' properties of a Fermi surface, these instabilities appear (at $T = 0$) even for infinitesimal values of the coupling constant of electron–phonon interaction [20]. After that, the metal acquires the new ground state (of a dielectric nature) so that all theoretical analysis is to be performed in a new way.

In the general case considered here, this instability appears at finite (large enough) values of the 'bare' constant of electron–phonon interaction. Naturally, the usual Eliashberg–McMillan theory 'works' only within the usual metallic phase, which is the main interest as far as the theory of superconductivity is concerned. In this sense, we are in certain disagreement with the terminology in Refs [21–23], where it was claimed that the Eliashberg theory becomes invalid for the values of $\lambda_0 \sim \lambda_0^c$. In reality, in this rather narrow region we are observing corrections due to the closeness of the system to instability — the phase transition into a new ground state (bipolarons, CDW), where fluctuations of the corresponding order parameter become important. The Eliashberg theory, considered a mean-field theory, nicely describes almost all the metallic region, except this 'critical' neighborhood of λ_0^c, including quite large values of *physical* coupling constant λ (which simply diverges at this transition).

It should be stressed here that all the above conclusions regarding the instability of the metallic phase were reached in the framework of purely *model* approaches (Fröhlich and Holstein models) and in terms of 'bare' parameters of these models like λ_0 and Ω_0, which, as was often noted in the literature, are not so well defined physically. This has been known for a long time and was discussed many times. The problem here is that the phonon spectrum in a metal, considered a system of ions and electrons, is usually assumed to be calculated in the adiabatic approximation [42]. This spectrum is relatively weakly renormalized due to nonadiabatic effects, which are small over the small parameter $\sqrt{m/M}$ [42, 43]. In this respect, it is drastically different from the 'bare' spectra of Fröhlich or Holstein models, which, as we have seen above, are significantly renormalized by electron–phonon interaction. The physical meaning of the 'bare' spectrum Ω_0 in these models remains not so clear, in contrast to the phonon spectrum in metals, calculated in the adiabatic approximation. In any case, it can not be determined from any experiments. Similarly, the same can be said about the parameters of electron–phonon interactions.

There were numerous attempts to build a consistent theory of electron–phonon interaction in the background of the physical (adiabatic) phonon spectrum [43], but they were not so successful. A rather detailed discussion of the modern state of this problem can be found in Ref. [44].

In short, a recipe for practical calculations is to identify the renormalized ('dressed') spectrum of phonons Ω in the Fröhlich or Holstein models with a physical (adiabatic) phonon spectrum, which is not to be further renormalized and should be taken from adiabatic calculations or from experiments.[3] Precisely this point of view is usually implicitly accepted in calculations within the Eliashberg–McMillan theory. As long as the system remains in the metallic phase, this point of view remains quite consistent. Then, there are practically no limitations on the value of physical (renormalized) coupling constant λ and the Eliashberg–McMillan theory remains valid even at very large values of λ (limited only by the Migdal theorem).

5. McMillan expression for electron–phonon coupling constant

McMillan derived a simple expression for the dimensionless electron–phonon coupling in the Eliashberg theory [16]. Let us write down Eliashberg–McMillan function (8) using (2) as

$$\begin{aligned}\alpha^2(\omega)F(\omega) &= \frac{1}{N(0)}\sum_{\mathbf{p}}\sum_{\mathbf{p}'}|g_{\mathbf{p}\mathbf{p}'}|^2\delta(\omega-\Omega_{\mathbf{p}-\mathbf{p}'})\delta(\varepsilon_{\mathbf{p}})\delta(\varepsilon_{\mathbf{p}'})\\ &= \frac{1}{N(0)}\sum_{\mathbf{p}}\sum_{\mathbf{p}'}\frac{1}{2M\Omega_{\mathbf{p}-\mathbf{p}'}}\left|I(\mathbf{p}-\mathbf{p}')\right|^2\\ &\times\delta(\omega-\Omega_{\mathbf{p}-\mathbf{p}'})\delta(\varepsilon_{\mathbf{p}})\delta(\varepsilon_{\mathbf{p}'})\,, \end{aligned} \tag{57}$$

where $\Omega_{\mathbf{p}-\mathbf{p}'}$ is assumed to be the physical frequency of phonons. Then, we immediately get

$$\int_0^\infty \mathrm{d}\omega\,\alpha^2(\omega)F(\omega)\omega = \frac{N(0)\langle I^2\rangle}{2M}\,. \tag{58}$$

Now, rewrite (13) as

$$\lambda = 2\int_0^\infty\frac{\mathrm{d}\omega}{\omega}\,\alpha^2(\omega)F(\omega) = \frac{2}{\langle\Omega^2\rangle}\int_0^\infty\mathrm{d}\omega\,\alpha^2(\omega)F(\omega)\omega\,, \tag{59}$$

[3] Ideologically, the situation here is quite analogous to the standard approach in quantum electrodynamics, where the physical charge and mass of an electron are defined by infinite series of the perturbation theory and are taken from the experiment.

where the mean square phonon frequency is defined as

$$\langle\Omega^2\rangle = \frac{\int_0^\infty \mathrm{d}\omega\,\alpha^2(\omega)F(\omega)\omega}{\int_0^\infty (1/\omega)\,\mathrm{d}\omega\,\alpha^2(\omega)F(\omega)} = \frac{2}{\lambda}\int_0^\infty \mathrm{d}\omega\,\alpha^2(\omega)F(\omega)\omega\,. \tag{60}$$

From this expression, we can immediately see that

$$\lambda = \frac{N(0)\langle I^2\rangle}{M\langle\Omega^2\rangle}\,, \tag{61}$$

where we have introduced the matrix element of the gradient of the electron–ion potential averaged over the Fermi surface:

$$\begin{aligned}\langle I^2\rangle &= \frac{1}{[N(0)]^2}\sum_{\mathbf{p}}\sum_{\mathbf{p}'}\left|I(\mathbf{p}-\mathbf{p}')\right|^2\delta(\varepsilon_{\mathbf{p}})\delta(\varepsilon_{\mathbf{p}'})\\ &= \frac{1}{[N(0)]^2}\sum_{\mathbf{p}}\sum_{\mathbf{p}'}\left|\left\langle\mathbf{p}\middle|\nabla V_{\mathrm{ei}}(\mathbf{r})\middle|\mathbf{p}'\right\rangle\right|^2\delta(\varepsilon_{\mathbf{p}})\delta(\varepsilon_{\mathbf{p}'})\\ &= \left\langle\left|\langle\mathbf{p}|\nabla V_{\mathrm{ei}}(\mathbf{r})|\mathbf{p}'\rangle\right|^2\right\rangle_{\mathrm{FS}}.\end{aligned} \tag{62}$$

Equation (61) gives a very useful representation for λ, which is often used in the literature and in practical calculations.

6. Eliashberg equations

The Eliashberg theory is based on a system of equations for normal and anomalous Green's functions of a superconductor [20]. Obviously, the solution of these *integral* equations, taking into account the real spectrum of phonons, represents a rather difficult problem. However, significant progress was achieved, and the theory of traditional superconductors, based on the picture of pairing due to electron–phonon interaction is an example of the very successful application of Green's functions. A very good presentation of methods used and applications of Eliashberg equations can be found in Ref. [16].

Below, we present some simplified derivations of Eliashberg equations, dropping some technical details. In particular, we shall not consider the role of direct Coulomb repulsion of electrons within a Cooper pair, which is accounted for in the complete Eliashberg–McMillan theory [16], limiting ourselves only to electron–phonon interaction. Accounting for Coulomb contributions is not especially difficult [16] and reduces in the end to the introduction of Coulomb pseudopotential $\mu^\star$ [16], which in typical metals is rather small and not so important in the limit of very strong coupling with phonons, which will be our main interest in what follows.[4]

Taking into account the Migdal theorem, in the adiabatic approximation, vertex corrections are irrelevant, so that the Eliashberg equations can be derived by calculating the diagram of Fig. 1, where the electron Green's function in the superconducting state is taken in the Nambu matrix representation [19]. Calculations are similar to the derivation of (10) and can be performed using the Matsubara technique ($T \neq 0$). In the Nambu formalism, the electronic Green's function of a superconductor is written in a standard way as [16]

$$\hat{G}^{-1}(\mathrm{i}\omega_n,\mathbf{p}) = \mathrm{i}\omega_n\hat{1} - \varepsilon_{\mathbf{p}}\hat{\sigma}_z - \hat{\Sigma}(\mathrm{i}\omega_n,\mathbf{p})\,, \tag{63}$$

where $\hat{\sigma}_i$ are Pauli matrices, and the matrix self-energy is represented as[5]

$$\hat{\Sigma}(\mathrm{i}\omega_n,\mathbf{p}) = \big(1 - Z(\mathrm{i}\omega_n)\big)\mathrm{i}\omega_n\hat{1} + Z(\mathrm{i}\omega_n)\Delta(\mathrm{i}\omega_n)\hat{\sigma}_x\,. \tag{64}$$

Here, we are introducing a number of simplifying assumptions like the independence of renormalization factor $Z(\mathrm{i}\omega_n)$ and gap function $\Delta(\mathrm{i}\omega_n)$ from momentum [16]. Then, we have

$$\hat{G}(\mathrm{i}\omega_n,\mathbf{p}) = \frac{Z(\mathrm{i}\omega_n)\mathrm{i}\omega_n\hat{1} + \varepsilon_{\mathbf{p}}\hat{\sigma}_z + Z(\mathrm{i}\omega_n)\Delta(\mathrm{i}\omega_n)\hat{\sigma}_x}{Z^2(\mathrm{i}\omega_n)(\mathrm{i}\omega_n)^2 - Z^2(\mathrm{i}\omega_n)\Delta^2(\mathrm{i}\omega_n) - \varepsilon_{\mathbf{p}}^2}\,. \tag{65}$$

The self-energy part corresponding to a diagram like Fig. 1 with a matrix Green's function of the electron (65) is written as

$$\begin{aligned}\hat{\Sigma}(\omega_n,\mathbf{p}) = -T\sum_m\sum_{\mathbf{p}'}|g_{\mathbf{p}\mathbf{p}'}|^2 D(\mathrm{i}\omega_n - \mathrm{i}\omega_m, \mathbf{p}-\mathbf{p}')\\ \times\,\hat{\sigma}_z\hat{G}(\mathrm{i}\omega_m,\mathbf{p}')\hat{\sigma}_z\,,\end{aligned} \tag{66}$$

where the phonon Green's function $D(\mathrm{i}\omega_n - \mathrm{i}\omega_m, \mathbf{p}-\mathbf{p}')$ can be taken as in Eqn (39), denoting the phonon frequency $\Omega_{\mathbf{p}-\mathbf{p}'}$ as in Eqn (6).

As we know, all physics of conventional superconductivity develops in a layer with a width of the order of $2\Omega_{\mathrm{D}} \ll E_{\mathrm{F}}$ close to the Fermi surface. Thus, we can make here the substitution (8) and obtain from (66) the expression for the self-energy part averaged over momenta on the Fermi surface (similar to (10)). As a result, we obtain the general system of equations for the gap $\Delta(\omega_n)$ and renormalization factor $Z(\omega_n)$ of the following form:

$$\begin{aligned}\Delta(\omega_n)Z(\omega_n) = T\sum_{n'}\int_{-\infty}^{\infty}\mathrm{d}\xi\int_0^\infty \mathrm{d}\omega\,\alpha^2(\omega)F(\omega)\\ \times\,D(\omega_n-\omega_{n'};\omega)\frac{\Delta(\omega_{n'})}{\omega_{n'}^2+\xi^2+\Delta^2(\omega_{n'})}\,,\end{aligned} \tag{67}$$

$$\begin{aligned}1 - Z(\omega_n) = \frac{\pi T}{\omega_n}\sum_{n'}\int_{-\infty}^{\infty}\mathrm{d}\xi\int_0^\infty \mathrm{d}\omega\,\alpha^2(\omega)F(\omega)\\ \times\,D(\omega_n-\omega_{n'};\omega)\frac{\omega_{n'}}{\omega_{n'}^2+\xi^2+\Delta^2(\omega_{n'})}\,,\end{aligned} \tag{68}$$

where we have introduced

$$D(\omega_n-\omega_{n'};\omega) = \frac{2\omega}{(\omega_n-\omega_{n'})^2+\omega^2}\,. \tag{69}$$

The integral over ξ here is easily calculated and gives

$$\begin{aligned}\int_{-\infty}^{\infty}\mathrm{d}\xi\,\frac{1}{\omega_{n'}^2+\xi^2+\Delta^2(\omega_{n'})} &= \frac{\pi}{\sqrt{\omega_{n'}^2+\Delta^2(\omega_{n'})}}\\ &\to \frac{\pi}{|\omega_{n'}|}\quad\text{for}\quad \Delta(\omega_{n'})\to 0\,.\end{aligned} \tag{70}$$

Then, the linearized gap equation (equation for T_{c}) has the form

$$\Delta(\omega_n)Z(\omega_n) = \pi T\sum_{n'}\int_0^\infty \alpha^2(\omega)F(\omega)D(\omega_n-\omega_{n'};\omega)\frac{\Delta(\omega_{n'})}{|\omega_{n'}|}\,, \tag{71}$$

[4] Surely, accounting for $\mu^\star$ is very important for quantitative estimates of the superconducting transition temperature in the weak and intermediate coupling regions.

[5] The possible contribution proportional to $\hat{\sigma}_y$ is removed by the appropriate choice of the phase of the superconducting order parameter, while the term proportional to $\hat{\sigma}_z$ reduces to renormalization of the chemical potential [16].

where

$$1 - Z(\omega_n) = \frac{\pi T}{\omega_n} \sum_{n'} \int_{-\infty}^{\infty} \mathrm{d}\xi \int_0^{\infty} \mathrm{d}\omega\, \alpha^2(\omega) F(\omega) \times D(\omega_n - \omega_{n'}; \omega) \frac{\omega_{n'}}{|\omega_{n'}|} . \quad (72)$$

The general gap equation is

$$\Delta(\omega_n) Z(\omega_n) = \pi T \sum_{n'} \int_0^{\infty} \alpha^2(\omega) F(\omega) \times D(\omega_n - \omega_{n'}; \omega) \frac{\Delta(\omega_{n'})}{\sqrt{\omega_{n'}^2 + \Delta^2(\omega_{n'})}} , \quad (73)$$

where factor $Z(\omega_n)$ is determined from the following equation:

$$1 - Z(\omega_n) = \frac{\pi T}{\omega_n} \sum_{n'} \int_0^{\infty} \mathrm{d}\omega\, \alpha^2(\omega) F(\omega) \times D(\omega_n - \omega_{n'}; \omega) \frac{\omega_{n'}}{\sqrt{\omega_{n'}^2 + \Delta^2(\omega_{n'})}} , \quad (74)$$

to be solved jointly with (73). In a model with an Einstein spectrum of phonons, Eqn (73) reduces to

$$\Delta(\omega_n) Z(\omega_n) = \pi T \lambda \sum_{n'} \frac{\Omega_0^2}{(\omega_n - \omega_{n'})^2 + \Omega_0^2} \times \frac{\Delta(\omega_{n'})}{\sqrt{\omega_{n'}^2 + \Delta^2(\omega_{n'})}} , \quad (75)$$

while Eqn (74) becomes

$$Z(\omega_n) = 1 + \frac{\pi T \lambda}{\omega_n} \sum_{n'} \frac{\Omega_0^2}{(\omega_n - \omega_{n'})^2 + \Omega_0^2} \frac{\omega_{n'}}{\sqrt{\omega_{n'}^2 + \Delta^2(\omega_{n'})}} , \quad (76)$$

where the coupling constant λ, determined by standard expressions (13) or (28), appears explicitly.

To determine T_c (in the limit of $\Delta(\omega_{n'}) \to 0$) in a system with an Einstein spectrum of phonons, we obtain the following system of linear homogeneous Eliashberg equations:

$$\Delta(\omega_n) Z(\omega_n) = \pi T \lambda \sum_{n'} \frac{\Omega_0^2}{(\omega_n - \omega_{n'})^2 + \Omega_0^2} \frac{\Delta(\omega_{n'})}{|\omega_{n'}|} , \quad (77)$$

where

$$Z(\omega_n) = 1 + \frac{\pi T \lambda}{\omega_n} \sum_{n'} \frac{\Omega_0^2}{(\omega_n - \omega_{n'})^2 + \Omega_0^2} \frac{\omega_{n'}}{|\omega_{n'}|} . \quad (78)$$

It is clear that the value of T_c is determined by the zero determinant of this system of equations.

Note that, in general equations (73), (74), the coupling constant λ does not appear explicitly. Usually, this is achieved by reducing these equations to the 'Einstein' form like (75), (76) by introducing the average square of the phonon frequency, defined as

$$\langle \Omega^2 \rangle = \frac{2}{\lambda} \int_0^{\infty} \mathrm{d}\omega\, \alpha^2(\omega) F(\omega) \omega , \quad (79)$$

and the following replacement in (73), (74):

$$\frac{1}{(\omega_n - \omega_{n'})^2 + \omega^2} \to \frac{1}{(\omega_n - \omega_{n'})^2 + \langle \Omega^2 \rangle} , \quad (80)$$

which gives (75), (76) and also the equations for T_c (77), (78) with simple replacement of Ω_0^2 by $\langle \Omega^2 \rangle$. In this sense, the general structure 'Einstein' Eliashberg equations are also conserved for the case of a general phonon spectrum. This approximation with the identification of Ω_0^2 and $\langle \Omega^2 \rangle$ is always assumed in the following.

For the model of a phonon spectrum consisting of a discreet set of Einstein phonons,

$$\alpha^2(\omega) F(\omega) = \sum_i \alpha^2(\Omega_i) \delta(\omega - \Omega_i) = \sum_i \frac{\lambda_i}{2} \Omega_i \delta(\omega - \Omega_i) . \quad (81)$$

In this case, from (79), we simply obtain

$$\langle \Omega^2 \rangle = \frac{1}{\lambda} \sum_i \lambda_i \Omega_i^2 , \quad (82)$$

where $\lambda = \sum_i \lambda_i$.

6.1 Weak and intermediate coupling

There is a vast literature on solving Eliashberg equations in the weak or intermediate coupling region $\lambda < 1$ [13, 14, 16]. Here, we only present qualitative results for T_c, dropping unimportant (for our aims) numerical coefficients ~ 1. In a model with an Einstein spectrum of phonons and Coulomb potential $\mu^\star = 0$, we have [20]

$$T_c \sim \Omega_0 \exp\left(-\frac{1 + \lambda}{\lambda} \right) . \quad (83)$$

This expression is in fact close to the results of an exact numerical analysis performed at the time by McMillan [6] [13, 14, 16].

Similar estimates of T_c can also be obtained in the strong antiadiabatic limit, considering Eliashberg equations for $\lambda < 1$ in the problem with a narrow electron band of half-width $D \sim E_F \ll \Omega_0$ [24–26]. Then, the appropriately generalized Eliashberg equations give for the same model with the Einstein spectrum

$$T_c \sim \frac{D}{1 + D/\Omega_0} \exp\left(-\frac{1 + \tilde{\lambda}}{\lambda} \right) , \quad (84)$$

where the effective constant $\tilde{\lambda}$ was defined above in Eqns (24), (27), and (30).

Equation (84) interpolates between the adiabatic and antiadiabatic limits. For $D \gg \Omega_0$, it gives (83), while for $D \ll \Omega_0$, it reduces to

$$T_c \sim D \exp\left(-\frac{1}{\tilde{\lambda}} \right) , \quad (85)$$

i.e., to a BCS-like expression (weak coupling!), where the pre-exponential factor is determined not by the phonon frequency but by the electron band half-width (Fermi energy), which

[6] Here, we drop some numerical coefficients ~ 1. If we remember a number of (not so well controlled) approximations made during the derivation of the Eliashberg equations, it becomes clear that we are not losing much accuracy here.

now plays the role of cutoff parameter for divergence in the Cooper channel. This fact was first noted by Gor'kov in Refs [29–31].

For a more general model of the phonon spectrum consisting of a discrete set of Einstein phonons (81), these relations are obviously generalized to [25, 26]

$$\lambda = 2\sum_i \frac{\alpha^2(\Omega_i)}{\Omega_i} \equiv \sum_i \lambda_i\,, \tag{86}$$

$$\tilde{\lambda} = 2\sum_i \frac{\alpha^2(\Omega_i)D}{\Omega_i(\Omega_i + D)} = \sum_i \lambda_i \frac{D}{\Omega_i + D} \equiv \sum_i \tilde{\lambda}_i\,, \tag{87}$$

and instead of (84) we have

$$T_c \sim \prod_i \left(\frac{D}{1 + D/\Omega_i}\right)^{\lambda_i/\lambda} \exp\left(-\frac{1+\tilde{\lambda}}{\lambda}\right). \tag{88}$$

In the simplest case of two Einstein phonons with frequencies Ω_1 and Ω_2, this gives

$$T_c \sim \left(\frac{D}{1 + D/\Omega_1}\right)^{\lambda_1/\lambda} \left(\frac{D}{1 + D/\Omega_2}\right)^{\lambda_2/\lambda} \exp\left(-\frac{1+\tilde{\lambda}}{\lambda}\right), \tag{89}$$

where $\tilde{\lambda} = \tilde{\lambda}_1 + \tilde{\lambda}_2$ and $\lambda = \lambda_1 + \lambda_2$. In the case of $\Omega_1 \ll D$ (adiabatic phonon) and $\Omega_2 \gg D$ (antiadiabatic phonon), (89) reduces to

$$T_c \sim (\Omega_1)^{\lambda_1/\lambda} (D)^{\lambda_2/\lambda} \exp\left(-\frac{1+\tilde{\lambda}}{\lambda}\right). \tag{90}$$

Equation (88) is easily rewritten as

$$T_c \sim \langle\Omega_{\ln}\rangle \exp\left(-\frac{1+\tilde{\lambda}}{\lambda}\right), \tag{91}$$

where we have introduced the mean logarithmic frequency $\langle\Omega_{\ln}\rangle$:

$$\ln\langle\Omega_{\ln}\rangle = \ln\prod_i \left(\frac{D}{1 + D/\Omega_i}\right)^{\lambda_i/\lambda} = \sum_i \frac{\lambda_i}{\lambda} \ln\frac{D}{1 + D/\Omega_i}\,. \tag{92}$$

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

$$\ln\langle\Omega_{\ln}\rangle = \frac{2}{\lambda}\int \frac{d\omega}{\omega}\,\alpha^2(\omega)F(\omega)\ln\frac{D}{1 + D/\omega}\,, \tag{93}$$

where λ is given by the usual relation (13).

In general, the pre-exponential factor in the expression for T_c in the Eliashberg theory for weak or intermediate coupling is always given by the mean logarithmic phonon frequency [16], and Eqn (93) gives a generalization of the standard expression for this frequency for an electron band of finite width. From Eqn (93), we can easily obtain the standard expression [16] (see also Section 6.2) for the adiabatic limit, when $D \to \infty$.

6.2 Lower bound for superconducting transition temperature in the limit of very strong coupling

To achieve really high values of T_c, the region of strong and very strong coupling $\lambda > 1$ is of the main interest and will be discussed in the following. The general Eliashberg equations in the Matsubara representation, determining superconducting gap $\Delta(\omega_n)$ at arbitrary temperatures, are given in (73), (74) [13, 14].

Limitations on the value of T_c in the limit of very strong coupling are easily derived analytically. We shall see shortly that the appropriate behavior follows from the estimate of the *lower* bound for T_c [45].

Consider the linearized gap equation (71) determining T_c:

$$\Delta(\omega_n)Z(\omega_n) = \pi T\sum_{n'}\int_0^\infty \alpha^2(\omega)F(\omega)D(\omega_n - \omega_{n'};\omega)\frac{\Delta(\omega_{n'})}{|\omega_{n'}|}\,, \tag{94}$$

where the phonon Green's function is defined in (69). Let us consider the term with $n = 0$. Then, leaving in the sum in Eqn (78) only the contribution from $n' = 0$, we obtain

$$Z(0) = 1 + \lambda\,, \tag{95}$$

which, after substitution into Eqn (94) for $n = 0$, just cancels the similar (corresponding to $n' = 0$) term on the right-hand side of equation [15, 46], so that the equation for $\Delta(0) = \Delta(\pi T)$ takes the form

$$\Delta(0) = \pi T\sum_{n'\neq 0}\int_0^\infty \alpha^2(\omega)F(\omega)\frac{2\omega}{(\pi T - \omega_{n'})^2 + \omega^2}\frac{\Delta(\omega_{n'})}{|\omega_{n'}|}\,. \tag{96}$$

All terms on the right-hand side here are positive. Let us leave only the contribution from $n' = -1$, so that, taking into account $\Delta(-1) = \Delta(-\pi T) = \Delta(\pi T) = \Delta(0)$ and canceling $\Delta(0)$ on the left-hand side and right-hand side, we immediately get the *inequality* [45]

$$1 > \int_0^\infty d\omega\,\frac{2\alpha^2(\omega)F(\omega)\omega}{(2\pi T)^2 + \omega^2}\,. \tag{97}$$

Actually, here, $T = T_c$, and this equation gives the *lower* estimate of T_c. In particular, in the model with the Einstein spectrum of phonons, $F(\omega) = \delta(\omega - \Omega_0)$, and this inequality is immediately rewritten as

$$1 > 2\alpha^2(\Omega_0)\frac{\Omega_0}{(2\pi T)^2 + \Omega_0^2} = \lambda\frac{\Omega_0^2}{(2\pi T)^2 + \Omega_0^2}\,, \tag{98}$$

so that for T_c we get

$$T_c > \frac{1}{2\pi}\sqrt{\lambda - 1}\,\Omega_0\,, \tag{99}$$

which for $\lambda \gg 1$ reduces to

$$T_c > \frac{1}{2\pi}\sqrt{\lambda}\,\Omega_0 \approx 0.16\sqrt{\lambda}\,\Omega_0\,. \tag{100}$$

For a discrete spectrum of phonons (81), inequality (97) reduces to

$$1 > \sum_i \lambda_i \frac{\Omega_i^2}{(2\pi T)^2 + \Omega_i^2}\,, \tag{101}$$

which, in the limit of very strong coupling for $2\pi T \gg \Omega_i$, immediately gives the natural generalization of (100):

$$T_c > \frac{1}{2\pi}\sqrt{\lambda\langle\Omega^2\rangle}\,, \tag{102}$$

where $\lambda = \sum_i \lambda_i$ and $\langle\Omega^2\rangle$ were defined above in Eqn (82).

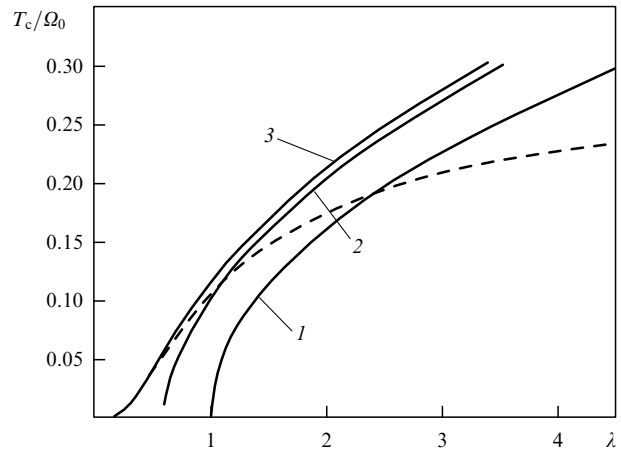

Figure 6. Temperature of superconducting transition in Einstein model of phonon spectrum in units of T_c/Ω_0 as a function of pairing constant λ [45]: *1* — lower bound (99), *2* — solution of the system of two linear equations ($n = 0, \pm 1$), *3* — numerically exact solution of the full system of equations ($n \leqslant 63$) [45]. McMillan expression for T_c [16] is shown by dashed line (for $\mu^\star = 0$).

If we solve the 2×2 system of equations and appropriate quadratic equation for T_c, following from Eqns (77), (78) for $n = 0; \pm 1$, the constant 0.16 in (100) is replaced by 0.18. The solution of the system with $n \leqslant 63$, performed in Ref. [45], leads to the replacement of 0.18 by 0.182, which practically corresponds to the numerically exact solution. It is obvious that even the simplest solution (99) is quite sufficient for qualitative estimates of T_c in the limit of very strong coupling. The general situation is illustrated in Fig. 6, from which it can be seen, in particular, that the asymptotic behavior of T_c for $\lambda \gg 1$ (100) with coefficient 0.18 rather well approximates the values of the critical temperature already starting from the values of $\lambda > 1.5-2.0$ (cf. curve *2* in this figure).

Consider now the very strong coupling case in the strong antiadiabatic limit, though realizing such a coupling in this limit is rather doubtful, as pairing constant λ, defined according to (17), typically rapidly drops with the growth of phonon frequency, as it exceeds the Fermi energy [24, 26].

Consider again an electron band of finite width $2D$ (constant density of states). Then, in the general Eliashberg equations considered above, instead of an integral in infinite limits (70), we have

$$\int_{-D}^{D} \mathrm{d}\xi \, \frac{1}{\omega_{n'}^2 + \xi^2 + \Delta^2(\omega_{n'})} = \frac{2}{\sqrt{\omega_{n'}^2 + \Delta^2(\omega_{n'})}} \arctan \frac{D}{\sqrt{\omega_{n'}^2 + \Delta^2(\omega_{n'})}} \to \frac{2}{|\omega_{n'}|} \arctan \frac{D}{|\omega_{n'}|} \quad \text{for} \quad \Delta(\omega_{n'}) \to 0 \,. \tag{103}$$

Then, the linearized Eliashberg equations take the following general form:

$$\Delta(\omega_n) Z(\omega_n) = T \sum_{n'} \int_0^\infty \mathrm{d}\omega \, \alpha^2(\omega) F(\omega) D(\omega_n - \omega_{n'}; \omega) \times \frac{2\Delta(\omega_{n'})}{|\omega_{n'}|} \arctan \frac{D}{|\omega_{n'}|} \,, \tag{104}$$

where

$$Z(\omega_n) = 1 + \frac{T}{\omega_n} \sum_{n'} \int_0^\infty \mathrm{d}\omega \, \alpha^2(\omega) F(\omega) \times D(\omega_n - \omega_{n'}; \omega) \frac{\omega_{n'}}{|\omega_{n'}|} \arctan \frac{D}{|\omega_{n'}|} \,. \tag{105}$$

We now directly obtain the equation for $\Delta(0)$:

$$\Delta(0) = T \sum_{n' \neq 0} \int_0^\infty \mathrm{d}\omega \, \alpha^2(\omega) F(\omega) \frac{2\omega}{(\pi T - \omega_{n'})^2 + \omega^2} \times \frac{2\Delta(\omega_{n'})}{|\omega_{n'}|} \arctan \frac{D}{|\omega_{n'}|} \,. \tag{106}$$

Again, taking into account only the contribution of $n' = -1$ on the right-hand side, we immediately obtain the inequality

$$1 > \frac{2}{\pi} \int_0^\infty \mathrm{d}\omega \, \alpha^2(\omega) F(\omega) \frac{2\omega}{(2\pi T)^2 + \omega^2} \arctan \frac{D}{\pi T} \,. \tag{107}$$

In the Einstein model of the phonon spectrum, we have $F(\omega) = \delta(\omega - \Omega_0)$, so that Eqn (107) reduces to

$$1 > \frac{2}{\pi} \lambda \arctan \frac{D}{\pi T} \frac{\Omega_0^2}{(2\pi T)^2 + \Omega_0^2} \,. \tag{108}$$

For $D \gg \pi T$, it immediately gives the result of Allen and Dynes:

$$T_c > \frac{1}{2\pi} \sqrt{\lambda - 1} \Omega_0 \to 0.16 \sqrt{\lambda} \Omega_0 \quad \text{for} \quad \lambda \gg 1 \,. \tag{109}$$

For $D \ll \pi T$, Eqn (108) gives

$$T > \frac{1}{2\pi} \sqrt{\lambda^*(T) - 1} \Omega_0 \,, \tag{110}$$

where

$$\lambda^*(T) = \frac{2D}{\pi^2 T} \lambda \,, \tag{111}$$

so that in the strong antiadiabatic limit we have

$$T_c > (2\pi^4)^{-1/3} (\lambda D \Omega_0^2)^{1/3} \approx 0.17 (\lambda D \Omega_0^2)^{1/3} \,. \tag{112}$$

From the obvious condition $\lambda^*(T) > 0$, we get

$$T_c < \frac{2}{\pi^2} \lambda D \approx 0.202 \lambda D \,, \tag{113}$$

which bounds T_c from above.

Thus, we have to satisfy the inequality

$$(2\pi^4)^{-1/3} (\lambda D \Omega_0^2)^{1/3} < T_c < \frac{2}{\pi^2} \lambda D \,, \tag{114}$$

which reduces to the condition

$$\Omega_0 < \frac{4}{\pi} \lambda D \approx 1.27 \lambda D \quad \text{or} \quad \frac{D}{\Omega_0} > \frac{0.78}{\lambda} \,, \tag{115}$$

so that for self-consistency of our analysis we have to satisfy the condition

$$\lambda \gg \frac{\Omega_0}{D} \gg 1 \,, \tag{116}$$

where the last equality corresponds to the limit of strong antiadiabaticity. Correspondingly, all the previous estimates

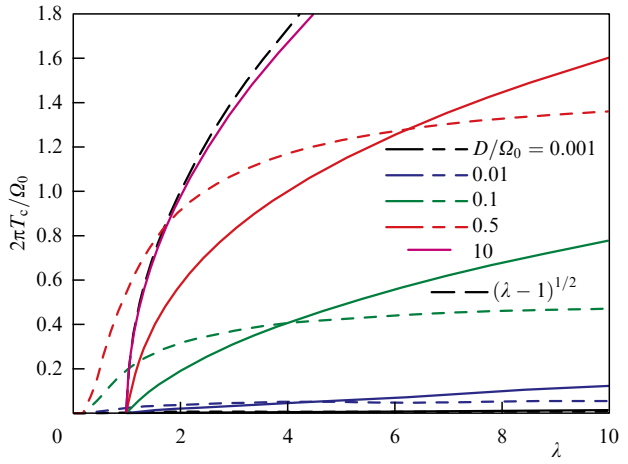

Figure 7. (Color online.) Temperature of superconducting transition (lower bound) in the Einstein model of the phonon spectrum in units of $2\pi T_c/\Omega_0$ as a function of pairing constant λ for different values of inverse adiabaticity parameter D/Ω_0. Dashed lines show appropriate dependences for $2\pi T_c/\Omega_0$ in the regions of weak and intermediate coupling (84). Black dashed line — Allen–Dynes estimate (99), valid in the adiabatic limit [45].

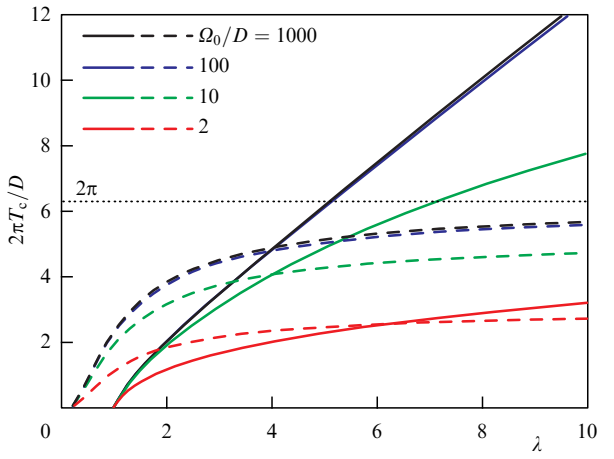

Figure 8. (Color online.) Temperature of superconducting transition (lower bound) in the Einstein model of the phonon spectrum in units of $2\pi T_c/D$ as a function of pairing constant λ for different values of adiabaticity parameter Ω_0/D. Dashed lines show appropriate dependences for $2\pi T_c/D$ in the weak and intermediate coupling regions (84).

become invalid for $\lambda \sim 1$ and can describe only the limit of very strong coupling.

In Figs 7 and 8, we show the results of numerical calculations of T_c boundaries, following from the solution of (108), as compared to the values of T_c in the region of weak and intermediate coupling (84), for different values of adiabaticity parameter Ω_0/D. It is clear that, in the vicinity of crossing dashed and continuous lines in the graphs shown in Figs 7 and 8, we actually have a smooth crossover from T_c behavior in the region of weak and intermediate coupling to its asymptotic behavior in the very strong coupling region of $\lambda \gg 1$. From Fig. 8, it is seen that the boundary (113) is practically reached in the region of large values of λ and Ω_0/D. From these figures, we can also see that a simple rise in phonon frequency and a transition to the antiadiabatic limit do not lead, in general, to an increase in T_c, as opposed to the adiabatic case.

7. Maximal temperature of superconducting transition?

The problem of the maximal possible temperature of superconducting transition arose immediately after the creation of the BCS theory. It was studied in numerous papers with sometimes contradictory results. Among these papers was the notorious one by Cohen and Anderson [47], where rather elegant arguments were given, seemingly quite convincing, that the characteristic scale of T_c values due to the electron–phonon mechanism, or any other similar mechanism, based on the exchange of Bose-like excitations in metals can be of the order of about 10–30 K only. This paper was immediately seriously criticized in Refs [34, 48], with the conclusion that, in reality, there are no such limitations. Even more, the analysis performed in these papers has shown that Ref. [47] is just erroneous.

However, the point of view expressed in the Cohen–Anderson paper became popular in the physics community (Anderson himself till the end of his life adhered to the view expressed in Ref. [47]), so that, at the time of the discovery of high-temperature superconductivity in cuprates (1986–1987), it was almost totally believed that the 'usual' electron–phonon mechanism does not allow values of T_c higher than 30–40 K. Because of this, after the discovery of superconductivity in cuprates, the 'great race' was on for new theoretical models and mechanisms of superconductivity, which may explain the high values of T_c. The problems of superconductivity in cuprates are outside the scope of this work. Most probably, in cuprates, some kind of nonphonon pairing mechanism really dominates (due to antiferromagnetic fluctuations). But the most important result of the discovery of record values of T_c in hydrides under high pressures, in our opinion, is the final (and experimental!) rebuttal of the point of view expressed in Ref. [47].

Thus, the problem of the maximal value of T_c, which may be achieved due to the electron–phonon mechanism of Cooper pairing, is as important as ever. Below, we try to discuss this problem once again within the standard approach based on Eliashberg equations as the most successful theory describing superconductivity in a system of electrons and phonons in metals.

There is a vast amount of literature on numerically solving the Eliashberg equations for different temperatures and different models of the phonon spectrum [14, 16]. A number of analytic expressions for T_c have been proposed by various authors to approximate the results of numerical computations. As an example, we quote here the popular interpolation formula for T_c due to Allen and Dynes [14], which is appropriate for a rather wide interval of values of the dimensionless coupling constant of electron–phonon interaction λ, including the strong coupling region of $\lambda > 1$:

$$T_c = \frac{f_1 f_2}{1.20} \langle \Omega_{\ln} \rangle \exp\left[-\frac{1.04(1+\lambda)}{\lambda - \mu^*(1+0.62\lambda)} \right], \qquad (117)$$

where

$$f_1 = \left[1 + \left(\frac{\lambda}{\Lambda_1} \right)^{3/2} \right]^{1/3}, \quad f_2 = 1 + \frac{\left[\langle \Omega^2 \rangle^{1/2} / \langle \Omega_{\ln} \rangle - 1 \right] \lambda^2}{\lambda^2 + \Lambda_2^2},$$

$$\Lambda_1 = 2.46(1 + 3.8\mu^*), \quad \Lambda_2 = 1.82(1 + 6.3\mu^*) \frac{\langle \Omega^2 \rangle^{1/2}}{\langle \Omega_{\ln} \rangle}. \qquad (118)$$

Here, $\langle\Omega_{\ln}\rangle$ is the mean logarithmic frequency of phonons,

$$\ln\langle\Omega_{\ln}\rangle = \frac{2}{\lambda}\int_0^\infty \frac{\mathrm{d}\omega}{\omega}\,\alpha^2(\omega)F(\omega)\,\ln\omega = \frac{\int_0^\infty (1/\omega)\,\mathrm{d}\omega\,\ln\omega\,\alpha^2(\omega)F(\omega)}{\int_0^\infty (1/\omega)\,\mathrm{d}\omega\,\alpha^2(\omega)F(\omega)}\,, \tag{119}$$

$\langle\Omega^2\rangle$ is the average (over the phonon spectrum) square of the frequency, defined in Eqn (79):

$$\langle\Omega^2\rangle = \frac{2}{\lambda}\int_0^\infty \mathrm{d}\omega\,\alpha^2(\omega)F(\omega)\omega = \frac{\int_0^\infty \mathrm{d}\omega\,\omega\alpha^2(\omega)F(\omega)}{\int_0^\infty (1/\omega)\,\mathrm{d}\omega\,\alpha^2(\omega)F(\omega)}\,. \tag{120}$$

The Coulomb pseudopotential $\mu^\star$ determines repulsion between electrons within a Cooper pair. According to most calculations [14, 16], its values are small and belong to the interval 0.1–0.15.

In the limit of very strong coupling $\lambda > 10$, this gives the expression for T_c, which was, in fact, obtained above from simple inequality (99):

$$T_c \approx 0.18\sqrt{\lambda\langle\Omega^2\rangle}\,. \tag{121}$$

It may seem now that limitations on the values of T_c are simply absent, so that in the limit of very strong coupling very high T_c can be obtained from the electron–phonon mechanism. The only more or less obvious limit is related to the limits of the adiabatic approximation, which is usually considered to be the cornerstone of the Eliashberg theory. However, we have seen above that similar results can also be obtained in the strong antiadiabatic limit (cf. estimates for T_c given in Eqns (112), (113)).

In the model with the Einstein spectrum of phonons, we simply have $\langle\Omega_{\ln}\rangle = \langle\Omega^2\rangle^{1/2} = \Omega$, where Ω is assumed to be the renormalized phonon frequency. Then, (121) reduces to

$$T_c = 0.18\sqrt{\lambda}\Omega\,, \tag{122}$$

so that seemingly for $\lambda \gg 1$ we can, in principle, obtain even $T_c > \Omega$. However, if we remember the renormalization of the phonon spectrum and take into account Eqn (50), we immediately obtain from Eqn (122)

$$T_c = 0.18\sqrt{\lambda}\Omega = 0.18\Omega_0\sqrt{\frac{\lambda}{1+2\lambda}}, \tag{123}$$

which, in the limit of $\lambda \gg 1$, tends to the value $T_c^{\max} \approx 0.13\Omega_0$ because of significant softening of the phonon spectrum. At the same time, as noted above, the physical meaning of 'bare' frequency Ω_0 in a metal is poorly defined, and in particular it can not be determined from experiments. Correspondingly, the estimate of Eqn (123) is somehow up in the air.

However, this analysis is valid only under the condition of a rigid fixation of all relations between 'bare' and 'dressed' phonon spectra. If we 'forget' about the 'bare' spectrum of phonons and consider parameters Ω and λ to be *independent*, we can obtain from Eqn (122) very high values of T_c. A certain, though rather artificial, model leading precisely to this kind of behavior was recently introduced in Ref. [49]. It considers the interaction of N-component electrons with an $N \times N$-component system of Einstein phonons in the limit of $N \to \infty$. It was shown that in this model the renormalization of a phonon spectrum due to interaction with conduction electrons is suppressed, so that in the limit of very strong coupling with $1 \ll \lambda \ll N$ we always have the Allen–Dynes estimate (122) with $\Omega = \Omega_0$.

However, the problem here is that in a real situation we can never consider Ω and λ to be independent parameters simply because of the general relations (13) and (79), which express λ and $\langle\Omega^2\rangle$ via integrals of Eliashberg–McMillan function $\alpha^2(\omega)F(\omega)$. In fact, we may rewrite the expression for T_c in the region of very strong coupling as

$$T_c = 0.18\sqrt{\lambda\langle\Omega^2\rangle} = 0.25\left(\int_0^\infty \mathrm{d}\omega\,\alpha^2(\omega)F(\omega)\omega\right)^{1/2} \tag{124}$$

in the adiabatic case and, correspondingly,

$$T_c = (2\pi^4)^{-1/3}\left(\lambda D\langle\Omega^2\rangle\right)^{1/3} = (2\pi)^{-1/3}\left(2D\int_0^\infty \mathrm{d}\omega\,\alpha^2(\omega)F(\omega)\omega\right)^{1/3} \tag{125}$$

in the antiadiabatic limit. We see that these expressions for T_c are completely determined by integrals of $\alpha^2(\omega)F(\omega)$.

In the famous Ref. [50], a simple inequality for T_c was proposed, limiting its value by the square A under $\alpha^2(\omega)F(\omega)$:

$$T_c \leqslant 0.2309\int_0^\infty \mathrm{d}\omega\,\alpha^2(\omega)F(\omega) \equiv 0.2309A\,. \tag{126}$$

For the case of an Einstein spectrum of phonons, taking into account Eqn (28), this inequality can be rewritten as

$$T_c \leqslant 0.115\lambda\Omega_0\,. \tag{127}$$

This inequality is relatively often used in calculations.

The limitation given by Eqn (113) obtained above in the antiadiabatic limit is essentially quite similar to Eqn (127), with the replacement $\Omega_0 \to 2D$, which is quite natural in the antiadiabatic limit.

The connection between λ and $\langle\Omega^2\rangle$ is markedly expressed in McMillan formula (61) for λ. If we use this expression in (121), we immediately obtain

$$T_c = 0.18\sqrt{\frac{N(0)\langle I^2\rangle}{M}}, \tag{128}$$

where

$$\langle I^2\rangle = \frac{1}{\left[N(0)\right]^2}\sum_{\mathbf{p}}\sum_{\mathbf{p}'}\left|I(\mathbf{p}-\mathbf{p}')\right|^2\delta(\varepsilon_{\mathbf{p}})\delta(\varepsilon_{\mathbf{p}'}) = \frac{1}{\left[N(0)\right]^2}\sum_{\mathbf{p}}\sum_{\mathbf{p}'}\left|\langle\mathbf{p}|\nabla V_{\mathrm{ei}}(\mathbf{r})|\mathbf{p}'\rangle\right|^2\delta(\varepsilon_{\mathbf{p}})\delta(\varepsilon_{\mathbf{p}'}) = \left\langle\left|\langle\mathbf{p}|\nabla V_{\mathrm{ei}}(\mathbf{r})|\mathbf{p}'\rangle\right|^2\right\rangle_{\mathrm{FS}}\,, \tag{129}$$

so that both λ and $\langle\Omega^2\rangle$ just drop out of the expression for T_c, which is now expressed simply via the Fermi surface matrix element of the gradient of the electron–ion potential, ion mass, and electron density of states averaged over at the Fermi level. Expression (128) is convenient for 'first principle' calculations, where it is often used, but it does not contain illustrative physical parameters in terms of which we usually treat T_c.

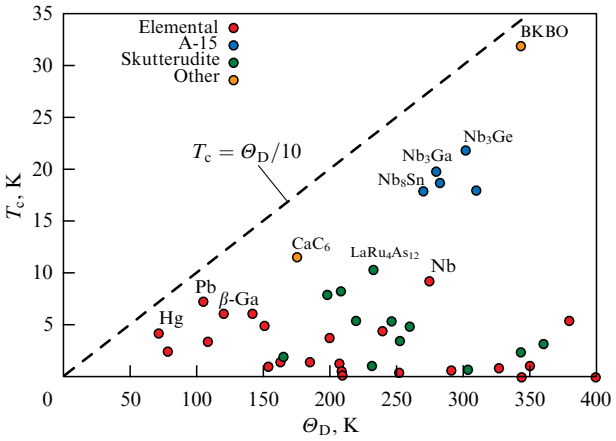

Figure 9. (Color online.) Experimental values of the temperature of the superconducting transition for conventional superconductors depending on their Debye temperature Θ_D [51].

In Ref. [51], a new semiempirical limit for T_c was proposed for conventional (electron–phonon) semiconductors, which is written in a very simple form:

$$k_B T_c \leqslant A_{\max}\Theta_D = A_{\max}\hbar\Omega_D\,, \tag{130}$$

where $A_{\max} \approx 0.10$, and $\Theta_D = \hbar\Omega_D$ is the Debye temperature, which may be determined, for example, from standard measurements of specific heat. This inequality correlates fairly well with $T_c^{\max}$, obtained above in the limit of $\lambda \to \infty$ in Eqn (123), if we identify Ω_0 with Ω_D. It is seen from Fig. 9 that this limitation is satisfied for most conventional superconductors [51]. Below, we shall see that this is probably not so in superhydrides.

8. Superhydrides and Eliashberg theory

In this section, we shall briefly discuss some results of the application of the Eliashberg theory to T_c calculations in hydrides under high pressures. Our presentation here will be very short; much more detail may be found, for example, in reviews [4–6] and in original papers, some of which will be quoted below.

Eliashberg equations were widely used for calculations of T_c in hydrides. Actually, both the crystal structure of H_3S under high pressures and high values of $T_c \sim 200$ K were *predicted* in Ref. [52]. For the structure $Im-3m$ under a pressure of 200 GPa, they obtained the value of the pairing constant $\lambda \approx 2.2$ and mean logarithmic frequency of phonons $\Omega_{\ln} \approx 1335$ K, so that, for T_c calculated from Allen–Dynes expression (117) with Coulomb pseudopotential values $\mu^\star = 0.1-0.13$, values of $T_c = 191-204$ K were obtained. These results were found to be in quite satisfactory agreement with experiment [1].

The achievement of room temperature values of T_c in C–S–H system [12] was reasonably explained in recent paper [53], where it was shown that hole doping of the $Im-3m$ structure of H_3S by introducing carbon shifts the Fermi level to a maximum of Van Hove singularity in the density of states and a certain softening of the phonon spectrum. Combined, all these lead to the growth of λ up to the value of 2.4, which is sufficient, in principle, to explain the values of $T_c \approx 288$ K.

In the Table, we show the calculated parameters of several hydrides of rare-earth elements from Ref. [6], for which record values of T_c were predicted. In the last two columns of the Table, we give the boundaries for T_c, calculated from inequality (99) and from the asymptotic expression of Allen and Dynes (122), under the simplest assumption of $\langle\Omega_{\ln}\rangle = \langle\Omega^2\rangle^{1/2} = \Omega$. We can see that these values are close enough to those obtained from more detailed calculations of Ref. [6] and determine, in fact, the lower and upper bounds for T_c. This clearly shows that systems with the highest achieved values of T_c are practically already in the very strong coupling region of the Eliashberg theory.

In recent paper [54], extensive calculations of T_c were performed for practically all possible binary compounds of hydrogen with other elements of the periodic system for values of the external pressure of 100, 200, and 300 GPa (for which stable crystal structures were also determined). As many as 36 new systems were discovered for which T_c may exceed 100 K, and in 18 cases T_c exceeded 200 K. In particular, for the NaH_6 system, values of $T_c = 248-279$ K were obtained, and for CaH_6, $T_c = 216-253$ K, already for pressures of 100 GPa. The results of this paper clearly show that the highest possible values of T_c are achieved in the region of very strong coupling, up to values of $\lambda = 5.81$ in NaH_6 (under 100 GPa).

Summarizing, we may say that the record values of T_c in superhydrides are achieved for typical values of $\lambda = 2-3.5$ (or even more) and for characteristic phonon frequencies from 1000 to 2000 K. We must also note that the upper bound expressed by Eqn (130) has already been significantly surpassed in some of the known superhydrides.

9. Conclusions

We consciously presented all the problems related to the derivation and use of Eliashberg equations on a fairly elementary level, trying to stress all approximations and simplifications.

The Eliashberg theory remains the main theory which completely explains the values of the critical temperature in superconductors with the electron–phonon mechanism of pairing. This theory is also applicable in the region of strong electron–phonon coupling, limited only by the applicability of the adiabatic approximation based on the Migdal theorem, which is valid in the vast majority of metals, including the

Table. Calculated values of T_c for La–H and Y–H compounds obtained from a numerical solution of Eliashberg equations [6] compared with their boundary values.

Compound	Pressure, GPa	λ	$\Omega_{\ln}$, K	T_c ($\mu^\star = 0.1$), K	T_c ($\mu^\star = 0.13$), K	$\frac{1}{2\pi}\sqrt{\lambda-1}\Omega$	$0.18\sqrt{\lambda}\Omega$
LaH_{10}	210	3.41	848	286	274	209	282
LaH_{10}	250	2.29	1253	274	257	226	341
LaH_{10}	300	1.78	1488	254	241	209	357
YH_{10}	250	2.58	1282	326	305	256	370
YH_{10}	300	2.06	1511	308	286	247	390

new superhydrides with record values of T_c. The values of (renormalized, physical) pairing coupling constant λ can surely exceed unity until the system possesses a metallic ground state. This is not so in the vicinity of a phase transition to a new ground state like a charge density wave or Bose-condensate of bipolarons.

Furthermore, the Eliashberg theory is also qualitatively applicable in the strong antiadiabatic limit. Simple interpolation expressions for T_c can be constructed, connecting adiabatic and antiadiabatic regions. The strong antiadiabatic limit may be of importance in quite exotic systems with very narrow electronic bands and/or anomalously small values of Fermi energy (like monolayers of FeSe, $SrTiO_3$, and, probably, some hydrides).

Unfortunately, this theory does not produce a simple expression for maximal values of T_c in terms of experimentally measurable (or calculated) parameters like characteristic (average) values of phonon frequencies and the pairing coupling constant. Formally, such a limit is generally absent if we consider these parameters independent. However, if we take into account their interdependence, the maximal values of T_c are in fact determined by some 'game' of atomic constants. However, all new data on superhydrides strongly indicate that all these systems are very close to the strong coupling region of the Eliashberg theory, which means that maximal values of T_c for 'usual' metals have already been reached. True, we can still hold out hope for metallic hydrogen [55].

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