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CONDENSED MATTER

Upper Limit for the Superconducting Transition Temperature in Eliashberg–McMillan Theory

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We present simple qualitative estimates for the maximal superconducting transition temperature, which may be achieved due to electron–phonon coupling in Eliashberg–McMillan theory. It is shown that in the limit of very strong coupling the upper limit for transition temperature is determined in fact by a combination of atomic constants and density of conduction electrons.

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Experimental discovery of high-temperature superconductivity in hydrides under high (megabar) pressures [1, 2] stimulated the search for the ways to achieve superconductivity at room temperature [3]. At the moment the common view [4, 5] is that the high-temperature superconductivity in hydrides can be described in the framework of the standard Eliashberg–McMillan theory [6–8]. Within this theory many attempts were undertaken to estimate the maximal achievable superconducting transition temperature and the discussion of some of these attempts can be found in the reviews [4, 5, 9]. In the recent paper [10] a new upper limit for T_c was proposed, expressed as some combination of fundamental constants. Below we shall show that with minor modifications such T_c limit follows directly from Eliashberg–McMillan theory.

Traditionally, after the appearance of BCS theory, in most papers devoted to possible ways of increasing T_c, discussion develops in terms of dimensionless constant of electron–phonon coupling λ and characteristic (average) frequency $\langle\Omega\rangle$ of phonons, responsible for Cooper pairing. In their fundamental paper [11] Allen and Dynes obtained in the limit of very strong coupling $\lambda > 10$ the following expression for T_c:[1]

$$T_c = 0.18\sqrt{\lambda\langle\Omega^2\rangle}. \tag{1}$$

Then it seems that limitations for the value of T_c are just absent, so that quite high values of T_c can be obtained with electron–phonon pairing mechanism. In reality the situation is more complicated. Actually parameters λ and $\langle\Omega^2\rangle$ in Eliashberg–McMillan theory are not independent, which is well known for quite a time [4, 5, 9, 12].

The relation of λ and $\langle\Omega^2\rangle$ is clearly expressed by McMillan's formula for λ, first derived in [8]:

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

where M is an ion mass, $N(0)$ is electronic density of states at the Fermi level and we introduced the matrix element of the gradient of electron–ion potential, averaged over the Fermi surface:

$$\langle I^2\rangle = \frac{1}{[N(0)]^2}\sum_{\mathbf{p}}\sum_{\mathbf{p}'}\left|\langle\mathbf{p}|\nabla V_{ei}(\mathbf{r})|\mathbf{p}'\rangle\right|^2\delta(\varepsilon_{\mathbf{p}})\delta(\varepsilon_{\mathbf{p}'}) = \left\langle\left|\langle\mathbf{p}|\nabla V_{ei}(\mathbf{r})|p'\rangle\right|^2\right\rangle_{FS}. \tag{3}$$

Here, $\varepsilon_{\mathbf{p}}$ is the spectrum of free electrons, with energy zero chosen at the Fermi surface. Equation (2) gives very useful representation for the coupling constant λ, which is routinely used in the literature and in practical (ab initio) calculations [5].

Using Eq. (2) in Eq. (1) we immediately obtain:

$$T_c^{\star} = 0.18\sqrt{\frac{N(0)\langle I^2\rangle}{M}} \tag{4}$$

so that both λ and $\langle\Omega^2\rangle$ just drop out from the expression for $T_c^{\star}$, which is now expressed via Fermi surface averaged matrix element of electron–ion potential, ion mass and electron density of states at the Fermi level. The only deficiency of this expression is the loss of intuitive understanding due to the absence of parameters in terms of which T_c is usually treated.

[1] In fact this asymptotic behavior works rather satisfactorily already for $\lambda > 2$.

As was already noted, all parameters entering this expression can be rather simply obtained during the ab initio calculations of T_c for specific materials (compounds) [5]. Let us also stress that the value of $T_c^\star$ defined in Eq. (4), calculated for any specific material does not have any direct relation to real value of T_c, but just defines precisely the upper limit of T_c, which "would be achieved" in the limit of strong enough electron–phonon coupling. Below we shall present some elementary qualitative estimates of its value.

In the following we shall assume to be dealing with three-dimensional metal with cubic symmetry with an elementary cell with lattice constant a and just one conduction electron per atom. Then we have:

$$N(0) = \frac{mp_F}{2\pi^2\hbar^3}a^3, \tag{5}$$

where $p_F \sim \hbar/a$ is the Fermi momentum, m is the mass of free (band) electron. Electron–ion potential (single-charged ion, e is electron charge) can be estimated as:

$$V_{ei} \sim \frac{e^2}{a} \sim e^2 p_F/\hbar \tag{6}$$

so that its gradient is:

$$\nabla V_{ei} \sim \frac{e^2}{a^2} \sim e^2 p_F^2/\hbar^2. \tag{7}$$

Then we easily obtain the estimate of (3):

$$I^2 \sim \left(\frac{e^2}{a^2}\right)^2 \sim (e^2 p_F^2/\hbar^2)^2. \tag{8}$$

Here, we have dropped different numerical factors of the order of unity. Collecting them back in the model of free electrons we get an estimate for $T_c^\star$ from Eq. (4) as:

$$T_c^\star \sim 0.2\sqrt{\frac{m}{M}}\frac{e^2}{\hbar v_F}E_F, \tag{9}$$

where $E_F = p_F^2/2m$ is the Fermi energy, $v_F = p_F/m$ is the electron velocity at the Fermi surface. The value of $\frac{e^2}{\hbar v_F}$, as is well known, represents the dimensionless coupling for Couloumb interaction and for typical metals it is of the order of or greater than unity. The factor of $\sqrt{\frac{m}{M}}$ determines isotopic effect.

Let us measure length in units of the Bohr radius a_B introducing the standard dimensionless parameter r_s by relation $a^3 = \frac{4\pi}{3}(r_s a_B)^3$. Then we have:

$$a \sim r_s a_B = r_s\frac{\hbar^2}{me^2} = r_s\frac{\hbar}{mc\alpha}, \tag{10}$$

where we have introduced the fine structure constant $\alpha = \frac{e^2}{\hbar c}$. Correspondingly the Fermi momentum is given by:

$$p_F \sim \frac{\hbar}{r_s a_B} = \frac{me^2}{\hbar r_s} = \frac{mc}{\hbar r_s}\alpha. \tag{11}$$

Then $T_c^\star$ (4) can be rewritten as:

$$\begin{aligned} T_c^\star &\sim \frac{0.2}{r_s}\sqrt{\frac{m}{M}}\alpha^2 mc^2 = \frac{0.2}{r_s}\sqrt{\frac{m}{M}}\frac{me^4}{\hbar^2} \\ &= \frac{0.2}{r_s}\sqrt{\frac{m}{M}}\,\mathrm{Ry}, \end{aligned} \tag{12}$$

where $\mathrm{Ry} = me^4/\hbar^2 \approx 13.6$ eV is the Rydberg constant. Here we have obtained the same combination of fundamental (atomic) constants, which was suggested in [10], by some quite different reasoning, as determining the upper limit of superconducting critical temperature. However, our expression contains an extra factor of r_s^{-1}, which necessarily reflects the specifics of a material under consideration (density of conduction electrons), so that the value of $T_c^\star$ is in no sense universal.

As was already noted above the value of $T_c^\star$ strictly speaking has no relation at all to the real superconducting transition temperature T_c. However, expressions (9) and (12) may be useful to estimate "potential perspectives" of some material in the sense of achieving high values of transition temperatures under the conditions of strong electron–phonon coupling. For example in metallic hydrogen M is equal to proton mass and we have $\sqrt{\frac{m}{m_p}} \sim 0.02$, so that for $r_s = 1$ we get an estimate of $T_c^\star \sim 650$ K. This is in nice agreement with the result of $T_c = 600$ K, obtained in [12] solving Eliashberg equations for FCC lattice of metallic hydrogen with $r_s = 1$, taking into account the calculated softening of the phonon spectrum, leading to realizations of very strong coupling ($\lambda = 6.1$). At the same time in the recent paper [13] an elegant numerical study of superconductivity of metallic hydrogen within jellium model has shown, that the maximal value of T_c can be achieved at $r_s \sim 3$, not exceeding 30 K. This is obviously related to the fact that in the "jellium" model the weak coupling is realized and there is no softening of the phonon spectrum. Finally we hope that Eqs. (9) and (12) can be relevant for preliminary estimates of T_c in some of the metallic hydrides, which are currently under intensive study in the search for room-temperature superconductivity.

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CONFLICT OF INTEREST

The author of this work declares that he has no conflicts of interest.

REFERENCES

1. A. P. Drozdov, M. I. Eremets, I. A. Troyan, V. Ksenofontov, and S. I. Shylin, Nature (London, U. K.) **525**, 73 (2015).
2. J. A. Flores-Livas, L. Boeri, A. Sanna, G. Pinofeta, R. Arita, and M. Eremets, Phys. Rep. **856**, 1 (2020).
3. I. A. Troyan, D. V. Semenok, A. V. Sadakov, I. S. Lyubutin, and V. M. Pudalov, J. Exp. Theor. Phys. **139**, (2024, in press); arXiv: 2406.11344.
4. L. P. Gor'kov and V. Z. Kresin, Rev. Mod. Phys. **90**, 01001 (2018).
5. W. E. Pickett, Rev. Mod. Phys. **95**, 021001 (2023).
6. G. M. Eliashberg, Sov. Phys. JETP **11**, 696 (1960).
7. G. M. Eliashberg, Sov. Phys. JETP **12**, 1000 (1961).
8. W. L. McMillan, Phys. Rev. **167**, 331 (1968).
9. M. V. Sadovskii, Phys. Usp. **65**, 724 (2022).
10. K. Trachenko, D. Montserrat, M. Hutcheon, and C. J. Pickard, arXiv: 2406.08129.
11. P. B. Allen and R. C. Dynes, Phys. Rev. **12**, 905 (1975).
12. E. G. Maksimov, Phys. Usp. **51**, 567 (2008).
13. D. van der Marel and C. Berthod, arXiv: 2404.05554.

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