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Simplified function for predicting superconducting critical temperature

Pakin TASEE[1,*], Nattawut NATKUNLAPHAT[1], and Udomsilp PINSOOK[1]

[1] *Department of Physics, Faculty of Science, Chulalongkorn University, Bangkok, 10330, Thailand*

***Corresponding author e-mail**: pakin613@hotmail.com

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Abstract

Currently, there is intense competition to develop models that can accurately estimate the critical temperature across a wide range of superconductors, while striving for straightforward derivations and comprehensive predictions. In this work, we present an approach to determining the critical temperature based on the linearized Eliashberg gap equations employing the bandwidth model. To verify the accuracy of our model, we collect Eliashberg spectral functions from various independent studies, compute the necessary parameters, and solve the Eliashberg gap equations numerically to obtain the exact solutions, along with utilizing the modified Allen-Dynes equation. The findings suggest that both models are in good agreement and exhibit a strong correlation with the exact solutions, although minor deviations are observed. The present study may provide a more effective approach to predicting the critical temperature of superconductors, particularly for materials exhibiting elevated transition temperatures, in future investigations.

1. Introduction

Superconductors are a special class of materials that exhibit superconducting properties—zero electrical resistance and the expulsion of external magnetic fields—at temperatures below a specific value, known as the critical temperature (T_c). One of the fundamental mechanisms underlying the superconducting phenomenon is the electron–phonon (e–ph) interaction, which leads to the formation of Cooper pairs through phonon exchange. This interaction forms the basis of the Bardeen-Cooper-Schrieffer (BCS) theory [1] and, by extension, the Eliashberg theory. The Eliashberg theory generalizes the BCS theory by incorporating strong-coupling effects and providing a more detailed treatment of the e–ph interaction. At its core, the framework relies on the frequency-dependent spectral function $\alpha^2F(\omega)$, which governs various physical properties. Superconducting materials of this type are commonly referred to as conventional superconductors. According to the BCS formalism, the analytic form of T_c is given by

$$T_c^{BCS} \approx 1.13\omega_D \exp\left\{-\frac{1}{N(\varepsilon_F)V_{eff}}\right\} \qquad (1)$$

Where ω_D is the Debye frequency and the exponential term involves the electronic density of state at the Fermi level, $N(\varepsilon_F)$, and the effective pairing potential, V_{eff}. However, several conventional superconductors deviate from the BCS prediction. Consequently, the Eliashberg formalism is required. In theory, T_c can be determined by solving the linearized Eliashberg gap equations (LEGE) [3]. Following the notations introduced in [4], the LEGE are expressed as follows:

$$\left.\begin{aligned} \Delta_n Z_n &= \pi T_c \sum_{m=-m_c}^{m_c} [\lambda_{mn} - \mu^*] \frac{\Delta_m}{|\Omega_m|}, \\ Z_n &= 1 + \frac{\pi T_c}{\Omega_n} \sum_{m=-m_c}^{m_c} \lambda_{mn}\, sgn(\Omega_m) \end{aligned}\right\} \qquad (2)$$

Equation (2) is a coupled equation involving the Matsubara gap function, Δ_n, and the renormalization function, Z_n. The index m is an integer corresponding to the Matsubara frequencies, $\Omega_m = \pi T_c(2m - 1)$, where $m \in \{-m_c,\ldots,0,\ldots,m_c\}$, with m_c being the cutoff value. The information about T_c of a given system is contained in the e–ph interaction kernel:

$$\lambda_{mn} \equiv \int_{\omega_{min}}^{\omega_{max}} \frac{2\omega\, \alpha^2F(\omega)d\omega}{\omega^2 + (\Omega_m - \Omega_n)^2} \qquad (3)$$

The central quantity is the (isotropic) Eliashberg spectral function, $\alpha^2F(\omega)$, which is defined on the phonon frequency domain $\omega_{min} \le \omega \le \omega_{max}$. Typically, $\alpha^2F(\omega)$ is a material-dependent quantity with a complex structure. Before proceeding further, let us highlight two essential limits of λ_{mn}, namely,

$$\lambda \equiv \lambda_{m=n} \equiv \int_{\omega_{min}}^{\omega_{max}} \frac{2\,\alpha^2F(\omega)}{\omega}\, d\omega \qquad (4)$$

$$\lim_{\Omega_{mn} \gg \omega_{max}} \lambda_{mn} = \int_{\omega_{min}}^{\omega_{max}} \frac{2\omega\,\alpha^2F(\omega)}{\Omega_{mn}^2}\, d\omega = \frac{\lambda\omega_2^2}{\Omega_{mn}^2} \qquad (5)$$

The parameters λ is the average e–ph coupling constant and ω_2 is the root mean square phonon frequency defined as:

$$\omega_2 \equiv \sqrt{\int_{\omega_{\min}}^{\omega_{\max}} g(\omega)\, \omega^2\, d\omega} \tag{6}$$

where $g(\omega) \equiv 2\alpha^2F(\omega)/(\lambda\omega)$ denotes the normalized distribution function.

In principle, the exact value of T_c can be determined by numerically solving Equation (2), given a specific form of $\alpha^2F(\omega)$. However, in practice, it is widely accepted to estimate T_c using four key parameters: λ, $\omega_{\ln}$, ω_2, and μ^*. For this reason, several mathematical formulas for estimating T_c have been proposed. One of the well-known formulas is the Allen-Dynes semi-empirical Equation [5], which is a modification of the result earlier proposed by McMillan [6]. It takes the form:

$$T_c^{\mathrm{AD}} = f_1 f_2 T_c^{\mathrm{weak}} \tag{7}$$

where

$$T_c^{\mathrm{weak}} = \frac{\omega_{\ln}}{1.2} \exp\left\{-\frac{1.04(1+\lambda)}{\lambda-\mu^*(1+0.62\lambda)}\right\} \tag{8}$$

The two correct factors are respectively given by:

$$f_1 = \left[1 + \left(\frac{\lambda}{2.46(1+3.8\mu^*)}\right)^{3/2}\right]^{1/3} \tag{9}$$

$$f_2 = 1 + \frac{\left(\frac{\omega_2}{\omega_{\ln}} - 1\right)\lambda^2}{\lambda^2 + \left[1.82(1+6.3\mu^*)\left(\frac{\omega_2}{\omega_{\ln}}\right)\right]^2} \tag{10}$$

It is worth noting that T_c^{weak} resembles the McMillan formula, except that the prefactor $\omega_{\ln}/1.2$ is replaced by $\omega_D/1.45$. The factor f_1 is inserted due to underestimation of T_c^{weak} in the strong coupling regime ($\lambda \geq 1.5$), whereas the factor f_2 reflects the dependency of the shape of $\alpha^2F(\omega)$ through the ratio $\omega_2/\omega_{\ln}$. In the limit of $\lambda \to \infty$ (extreme case), or approximately $\lambda \geq 10$,

$$T_c^{\mathrm{AD}} \longrightarrow F(\mu^*)\sqrt{\lambda}\omega_2 \tag{11}$$

where $F(\mu^*)$ is a function of the Coulomb pseudopotential, μ^*, due to the screened Coulomb interactions between electrons. The value of μ^* typically ranges from 0 to approximately 0.2. Therefore, it is a small parameter, but it still contributes to the reduction of T_c. The expression in Equation (11) is regarded as the asymptotic behavior of T_c. Nevertheless, it is more rigorous to derive Equation (11) under the condition $\omega_{\max}/2\pi T_c >> 1$, rather than relying solely on the parameter λ [7].

Recently, Pinsook *et al.* [4] proposed an analytic approach for evaluating T_c based on the Equation (12).

$$L(T_c; m_c) \equiv \sum_{m=-m_c}^{m_c} \frac{\lambda_{m1}}{|2m-1|} = 1 + \lambda + \sum_{m=-m_c}^{m_c} \frac{\mu^*}{|2m-1|} \tag{12}$$

In their analysis, two simple models of $\alpha^2F(\omega)$, namely the Einstein and Debye models, are employed. The Einstein model [5,8] is an idealized representation that assumes all optical phonons share the same frequency, termed the Einstein frequency (ω_E). As a result, its spectral function is given by

$$\alpha^2F(\omega) = \frac{\lambda\omega_E}{2}\delta(\omega - \omega_E) \tag{13}$$

Obviously, this model specifies

$$\lambda = \lambda \text{ and } \omega_{\ln} = \omega_2 = \omega_E \tag{14}$$

Next, the Debye model is often adopted as a generic model to examine systems mediated by acoustic phonons [8]. The spectral function takes the form

$$\alpha^2F(\omega) = \frac{\lambda}{\omega_D^2}\omega^2 \tag{15}$$

defined on the frequency domain $0 \leq \omega \leq \omega_D$. The corresponding parameters can be calculated as

$$\lambda = \lambda,\ \omega_{\ln} = \omega_D/\sqrt{e}, \text{ and } \omega_2 = \omega_D/\sqrt{2} \tag{16}$$

In contrast to the Einstein model, Equation (16) gives the $\omega_2/\omega_{\ln} = \sqrt{e/2} > 1$. The significant finding of [4] is the logarithmic behavior of the predictive function L, which results in a simple T_c formula:

$$T_c = \frac{2e^{\gamma-1}}{\pi}\omega_{\ln}\exp\left\{-\frac{1+\mu^*\ln(4e^{\gamma}m_c)}{\lambda}\right\} \tag{17}$$

The expression is suitable for the range $a^2 > 0.5$, where the dimensionless parameter is defined as $a = \omega_{\ln}/2\pi T_c$. For $a^2 < 0.5$, the predictive function L behaves as a rational function of polynomials. Unfortunately, the analytic form of T_c has not yet been attained in this regime. Furthermore, our recent rigorous derivation of Equation (17) for a general $\alpha^2F(\omega)$ is presented in reference [9]. One of the limitations of the Einstein and Debye models is that both consist of only two independent parameters. To extend this, the bandwidth (constant) model, defined by

$$\alpha^2F(\omega) = C \tag{18}$$

for $\omega_a < \omega < \omega_b$, has been suggested to provide insight into studies of T_c [10,11]. Additionally, the simple models mentioned herein are also applicable to other areas of research, such as the universal resistivity in the metallic phase of certain superconductors described by the Einstein model [12], and simplified approaches for examining electron self-energy [13]. In this paper, we aim to extend the result of Pinsook *et al.* to investigate T_c in the regime of relatively high T_c, i.e., $a^2 < 1$, using the bandwidth model. To supplement the analysis, we extract $\alpha^2F(\omega)$ from several superconducting materials and perform numerical calculations to find the exact values of T_c in accordance with Equation (12). Subsequently, we compute T_c directly using the modified Allen-Dynes formula. Finally, we compare the obtained calculated T_c with the exact values of T_c derived from the predictive function L.

2. Computational methods

This section elaborates on the theoretical procedures for computing the critical temperature by means of: (1) the exact solution to Equation

(12) (T_c^{Exact}), (2) the bandwidth model (T_c^{BW}), and (3) the modified Allen-Dynes model ($T_c^{\mathrm{AD(mod)}}$).

2.1 Exact solution

To numerically solve Equation (12) for (T_c^{Exact}), we need to consider λ_{m1}, which takes the form in Equation (3) with the index $n = 1$. Hence, the predictive function $L(T_c; m_c)$ is explicitly written as:

$$L(T_c; m_c) = \sum_{m=-m_c}^{m_c} \int_{\omega_{\min}}^{\omega_{\max}} \frac{2\omega\alpha^2F(\omega)}{|2m-1|(\omega^2+4\pi^2T_c^2(m-1)^2)} d\omega \quad (19)$$

In the following step, we focus on the summation accompanied by μ^*on right-hand side in Equation (12). As demonstrated by [4,9], under the condition $m_c >> 1$, one obtains

$$\sum_{m=-m_c}^{m_c} \frac{1}{|2m-1|} \approx \ln(4e^{\gamma}m_c) \quad (20)$$

Where γ is Euler-Mascheroni constant ($\gamma \approx 0.57721566$). Consequently, T_c^{Exact} is the solution to the Equation

$$L(T_c; m_c) = 1 + \lambda + \mu^* \ln(4e^{\gamma}m_c) \quad (21)$$

Our analysis indicates that the optimal cutoff value is $m_c = 95$. This value provides the best agreement between the T_c values computed from Equation (19) and Equation (21) and those obtained from experiments and DFT methods. This observation is also consistent with the findings reported by [4].

In this section, several forms of $\alpha^2F(\omega)$ are extracted from published graphs in recent studies by manually digitizing data points. These digitized points are then used to reconstruct the spectral function, which is subsequently interpolated for the calculation of essential parameters. For example, $\alpha^2F(\omega)$ of HC_8 [17] and PbH_8 [19] are shown in Figure 1. The extracted $\alpha^2F(\omega)$ will be used to calculate the predictive function L, and ultimately, T_c^{Exact}. A similar procedure is applied to 12 different superconducting compounds [14–23].

2.2 Critical temperature from the bandwidth model

From a broader perspective, the Einstein model can be viewed as a limiting case of the bandwidth model [11], where the bandwidth approaches zero ($\omega_b - \omega_a \rightarrow 0^+$), leading to all phonons sharing the same frequency —namely, an idealization rarely observed in real materials. Due to the limitations of this model [24], we utilize the bandwidth model, which offers a more realistic approximation. First, we can compute the essential parameters [10,11]:

$$\lambda = 2C\ln\left(\frac{\omega_b}{\omega_a}\right) \quad (22)$$

$$\omega_2 = \sqrt{\left(\frac{\omega_b^2 - \omega_a^2}{2\ln\left(\frac{\omega_b}{\omega_a}\right)}\right)} \quad (23)$$

$$\omega_{\ln} = \sqrt{\omega_a\omega_b} \quad (24)$$

For convenience, we define a frequency parameter as

$$\Delta = \ln\left(\frac{\omega_b}{\omega_a}\right) \quad (25)$$

$$\frac{\omega_2}{\omega_{\ln}} = \sqrt{\frac{\sin\mathrm{h}\,\Delta}{\Delta}} > 1 \quad (26)$$

Accordingly, the ratio can be obtained. It should be noted that, in the limit $\Delta \rightarrow 0^+$, the ratio $\omega_2/\omega_{\ln} \rightarrow 1^+$, which is consistent with the Einstein model.

At this point, let us briefly derive the explicit form of the predictive function based on the current model within a certain limit. As discussed in [4], in the limit $a \rightarrow 0^+$ of the Einstein model, the m_c– independent expression is given by

$$\frac{L(a)}{\lambda} \approx 1 + 1.545a^2 - \frac{\tau_0 a^4}{1+a^2} \quad (27)$$

Where $a = \omega_E/2\pi T_c$. The fitting parameter τ_0 is found to be optimal at the value $\tau_0 \approx 1.390$. Notably, Equation (27) remains approximately valid within the range $a^2 \lesssim 0.5$. To generalize this, we rewrite the predive function as:

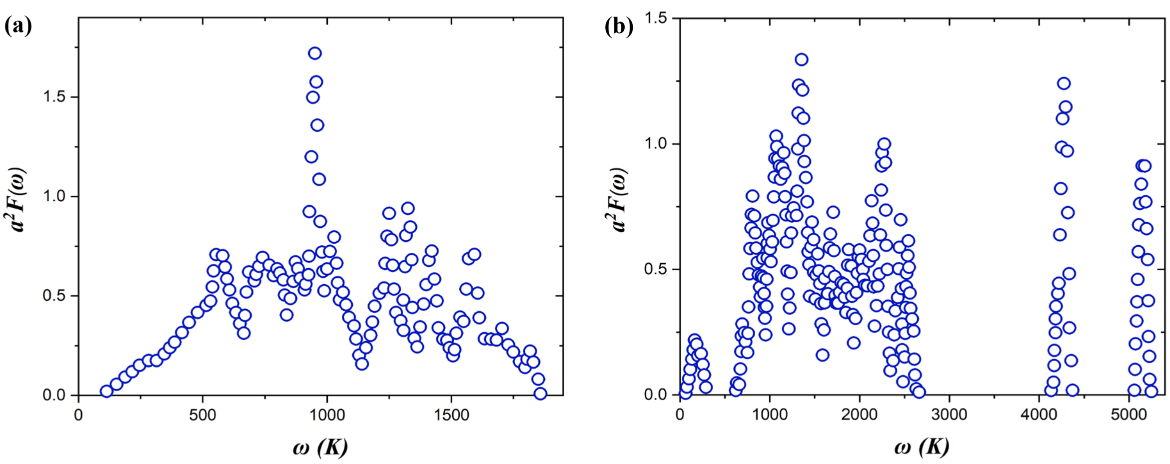

Figure 1. The Eliashberg spectral functions of HC_8 [17] (a), and PbH_8 [19] (b).

$$\frac{L(T_c;m_c)}{\lambda} = 1 + \frac{2}{\lambda}\int_{\rho_{\min}}^{\rho_{\max}} d\rho\, \frac{\alpha^2F(\omega)}{\rho}\left(\sum_{m=1}^{m_c} \frac{4m}{4m^2-1}\frac{\rho^2}{m^2+\rho^2}\right) \tag{28}$$

Where $\rho \equiv \omega/2\pi T_c$ [4,9]. By imposing the rigorous condition $\rho_{\max} = \omega_{\max}/2\pi T_c < 1$ [9], Equation (28) reduces to the following form:

$$\frac{L(T_c)}{\lambda} \approx 1 + \frac{2}{\lambda}\int_{\rho_{\min}}^{1} d\rho\, \alpha^2F(\omega)\left(1.545\rho - \frac{\tau_0\rho^3}{1+\rho^2}\right) \tag{29}$$

By substituting the definition of the bandwidth model, Equation (18), into Equation (29), we obtain the Equation:

$$\frac{L(a,\Delta)}{\lambda} \equiv \frac{L(T_c)}{\lambda} \approx 1 + (1.545 - \tau_0)\left(\frac{\sin h\,\Delta}{\Delta}\right)a^2 + \frac{\tau_0}{\Delta}\ln\left(\frac{a^2e^{\Delta}+1}{a^2e^{-\Delta}+1}\right) \tag{30}$$

Here, $a = \omega_{\ln}/2\pi T_c$, and Δ is defined in Equation (25). Note that Equation (30) provides an accurate description only within the range $a^2 \lesssim 0.5$. To extend its applicability to the range $a^2 \lesssim 1$, a slight modification is required: specifically, the coefficient 1.545 is replaced with 0.847. These coefficients arise from a Taylor expansion. In addition, the fitting parameter is adjusted to $\tau_0 = 0.764$. Eventually, to evaluate T_c within the model, we rely on the same extracted data as described in subsection 2.1. This can be achieved in a similar manner by numerically solving Equation (21) with the aid of Equation (30) and applying the adjusted parameters.

2.3 Critical temperature from the Allen-Dynes Model

In this part, we introduce a slight modification of the Allen-Dynes formula by adjusting the correction factor f_2 as follows:

$$f_2 \longrightarrow f_2^{\text{Mod}} \equiv 1 + \frac{\left(\frac{\omega_2}{\omega_{\ln}} - 1\right)\lambda^2}{\lambda^2 + [1.82(1+6.3\mu^*)]^2} \tag{31}$$

Due to the exclusion of the ratio $\omega_2/\omega_{\ln}$ in the denominator of f_2, we can immediately deduce that $f_2^{\text{Mod}} \geq f_2$ and $T_c^{\text{AD(Mod)}} \geq T_c^{\text{AD}}$ (with equality in the Einstein model) [9]. Again, we calculate $T_c^{\text{AD(Mod)}}$ based on the essential parameters extracted from the same set of data used in subsection 2.1.

3. Results and discussion

In this section, we discuss the results of the critical temperature calculations. The exact critical temperature (T_c^{Exact}) is compared with the critical temperatures obtained from the bandwidth model (T_c^{BW}) and the modified Allen-Dynes formula ($T_c^{\text{AD(Mod)}}$). First, the values of the necessary parameters deduced from the extracted $a^2F(\omega)$ [14–23] are shown in Table 1.

Once these parameters are obtained, we calculate the critical temperature from three different methods. The comparison of these critical temperatures is presented in Figure 2.

As illustrated in Figure 2, the exact critical temperatures are compared with those obtained from the bandwidth model and the modified Allen-Dynes formula, represented by green triangles and red circles, respectively. The black line denotes the unity line. We calculate the mean relative error based on the percentage deviations of the critical temperatures obtained from the bandwidth and the Allen-Dynes models relative to the exact critical temperature. The results show that the mean relative errors for the bandwidth and Allen-Dynes models are 6.89% and 5.92%, respectively, indicating good agreement with the exact values. Although the results from both models exhibit slight deviations from the unity line, they show a strong correlation with the exact critical temperatures. This suggests that, while the models are effective, further refinement or the development of more advanced models may be necessary to achieve higher predictive power.

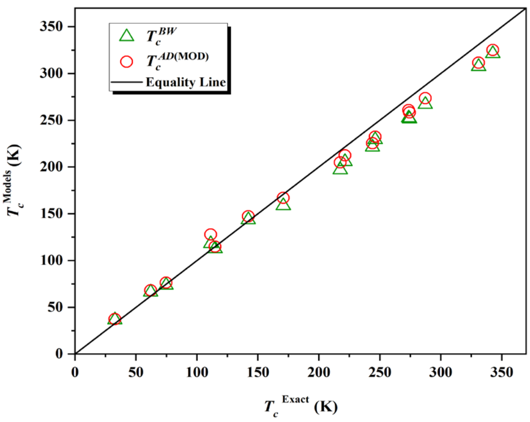

Figure 2. The exact critical temperature compared with the critical temperatures from the bandwidth and the modified Allen-Dynes models [14–23].

Table 1. The necessary parameters calculated from the Eliashberg spectral functions.

Material	λ	$\omega_{\ln}$	ω_2	Δ	μ^*	Ref.
Y_3EuH_{24} (200GPa)	2.29	1138.95	1521.10	1.97	0.10	[14]
					0.13	
Y_3EuH_{24} (250GPa)	2.04	1212.33	1672.36	2.09	0.10	[14]
					0.13	
HPC_3	1.72	421.87	648.61	2.46	0.10	[15]
LuH_{12} (400GPa,Pm3)	2.81	875.54	1618.57	3.03	0.10	[16]
HC_8	1.85	696.30	903.24	1.86	0.10	[17]
SBH_7 (90GPa)	1.80	883.72	1293.50	2.30	0.10	[18]
PbH_8 (200GPa)	1.98	921.50	1684.67	3.00	0.13	[19]
CuN (0GPa)	3.26	114.98	198.64	2.83	0.10	[20]
$Ti_2B_2H_4$	1.67	467.32	812.48	2.85	0.10	[21]
YSc_2H_{24} (300GPa)	3.47	1036.09	1568.64	2.41	0.10	[22]
					0.16	
YSc_2H_{24} (350GPa)	2.90	1175.95	1729.56	2.31	0.10	[22]

4. Conclusions

In this work, we collect the Eliashberg spectral functions of various superconducting compounds and calculate the necessary parameters: λ, $\omega_{\ln}$, ω_2, and Δ. These parameters are then applied to the relevant equations to compute the exact critical temperature, as well as those obtained from the bandwidth model and from the modified Allen-Dynes formula. The results show that the critical temperatures predicted by the bandwidth model and modified Allen-Dynes formula are in close agreement. However, both results slightly deviate from the exact critical temperature. Therefore, further investigation is required to develop a model that yields a critical temperature closer to the exact value.

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