

## The ratio $2\Delta_0/k_B T_c$ within Eliashberg theory

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We have calculated the ratio of the energy gap  $\Delta_0$  to the critical temperature  $T_c$  for a large number of known electron-phonon spectral densities with the use of the imaginary-axis formulation of Eliashberg theory with an analytic-continuation technique to the real axis. Agreement with experiment is within a few percent. It is found that the general trend obtained for  $2\Delta_0/k_B T_c$  against  $T_c/\omega_{\text{in}}$ , where  $\omega_{\text{in}}$  is the popular Allen-Dynes expression for the average phonon energy, can be reproduced by a two-parameter functional form of the general type first given by Geilikman and Kresin. The details, however, can only be understood with complete calculations.

### I. INTRODUCTION

To interpret carefully experimental data on the thermodynamics of superconductors it is necessary to consider and to account, in detail, for strong-coupling effects. These effects lead to modifications of BCS laws<sup>1-3</sup> and have their origin in the retardation of the electron-phonon interaction. In order to treat retardation it is necessary to introduce the Eliashberg gap equations<sup>4</sup> which need to be solved numerically because of their complexity. The imaginary-frequency-axis formulation<sup>4-6</sup> of these equations, which deals with discrete sums over Matsubara frequencies, is well suited for thermodynamic calculations.<sup>6,7</sup> Good agreement<sup>7</sup> with experiment can be obtained using the microscopic parameters derived from tunneling spectroscopy, namely the electron-phonon spectral density  $\alpha^2(\Omega)F(\Omega)$ , as a function of phonon energy  $\Omega$ , and the Coulomb pseudopotential  $\mu^*$ .

An index of strong-coupling effects is the deviation from the BCS value of 3.53 for the ratio  $2\Delta_0/k_B T_c$ , where  $\Delta_0$  is the zero-temperature gap edge and  $T_c$  is the critical temperature. To obtain  $\Delta_0$  it is necessary to make an analytic continuation of the imaginary-axis solutions of the Eliashberg equations at zero temperature to the real frequency axis.<sup>8</sup> This can be done by the method of Padé approximants. In Sec. II of this paper we present such calculations of  $\Delta_0$  for many superconductors for which  $\alpha^2(\Omega)F(\Omega)$  is known and compare the ratio  $2\Delta_0/k_B T_c$  with experimental results. We find agreement with experiment to within a few percent.

There exist in the literature several approximate analytic formulas, accurate at the 10% level, which relate the size of the critical temperature to the microscopic parameters  $\alpha^2(\Omega)F(\Omega)$  and  $\mu^*$ . The first such formula to be derived, and by far the most extensively used so far, is due

to McMillan<sup>9</sup> and its extension by Allen and Dynes.<sup>10</sup> An equally accurate but rarely used formula is that due to Leavens and Carbotte<sup>11,12</sup> who also consider, in the same approximation scheme, the gap edge  $\Delta_0$ , and find a ratio  $2\Delta_0/k_B T_c$  unchanged from the BCS value 3.53.

Using rather sweeping approximations as compared to those used in the previously mentioned works, Geilikman and Kresin<sup>13</sup> have derived an expression for  $2\Delta_0/k_B T_c$  of the form

$$\frac{2\Delta_0}{k_B T_c} = 3.53 \left[ 1 + 5.3 \left[ \frac{T_c}{\tilde{\omega}} \right]^2 \ln \left[ \frac{\tilde{\omega}}{T_c} \right] \right],$$

in which  $\tilde{\omega}$  is some phonon energy which is not sharply specified in the theory and remains uncertain.

In Sec. III we present a new derivation for  $2\Delta_0/k_B T_c$  which is tailored to yield a formula, of the same general form as found by Geilikman and Kresin,<sup>13</sup> but which makes clear the approximations that are introduced along the way. We note that in our work the underlying formula for  $T_c$  is that of Leavens and Carbotte which is accurate at the 10% level without introducing any fitting parameters. It is in the derivation of  $\Delta_0$  that the somewhat uncertain frequency  $\tilde{\omega}$  is introduced together with two constants. Once the definition of  $\tilde{\omega}$  is specified, the two constants can be determined by a fit to the exact results obtained in Sec. II. This is done in Sec. IV where we present a final formula for  $2\Delta_0/k_B T_c$  which is phenomenological in nature. While it cannot reproduce in detail the values of  $2\Delta_0/k_B T_c$  obtained from the full numerical solutions of the Eliashberg equations, it does give the general overall trend found over the entire set of systems considered.

## II. SOLUTION OF THE IMAGINARY-AXIS ELIASHBERG EQUATIONS

The Eliashberg equations, at temperature  $T$ , written on the imaginary frequency axis are<sup>4,6,7</sup>

$$\Delta(i\omega_n)Z_S(i\omega_n) = \pi k_B T \sum_{m=-\infty}^{+\infty} [\lambda(n-m) - \mu^*(\omega_c)\Theta(\omega_c - |\omega_m|)] \frac{\Delta(i\omega_m)}{[\omega_m^2 + \Delta^2(i\omega_m)]^{1/2}} \quad (1)$$

and

$$\omega_n Z_S(i\omega_n) = \omega_n + \pi k_B T \sum_{m=-\infty}^{+\infty} \lambda(n-m) \frac{\omega_m}{[\omega_m^2 + \Delta^2(i\omega_m)]^{1/2}}, \quad (2)$$

where  $\Delta$  is the gap and  $Z_S$  the renormalization factor at the  $n$ th Matsubara frequency:

$$i\omega_n = i\pi k_B T(2n-1), \quad n=0, \pm 1, \pm 2, \dots$$

with  $k_B$  the Boltzmann constant. In Eqs. (1) and (2)  $\omega_c$  is the cutoff frequency,  $\mu^*(\omega_c)$  is the Coulomb pseudopotential corresponding to the phonon cutoff  $\omega_c$ , and  $\lambda(n-m)$  is related to the electron-phonon spectral density  $\alpha^2(\Omega)F(\Omega)$  by

$$\lambda(n-m) = 2 \int_0^\infty \frac{\Omega \alpha^2(\Omega) F(\Omega)}{\Omega^2 + (\omega_n - \omega_m)^2} d\Omega. \quad (3)$$

There is an image of  $\alpha^2(\Omega)F(\Omega)$  and  $\mu^*(\omega_c)$  in the current ( $I$ ) voltage ( $V$ ) characteristics of a tunnel junction.  $I$ - $V$  data can be inverted to get these microscopic parameters. The McMillan-Rowell inversion procedure,<sup>14</sup> generally used for this task, makes use of the real-axis formulation of the Eliashberg equations. These can be obtained from Eqs. (1) and (2) by formal analytic continuation. The resulting equations are more complicated to write than the imaginary-axis version but would be fully equivalent if an infinite cutoff is used. In practice, finite cutoffs are introduced both in the real- and imaginary-axis versions, which in turn are reflected in the value of  $\mu^*$ . It is important to realize that a sharp cutoff in the real axis does not analytically continue to a sharp cutoff on the imaginary axis and vice versa.<sup>15</sup> In our calculations we use the spectral density  $\alpha^2(\Omega)F(\Omega)$  obtained from tunneling data in many superconductors and tabulated by Rowell, McMillan, and Dynes.<sup>16</sup> Because of the above-mentioned cutoff difficulties, we do not use the tunneling value of  $\mu^*$ , but fit  $\mu^*(\omega_c)$  in Eq. (1) to get the measured values of  $T_c$  when Eqs. (1) and (2) are solved at the critical temperature. In this case the equation can be linearized since  $\Delta(i\omega_n)$  tends to zero. We obtain the real gap at zero temperature analytically continuing  $\Delta(i\omega_n)$  from (1) and (2) to the real axis using Padé approximants.<sup>8</sup> The  $N$ -point Padé approximant to a complex function  $u(z)$  of the complex variable  $z$ , whose  $N$  values  $u_i$  ( $i=1, \dots, N$ ) are given at  $N$  complex points  $z_i$  ( $i=1, \dots, N$ ), is defined<sup>8,17</sup> as a continued fraction:

$$C_n(z) = \frac{a_1}{1 + \frac{a_2(z-z_1)}{1 + \frac{a_3(z-z_1)}{1 + \dots \frac{a_n(z-z_{n-1})}{1}}}} \quad (4)$$

such that

$$C_N(z_i) = u_i, \quad i=1, \dots, N. \quad (5)$$

The coefficients  $a_i$  are then given by the recursion

$$a_i = g_i(z_i), \quad g_1(z_i) = u_i, \quad i=1, \dots, N \quad (6)$$

$$g_p(z) = \frac{g_{p-1}(z_{p-1}) - g_{p-1}(z)}{(z - z_{p-1})g_{p-1}(z)}, \quad p \geq 2. \quad (7)$$

It can be shown that

$$C_N(z) = \frac{A_N(z)}{B_N(z)}, \quad (8)$$

where  $A_N$  and  $B_N$  are polynomials given by the recursion

$$A_{n+1}(z) = A_n(z) + (z - z_n)a_{n+1}A_{n-1}(z), \quad n=1, 2, \dots, N-1, \quad (9)$$

$$B_{n+1}(z) = B_n(z) + (z - z_n)a_{n+1}B_{n-1}(z), \quad n=1, 2, \dots, N-1,$$

and

$$A_0 = 0, \quad A_1 = a_1, \quad B_0 = B_1 = 1. \quad (10)$$

Vidberg and Serene<sup>8</sup> have tested this method on several general cases and applied it to the problem of obtaining the real-axis solutions  $\Delta(\omega)$  and  $Z_S(\omega)$  from the imaginary solutions  $\Delta(i\omega_n)$  and  $Z_S(i\omega_n)$  at the Matsubara frequencies. The main conclusions of their analysis are as follows:

(a) In order to get a good approximation to a function structured in the interval  $[0, \bar{\omega}]$  on the real axis one should use a sufficient number of inputs points from the interval  $[0, i\bar{\omega}']$  on the imaginary axis where  $i\bar{\omega}'$  belongs to the range of imaginary axis where the function attains its asymptotic form (usually  $i\bar{\omega}'$  is several times  $i\bar{\omega}$ ).

(b) The number of digits in the known values of the function  $u_i$  ( $i=1, \dots, N$ ) is crucial for obtaining a good analytic continuation.

(c) Overall agreement between the  $\Delta(\omega)$  and  $Z_S(\omega)$  obtained by means of the  $N$ -point Padé approximant and those tabulated by Rowell, McMillan and Dynes<sup>16</sup> is good, being excellent in the low-frequency range (from zero up to several meV).

For fixed frequency  $\omega_c$  we have fitted the  $\mu^*(\omega_c)$  to the experimental transition temperature  $T_c$  and then used the same cutoff and Coulomb-repulsion parameter to solve the Eliashberg equations (1) and (2) at some low temperature. Then we have applied the Padé scheme and determined  $\Delta_0$  from the condition  $\text{Re}\Delta(\omega=\Delta_0)=\Delta_0$ . Since the Padé scheme is supposed to work well in the low-frequency range [see (c)] one can hope that this method will give a good value for the  $\Delta_0$ . Furthermore, in view of (a), it is not necessary to take too large a cutoff  $\omega_c$  for the purposes of determining the gap edge at zero temperature. In most cases we have taken  $\omega_c$  to be three times the maximum phonon frequency  $\omega_M$  of the given material (see Table I). The temperature  $T$  at which the Eliashberg equations were solved was usually 0.4 K. The variation of  $\Delta_0(T)$ , the gap edge at temperature  $T$  with  $T$ , is negligible at very low temperature.

We give the results of our calculations in Table I. As

previously mentioned, most of the electron-phonon spectral densities  $\alpha^2(\Omega)F(\Omega)$  used come from the tabulation of Rowell, McMillan, and Dynes<sup>16</sup> from which  $\omega_M$ ,  $\mu_{\text{tunn}}^*$ , and  $\Delta_0^{\text{expt}}$  is available and reproduced here; the third column giving  $\omega_{\text{in}}$  is mainly taken from the tabulation in Allen and Dynes.<sup>10</sup> The exact definition of this average phonon energy will come in Sec. III where it becomes needed. For convenience, we also quote  $\lambda$ , the mass-renormalization parameter, and the measured  $T_c$  which is also the calculated one. The electron-phonon spectral density not found in the Rowell-McMillan-Dynes tabulation are now described. The one for Al is from the theoretical calculation of Leung *et al.*<sup>18</sup> The first Nb entry is from an early tunneling experiment by Robinson and Rowell.<sup>19</sup> The second is a theoretical calculation by Butler *et al.*<sup>20</sup> based on a calculation of phonon widths. The last is from the recent work of Arnold *et al.*<sup>21</sup> which accounts for the possibility of proximity in the tunnel junction. The vana-

TABLE I. Comparison of calculated and experimental gap edge. The theoretical ratio  $2\Delta_0/k_B T_c$ .

| System   | $\omega_M$<br>(meV) | $\omega_{\text{in}}$<br>(K) | $\lambda$ | $\omega_c/\omega_M$ | $\mu_{\text{tunn}}^*$ | $\mu_{\text{fitted}}^*$ | $T_c$<br>(K) | $\Delta_0^{\text{expt}}$<br>(meV) | $\Delta_0^{\text{calc}}$<br>(meV) | $(\Delta_0^{\text{calc}} - \Delta_0^{\text{expt}})/\Delta_0^{\text{expt}}$ | $(2\Delta_0/k_B T_c)_{\text{calc}}$ |
|--|---------------------|-----------------------------|-----------|---------------------|-----------------------|-------------------------|--------------|-----------------------------------|-----------------------------------|--|-------------------------------------|
| Al   | 41.4                | 296                         | 0.432     | 3                   |                       | 0.1472                  | 1.18         |                                   | 0.18                              |  | 3.54                                |
| Sn   | 18.4                | 99                          | 0.716     | 3                   | 0.11                  | 0.1143                  | 3.75         | 0.606                             | 0.599                             | -1.1   | 3.71                                |
| Nb <sub>3</sub> Sn                                       | 28.7                | 125                         | 1.68      | 6                   | 0.15                  | 0.1575                  | 18.0         | 3.1                               | 3.53                              | +13.9  | 4.55                                |
| Nb (Robinson)  | 29.0                | 124                         | 0.97      | 3                   | 0.11                  | 0.1158                  | 9.2          | 1.46                              | 1.57                              | +7.5   | 3.96                                |
| Nb (Butler)  | 28.88               | 166                         | 1.12      | 3                   |                       | 0.2735                  | 9.2          |                                   | 1.53                              |  | 3.86                                |
| Nb (Arnold)  | 28.29               | 147                         | 1.01      | 6                   | 0.16                  | 0.1854                  | 9.22         | 1.51                              | 1.54                              | +2   | 3.88                                |
| V  | 33.0                | 172                         | 0.81      | 3                   | 0.15                  | 0.19                    | 5.36         | 0.8                               | 0.85                              | +6   | 3.67                                |
| Nb <sub>0.75</sub> Zr <sub>0.25</sub>                    | 26.0                | 109                         | 1.31      | 6                   | 0.10±<br>0.02         | 0.1808                  | 10.8         | 1.9                               | 1.93                              | +1.6   | 4.15                                |
| Ta   | 20.9                | 132                         | 0.69      | 3                   | 0.11                  | 0.1169                  | 4.48         | 0.72                              | 0.71                              | -1.4   | 3.68                                |
| In   | 15.8                | 68                          | 0.805     | 3                   | 0.125                 | 0.1130                  | 3.40         | 0.541                             | 0.556                             | +2.8   | 3.80                                |
| In <sub>0.9</sub> Tl <sub>0.1</sub>                      | 16.2                | 63                          | 0.85      | 3                   | 0.12                  | 0.1271                  | 3.28         | 0.530                             | 0.540                             | +1.9   | 3.82                                |
| In <sub>0.73</sub> Tl <sub>0.27</sub>                    | 14.6                | 55                          | 0.934     | 3                   | 0.13                  | 0.1358                  | 3.36         | 0.57                              | 0.564                             | -1.0   | 3.90                                |
| In <sub>0.67</sub> Tl <sub>0.33</sub>                    | 15.2                | 57                          | 0.90      | 3                   | 0.13                  | 0.1314                  | 3.26         | 0.54                              | 0.543                             | +0.6   | 3.87                                |
| In <sub>0.57</sub> Tl <sub>0.43</sub>                    | 14.4                | 53                          | 0.85      | 3                   | 0.14                  | 0.1387                  | 2.6          | 0.42                              | 0.426                             | +1.4   | 3.80                                |
| In <sub>0.50</sub> Tl <sub>0.50</sub>                    | 14.8                | 53                          | 0.83      | 3                   | 0.13                  | 0.1377                  | 2.52         | 0.41                              | 0.41                              | 0.0  | 3.78                                |
| Pb <sub>0.8</sub> Tl <sub>0.2</sub>                      | 10.9                | 50                          | 1.53      | 3                   | 0.122                 | 0.1239                  | 6.80         | 1.28                              | 1.33                              | 3.9  | 4.54                                |
| In <sub>0.27</sub> Tl <sub>0.73</sub>                    | 13.6                | 42                          | 1.09      | 3                   | 0.11                  | 0.1164                  | 3.64         | 0.64                              | 0.64                              | 0.0  | 4.08                                |
| In <sub>0.17</sub> Tl <sub>0.83</sub>                    | 13.2                | 45                          | 0.98      | 3                   | 0.12                  | 0.1188                  | 3.19         | 0.535                             | 0.545                             | +1.9   | 3.96                                |
| In <sub>0.07</sub> Tl <sub>0.93</sub>                    | 11.8                | 49                          | 0.89      | 3                   | 0.13                  | 0.1311                  | 2.77         | 0.45                              | 0.46                              | +2.2   | 3.85                                |
| Tl   | 10.9                | 52                          | 0.795     | 3                   | 0.135                 | 0.1281                  | 2.36         | 0.366                             | 0.382                             | +4.0   | 3.76                                |
| Pb <sub>0.4</sub> Tl <sub>0.6</sub>                      | 11.0                | 48                          | 1.15      | 3                   | 0.113                 | 0.1149                  | 4.60         | 0.805                             | 0.822                             | +2.1   | 4.15                                |
| Pb <sub>0.6</sub> Tl <sub>0.4</sub>                      | 10.9                | 50                          | 1.38      | 3                   | 0.126                 | 0.1262                  | 5.90         | 1.08                              | 1.11                              | +2.8   | 4.37                                |
| Pb   | 11.0                | 56                          | 1.55      | 3                   | 0.131                 | 0.1446                  | 7.19         | 1.40                              | 1.40                              | 0.0  | 4.52                                |
| Pb <sub>0.9</sub> Bi <sub>0.10</sub>                     | 9.9                 | 50                          | 1.66      | 3                   | 0.095                 | 0.1120                  | 7.65         | 1.54                              | 1.55                              | +0.6   | 4.70                                |
| Pb <sub>0.8</sub> Bi <sub>0.2</sub>                      | 10.9                | 46                          | 1.88      | 3                   | 0.111                 | 0.1127                  | 7.95         | 1.61                              | 1.67                              | +3.7   | 4.88                                |
| Pb <sub>0.7</sub> Bi <sub>0.3</sub>                      | 10.4                | 47                          | 2.0       | 3                   | 0.11                  | 0.1154                  | 8.45         | 1.77                              | 1.82                              | +2.8   | 5.00                                |
| Pb <sub>0.65</sub> Bi <sub>0.35</sub>                    | 10.1                | 45                          | 2.13      | 3                   | 0.111                 | 0.0996                  | 8.95         | 1.84                              | 1.98                              | +7.6   | 5.13                                |
| Pb <sub>0.60</sub> Tl <sub>0.20</sub> Bi <sub>0.20</sub> | 10.2                | 48                          | 1.82      | 3                   | 0.137                 | 0.1538                  | 7.26         | 1.50                              | 1.49                              | -0.7   | 4.76                                |
| Tl <sub>0.90</sub> Bi <sub>0.10</sub>                    | 10.5                | 48                          | 0.78      | 3                   | 0.119                 | 0.1114                  | 2.3          | 0.354                             | 0.374                             | +5.6   | 3.77                                |
| Hg <sup>10</sup>   | 14.3                | 29                          | 1.62      | 3                   | 0.11                  | 0.1197                  | 4.19         | 0.83                              | 0.83                              | 0.0  | 4.60                                |
| Amorphous Bi   | 14.0                |                             | 2.46      | 3                   | 0.105                 | 0.0917                  | 6.11         | 1.21                              | 1.30                              | +7.4   | 4.94                                |
| Amorphous<br>Pb <sub>0.50</sub> Bi <sub>0.50</sub>       | 13.1                | 29                          | 3.00      | 3                   | 0.14                  | 0.1338                  | 6.99         | 1.51                              | 1.57                              | +4.0   | 5.21                                |
| Amorphous<br>Pb <sub>0.75</sub> Bi <sub>0.25</sub>       | 12.7                |                             | 2.76      | 3                   | 0.14                  | 0.1340                  | 6.91         | 1.48                              | 1.53                              | +3.4   | 5.14                                |
| Amorphous Ga   | 27.0                | 35                          | 2.25      | 3                   | 0.17                  | 0.1632                  | 8.56         | 1.68                              | 1.74                              | +3.6   | 4.72                                |

dium was also similarly obtained and is found in the work of Zasadzinski *et al.*<sup>22</sup> Finally, the  $\text{Nb}_{0.75}\text{Zn}_{0.25}$  alloy is from a paper by Wolf and Noer.<sup>23</sup> The amorphous metals are from the work of Chen *et al.*<sup>24</sup> and of Chen.<sup>25</sup>

We return now to the table and note that in the case of Pb and Hg the agreement between the calculated and experimental values of  $\Delta_0$  is perfect. Also, in the case of Al the calculated ratio is very close to the BCS result 3.53. Aluminum is a very weak coupling material for which the retardation and damping effects are not important and which can be well described within the BCS theory. We see that our procedure gives the correct weak-coupling limit of the Eliashberg theory.

Since the experimental results for the gap edge are accurate to at best 1% we can conclude that, except in a few cases, the agreement between the calculated value of the gap edge  $\Delta_0$  and the corresponding experimental value is quite good.

Two cases deserve special attention. The worst agreement is in the case of  $\text{Nb}_3\text{Sn}$ . For this material we have used the electron-phonon spectral function  $\alpha^2(\Omega)F(\Omega)$  obtained by Shen<sup>26</sup> from tunneling experiments. Recently, Moore, Zubeck, Rowell, and Beasley<sup>27</sup> have performed new tunneling experiments in a series of *A15* materials. They have used an improved technique for forming tunneling junctions with these difficult materials. In their experiments on  $\text{Nb}_3\text{Sn}$  the measured values of the zero-temperature gap edge  $\Delta_0$  are between 3.2 and 3.4 meV, which is larger than Shen's value of 3.1 meV and close to our calculated value of 3.53 meV.

The second example of poor agreement is the case of Nb when we used the  $\alpha^2(\Omega)F(\Omega)$  obtained by Robinson *et al.*<sup>19</sup> It has since been recognized, however, that Nb junctions can suffer from a proximity layer between Nb and oxide which needs to be accounted for.<sup>21</sup> This is now well understood<sup>21-23</sup> and our calculation with the spectrum of Arnold *et al.*<sup>19</sup> agrees well with the experiment.

At present we do not have an unambiguous explanation

for the large discrepancies between calculated and measured values of the gap edge  $\Delta_0$  for the alloy  $\text{Pb}_{0.65}\text{Bi}_{0.35}$  and amorphous Bi. The most probable answer for the first is that the measured values of the gap edge  $\Delta_0$  at zero temperature and/or transition temperature  $T_c$  are not accurate for this material.

For the second one, however, there may be another explanation. In general the values of  $\alpha^2(\Omega)F(\Omega)$  obtained from the inversion of tunneling data are not well known at low  $\Omega$ 's. In the amorphous materials there is a lot of weight under  $\alpha^2F$  at these energies and since the functional derivative  $\delta(2\Delta_0/k_B T_c)/\delta[\alpha^2(\Omega)F(\Omega)]$  indicates<sup>28</sup> that the most important phonons for  $2\Delta_0/k_B T_c$  are around  $\Delta_0/3$ , the uncertainties in the inverted  $\alpha^2(\Omega)F(\Omega)$ 's for amorphous materials at low frequencies may be the cause of a large discrepancy between calculated and experimental values for  $2\Delta_0/k_B T_c$  in amorphous Bi.

We can conclude this section by saying that the method of *N*-point Padé approximants for obtaining the zero-temperature gap edge from imaginary-axis solutions is quite reliable. Second, in most of the cases investigated here, standard Eliashberg theory predicts well the observed values of the ratio  $2\Delta_0/k_B T_c$ .

### III. DERIVATION OF A GEILIKMAN-KRESIN-TYPE FORMULA

In this section we turn to the problem of deriving a simple expression for  $2\Delta_0/k_B T_c$ . We follow closely the procedure of Leavens and Carbotte,<sup>11</sup> the only difference being that the zero-temperature value of the renormalization function in the superconducting state  $Z_S$  is not identified with the corresponding quantity  $Z_n$  in the normal state. The approximation  $Z_S = Z_n$ , which is excellent for the weak-coupling superconductors, produces no change in the value of  $2\Delta_0/k_B T_c$  from the BCS result 3.53, Ref. 11.

At  $T=0$  the Eliashberg equations written on the real frequency axis are

$$\Delta(\omega)Z_S(\omega) = \int_0^{\omega_c} d\omega' \text{Re} \left[ \frac{\Delta(\omega')}{[\omega'^2 - \Delta^2(\omega')]^{1/2}} \right] [K_+(\omega, \omega') - \mu^*(\omega_c)], \quad (11)$$

$$[1 - Z_S(\omega)]\omega = \int_0^{+\infty} d\omega' \text{Re} \left[ \frac{\omega'}{[\omega'^2 - \Delta^2(\omega')]^{1/2}} \right] K_-(\omega, \omega'), \quad (12)$$

where

$$K_{\pm}(\omega, \omega') = \int_0^{+\infty} d\Omega \alpha^2(\Omega)F(\Omega) \left[ \frac{1}{\omega' + \Omega + \nu + i0^+} \pm \frac{1}{\omega' + \Omega - \nu - i0^+} \right]. \quad (13)$$

We consider the real part of Eq. (11) at the gap edge  $\omega = \Delta_0$ , take the cutoff  $\omega_c$  to be equal to the maximum phonon frequency, and approximate  $\Delta(\omega)$  by  $\Delta_0$ . Leavens and Carbotte<sup>11</sup> have shown in detail that this will reduce Eq. (11) to

$$\Delta_0 Z_S(\Delta_0) = \left[ -\bar{\lambda} + (\lambda - \mu^*) \ln \left[ \frac{2\omega_c}{\Delta_0} \right] \right] \Delta_0, \quad (14)$$

where

$$\lambda \equiv 2 \int_0^{\omega_c} \frac{d\Omega}{\Omega} \alpha^2(\Omega) F(\Omega)$$

and

$$\bar{\lambda} \equiv 2 \int_0^{\omega_c} \frac{d\Omega}{\Omega} \alpha^2(\Omega) F(\Omega) \ln \left[ 1 + \frac{\omega_c}{\Omega} \right].$$

In obtaining (14) it has been assumed that the important frequencies in  $\alpha^2(\Omega)F(\Omega)$  are  $\gg \Delta_0$ . Equation (12) for  $Z_S$  in the limit  $\omega \rightarrow 0$  reduces to

$$\begin{aligned} Z_S(\omega) &\equiv 1 + \int_0^{+\infty} d\Omega \left[ 2\alpha^2(\Omega)F(\Omega) \int_{\Delta_0}^{+\infty} d\omega' \frac{\omega'}{(\omega'^2 - \Delta_0^2)^{1/2}} \frac{1}{(\omega' + \Omega)^2} \right] \\ &\equiv 1 + \int_0^{+\infty} d\Omega \frac{2\alpha^2(\Omega)F(\Omega)}{\Omega} \left[ 1 + \left[ \frac{\Delta_0}{\Omega} \right]^2 \ln \left[ \frac{\Delta_0}{2\Omega} \right] \right] \\ &= 1 + \lambda + \Delta_0^2 \int_0^{+\infty} d\Omega \frac{2\alpha^2(\Omega)F(\Omega)}{\Omega^3} \ln \left[ \frac{\Delta_0}{2\Omega} \right], \end{aligned} \quad (15)$$

where it has been assumed that  $\Delta_0/\Omega \ll 1$  for the important  $\Omega$ 's.

To proceed further we approximate the last integral in (15) by

$$\alpha \frac{\lambda}{\bar{\Omega}^2} \ln \left[ \frac{\Delta_0 \beta}{\bar{\Omega}} \right], \quad (16)$$

where  $\alpha$  and  $\beta$  are constants to be determined later through a phenomenological fit to the exact results of Sec. II (or experiment) and  $\bar{\Omega}$  is some suitably defined average phonon frequency. The value  $Z_S(\Delta_0)$  in Eq. (14) can be replaced by  $Z_S(0)$ . By substituting (15) and (16) into (14) we get

$$\Delta_0 = 2\omega_c \exp \left[ -\frac{1 + \lambda + \bar{\lambda}}{\lambda - \mu^*} - \alpha \left[ \frac{\Delta_0}{\bar{\Omega}} \right]^2 \frac{\lambda}{\lambda - \mu^*} \ln \left[ \frac{\Delta_0 \beta}{\bar{\Omega}} \right] \right]. \quad (17)$$

By using a similar approach Leavens and Carbotte<sup>11</sup> have obtained for the critical temperature  $T_c$

$$k_B T_c = 1.134 \omega_c \exp \left[ -\frac{1 + \lambda(T_c) + \bar{\lambda}}{\lambda - \mu^*} \right], \quad (18)$$

where

$$\lambda(T) = 2 \int_0^{+\infty} d\omega \left[ -\frac{\partial f(\omega)}{\partial \omega} \right] \int_0^{+\infty} d\Omega \frac{\alpha^2(\Omega)F(\Omega)}{\Omega + \omega}. \quad (19)$$

By setting  $\lambda(T_c) \equiv \lambda$  Eqs. (17) and (18) give

$$\frac{2\Delta_0}{k_B T_c} = 3.53 \left[ 1 - \alpha \left[ \frac{\Delta_0}{\bar{\Omega}} \right]^2 \frac{\lambda}{\lambda - \mu^*} \ln \left[ \frac{\Delta_0 \beta}{\bar{\Omega}} \right] \right] \quad (20)$$

assuming  $\Delta_0 \ll \bar{\Omega}$ . In Eq. (20)  $\lambda - \mu^*$  can be approximated by  $\lambda$  so as to get the very approximate, but simple formula

$$\frac{2\Delta_0}{k_B T_c} = 3.53 \left[ 1 + \alpha \left[ \frac{\Delta_0}{\bar{\Omega}} \right]^2 \ln \left[ \frac{\bar{\Omega}}{\Delta_0 \beta} \right] \right]. \quad (21)$$

Now, many different choices of  $\bar{\Omega}$  are possible. One popular choice is  $\omega_{\ln}$  defined by<sup>10</sup>

$$\omega_{\ln} \equiv \exp \left[ \frac{2}{\lambda} \int_0^{+\infty} \frac{d\omega}{\omega} \alpha^2(\omega) F(\omega) \ln \omega \right]. \quad (22)$$

Values of  $\omega_{\ln}$  are found in Table I. Most have been taken from the work of Allen and Dynes<sup>10</sup> with the remainder taken from the previously referred to literature.

In Fig. 1 we plot the exact results for  $2\Delta_0/k_B T_c$  against  $T_c/\omega_{\ln}$ . It is clear from the figure that there is enough scatter that no smooth curve will fit all the points. On the other hand, a general increase of  $2\Delta_0/k_B T_c$  with increasing  $T_c/\omega_{\ln}$  is clearly seen. It is this general trend that interests us and it is certainly, at best, only this general trend that a crude formula like Eq. (21) can describe. We have adjusted  $\alpha$  and  $\beta$  after making a change from  $\Delta$  to  $T_c$  (the more easily measured quantity) to get as good a fit as is possible to the data in Fig. 1 and found the dashed curve which corresponds to the formula

$$\frac{2\Delta_0}{k_B T_c} = 3.53 \left[ 1 + 12.5 \left[ \frac{T_c}{\omega_{\ln}} \right]^2 \ln \left[ \frac{\omega_{\ln}}{2T_c} \right] \right]. \quad (23)$$

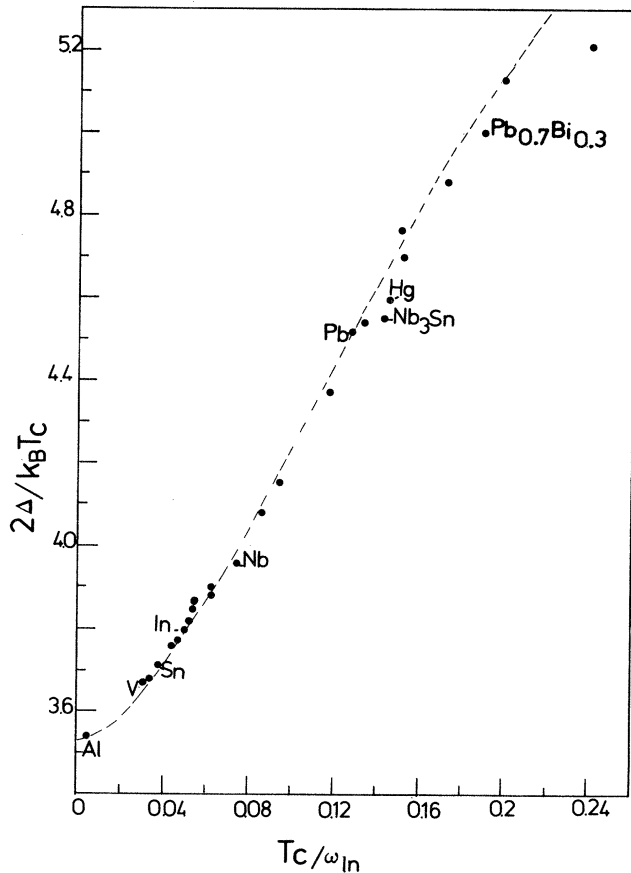


FIG. 1. The ratio  $2\Delta_0/k_B T_c$  vs  $T_c/\omega_{in}$ . The dots are the theoretical results from the full numerical solutions of the Eliashberg equations given by Table I. In increasing order of  $2\Delta_0/k_B T_c$  they correspond to the following systems: Al, V, Ta, Sn, Tl,  $Tl_{0.9}Bi_{0.1}$ , In,  $In_{0.9}Tl_{0.1}$ ,  $In_{0.07}Tl_{0.93}$ , Nb (Butler), Nb (Arnold),  $In_{0.73}Tl_{0.27}$ , Nb (Robinson),  $In_{0.27}Tl_{0.73}$ ,  $Pb_{0.4}Tl_{0.6}$ ,  $Pb_{0.6}Tl_{0.4}$ , Pb,  $Pb_{0.8}Tl_{0.2}$ ,  $Nb_3Sn$ , Hg,  $Pb_{0.9}Bi_{0.1}$ ,  $Pb_{0.6}Tl_{0.2}Bi_{0.2}$ ,  $Pb_{0.8}Bi_{0.2}$ ,  $Pb_{0.7}Bi_{0.3}$ ,  $Pb_{0.65}Bi_{0.35}$ , amorphous  $Pb_{0.5}Bi_{0.5}$ . The dashed curve corresponds to  $2\Delta_0/k_B T_c = 3.53 \times [1 + 12.5 T_c/\omega_{in}]^2 \ln(\omega_{in}/2T_c)$  and it is discussed in Sec. III.

This is our final formula. The fit to the data is excellent if one simply wants to know the general trend. For details it is necessary to go back to the full numerical solution of the Eliashberg equations as was done in Sec. II. It is seen from Fig. 1 that amorphous  $Pb_{0.5}Bi_{0.5}$  falls farthest off the dashed curve. Also, we have not included amorphous Bi and Ga which would fit even worse. It is likely that (23) simply does not apply to such extreme spectrum with a large amount of weight in the region where the functional derivative of  $2\Delta_0/k_B T_c$  peaks. Also, as previously remarked, the low-energy part of the spectral density is not well determined by tunneling so that the  $\omega_{in}$  values may not be very reliable for amorphous spectra where  $\alpha^2(\omega)F(\omega)$  is linear at low  $\omega$ .

#### IV. CONCLUSIONS

We have obtained numerous solutions of the Eliashberg equations for the ratio  $2\Delta_0/k_B T_c$  in systems for which the electron-phonon spectral density  $\alpha^2(\Omega)F(\Omega)$  is known from tunneling results. The agreement with experiment is in all cases at the few-percent level which is the expected accuracy of the Eliashberg equations themselves. We have found that the formula

$$\frac{2\Delta_0}{k_B T_c} = 3.53 \left[ 1 + 12.5 \left( \frac{T_c}{\omega_{in}} \right)^2 \ln \left( \frac{\omega_{in}}{2T_c} \right) \right]$$

reproduces well the general trend obtained for this ratio but does not give the details. In this formula  $\omega_{in}$  is the well-known phonon average introduced by Allen and Dynes.

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