Maximum $2\Delta_0/k_BT_c$ for electron-phonon superconductors

J. P. Carbotte and F. Marsiglio
Physics Department, McMaster University, Hamilton, Ontario, Canada L8S 4M1

B. Mitrović
Physics Department, Brock University, Saint Catharines, Ontario, Canada L2S 3A1

(Received 6 September 1985)

For an electron-phonon superconductor the question of a possible maximum value for the size of the ratio $2\Delta_0/k_BT_c$ is addressed. Here Δ_0 is the gap edge and T_c the critical temperature. We were able to obtain well-converged solutions of the Eliashberg equations for a δ-function electron-phonon spectral density centered at Ω_E with Ω_E as low as 0.75 meV, in which case $2\Delta_0/k_BT_c$ is still rising and equal to ~ 9. In the limit $\Omega_E \to 0$, we can prove analytically that both Δ_0 and T_c scale like $(\Omega_E)^{1/2}$ so that their ratio remains finite. A rough estimate gives a value of about 7 for the ratio in this limit. In the course of the discussion a new upper bound on Δ_0 is established and tested.

I. INTRODUCTION

In this paper we address the following question. For an electron-phonon superconductor, to which the Eliashberg gap equations apply, how big can the ratio of the gap Δ_0 to the critical temperature get? To answer this question we will use an appropriate generalization of a general approach already used in the literature to discuss limits on T_c. This problem was studied by Leavens and Carbotte[1] within the framework of the McMillan[2,3] equation. These authors point out the importance of the parameter A in high T_c superconductivity. Here A is the area under the electron-phonon spectral density $\alpha^2F(\omega)$. It is shown that under certain circumstances T_c grows linearly with A. A more sophisticated formulation of the problem using full Eliashberg theory was given by Leavens.[4] It is shown that, for any fixed value of A, the optimum shape for the spectral density is a δ function at a certain well-defined frequency ω_E^*. The proof is based on the properties of the functional derivative of T_c with $\alpha^2F(\omega)$ calculated by Bergmann and Rainer.[5] The functional derivative denoted by $\delta T_c/\delta\alpha^2F(\omega_0)$ gives the response of T_c to an infinitesimal increase in spectral weight at phonon energy ω_0. It is found to be positive definite for all ω_0, going to zero in both the $\omega_0 \to 0$ and $\omega_0 \to \infty$ limits with a broad maximum in between at about $\omega_0 \cong 7k_BT_c$. For a given $\alpha^2F(\omega)$, of area A, it is argued that T_c will be maximum when the entire area under $\alpha^2F(\omega)$ is transferred to the maximum in its own functional derivative, in which case $T_c = C(\mu^*)A$ where $C(\mu^*)$ is a constant which depends only on the Coulomb pseudopotential μ^*.

In a recent paper Mitrović, Leavens, and Carbotte[6] have calculated the functional derivative of the ratio $2\Delta_0/k_BT_c$ for several superconductors. For all cases considered

$$\delta[2\Delta_0/k_BT_c]/\delta[\alpha^2F(\omega)]$$

is found to be positive definite, tending to zero as $\omega \to 0, \infty$ with a very sharp maximum around $\omega^* \cong \frac{2}{3}\Delta_0$. *Assuming* this form to hold in *all* cases, arguments similar to those described in the case of the critical temperature would lead us to expect that $2\Delta_0/k_BT_c$ is maximized for a δ function spectrum placed at the maximum of its own functional derivative (an assumption—not proven)

$$\delta[2\Delta_0/k_BT_c]/\delta[\alpha^2F(\omega)] \ .$$

In Sec. II we introduce the gap equations and show that, for a δ-function spectrum $A\delta(\omega-\omega_E)$, the gap and critical temperature scale with A. This feature can be exploited to discover a new upper bound on Δ_0. In Sec. III we deal with results for $2\Delta_0/k_BT_c$. It will be found that our numerical techniques do not converge well when Ω_E becomes very small. For this reason we consider analytically the $\Omega_E \to 0$ limit in which case we are able to prove that both T_c and Δ_0 scale like $(A\Omega_E)^{1/2}$ so that the ratio $2\Delta_0/k_BT_c$ remains finite and is a universal number independent of material parameters. A rough analytic estimate for this universal constant is given in Sec. IV. In Sec. V conclusions are drawn.

II. OPTIMUM SPECTRUM FOR THE GAP EDGE

The imaginary frequency axis Eliashberg equations are[7,8]

$$\Delta(i\omega_n)Z(i\omega_n) = \pi k_BT \sum_{m=-\infty}^{+\infty} [\lambda(n-m)-\mu^*(\omega_c)\theta(\omega_c-|\omega_m|)] \times \frac{\Delta(i\omega_m)}{[\omega_m^2+\Delta^2(i\omega_m)]^{1/2}} \quad (1)$$

and

$$\omega_nZ(i\omega_n) = \omega_n + \pi k_BT \sum_{m=-\infty}^{+\infty} \lambda(n-m) \times \frac{\omega_m}{[\omega_m^2+\Delta^2(i\omega_m)]^{1/2}} \quad (2)$$

with Δ and Z the Matsubara gap and renormalization function evaluated on the imaginary frequency axis at the discrete points,

$$i\omega_n = i\pi k_B T_c(2n-1), \quad n=0,\pm 1,-\cdots .$$

In these equations T is the temperature, k_B is Boltzmann's constant, ω_c a cutoff on the Coulomb repulsion needed to get a convergent sum over m, $\mu^*(\omega_c)$ the Coulomb pseudopotential appropriate to the cutoff ω_c, and $\lambda(m-n)$ is given by

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

where $\alpha^2F(\Omega)$ is the electron-phonon spectral density.

We will want to consider the special case of a δ-function spectrum for $\alpha^2F(\Omega)$ of the form

$$\alpha^2F(\Omega)=A\delta(\Omega-\Omega_E) \tag{4}$$

with A the weight of the spectral density, i.e., the area under it and Ω_E some definite phonon energy. For this special case Eqs. (1) and (2) simplify. After dividing both sides of each equation by A and introducing $\bar{\Delta}\equiv\Delta/A$, $\bar{T}=T/A$, and $\bar{\omega}_n\equiv\omega_n/A$ so that $\bar{\omega}_n=\pi\bar{T}(2n-1)$, we arrive at the pair of equations

$$\bar{\Delta}(i\omega_n)Z(i\omega_n)=\pi k_B\bar{T}\sum_{m=-\infty}^{+\infty}\left[\frac{2\bar{\Omega}_E}{\bar{\Omega}_E^2+(\bar{\omega}_n-\bar{\omega}_n)^2}-\mu^*(\omega_c)\theta(\omega_c-|\bar{\omega}_m|A)\right]\frac{\bar{\Delta}(i\omega_m)}{[\bar{\omega}_m^2+\bar{\Delta}^2(i\omega_m)]^{1/2}} \tag{5}$$

and

$$\bar{\omega}_nZ(i\omega_n)=\omega_n+\pi k_B\bar{T}\sum_{m=-\infty}^{+\infty}\frac{2\bar{\Omega}_E}{\bar{\Omega}_E^2+(\bar{\omega}_n-\bar{\omega}_m)^2}\frac{\bar{\omega}_m}{[\bar{\omega}_m^2+\bar{\Delta}^2(i\omega_m)]^{1/2}} . \tag{6}$$

We will follow Leavens[4] and ignore the explicit dependence on A occurring in the Coulomb cutoff in Eq. (5). This is reasonable because μ^* is not an important parameter and its dependence on ω_c is small for a large cutoff. With this approximation, it is clear from the form of Eqs. (5) and (6) that $\bar{\Delta}$ and Z can depend only on the reduced parameters $\bar{T}$ and $\bar{\Omega}_E$ in addition to μ^*, of course. This means that for a given $\bar{\Omega}_E$ and μ^* the critical temperature $\bar{T}_c$ derived from the linearized version of Eqs. (5) and (6) is a function (f) of only these two parameters, i.e.,

$$\bar{T}_c\equiv\frac{T_c}{A}=f(\bar{\Omega}_E,\mu^*) \tag{7}$$

a result previously obtained by Leavens. If (5) and (6) are considered at low (or zero) temperature we can further conclude that the gap edge $\bar{\Delta}_0$ can only be a function (g) of $\bar{\Omega}_E$ and μ^* so that

$$\bar{\Delta}_0\equiv\frac{\Delta_0}{A}=g(\bar{\Omega}_E,\mu^*) \tag{8}$$

which is a new result.

To determine the function g we need to solve Eqs. (5) and (6) at some low temperature and use a technique of Padé approximants to obtain the analytic continuation of the gap to the real frequency axis [$\bar{\Delta}(\omega)$]. The gap edge follows from $\bar{\Delta}_0=\mathrm{Re}\bar{\Delta}(\omega=\bar{\Delta}_0)$.[8] Alternatively, one can return to (1) and (2) and solve them for spectrum (4) with a definite value of A and Ω_E. Since the choice of A is immaterial we will use throughout this paper the value 10.652 meV, appropriate for Nb_3Sn.[9]

We have solved (1) and (2) at low temperatures for three values of μ^*, namely 0, 0.1, and 0.227 [the value appropriate for Nb_3Sn (Ref. 8)] as a function of Ω_E. In all cases Δ_0 is found to exhibit a maximum at some definite frequency Ω_E^* which depends on μ^* and to drop slowly on either side of Ω_E^*. This behavior is shown in Fig. 1 where Δ_0 is plotted (in the region of its maximum value) against Ω_E [Fig. 1(a)] and also against $\lambda_E=2A/\Omega_E\equiv 2/\Omega_E$ [Fig. 1(b)]. The shape of the function $g(\bar{\Omega}_E,\mu^*)$ obtained was really expected from the previous work of Mitrović, Leavens, and Carbotte[6] who calculated the functional derivative of Δ_0 with respect to $\alpha^2F(\omega)$ for several materials. In all cases they find that $\delta\Delta_0/\delta\alpha^2F(\omega)$ goes to zero at high and at low frequencies displaying a broad maximum somewhere in between. Although the position of the maximum varies somewhat from material to material, the rule of thumb developed in Ref. 8 is that it occurs around $4k_BT_c$. For $\mu^*=0.227$ the peak in Fig. 1 is found to occur at approximately 5.5 meV for which case $k_BT_c=1.39$ meV. This is in close agreement with the rule developed for the case of the functional derivative.

To check on the validity of Eq. (8) we have made an extra calculation of Δ_0 with $\Omega_E=3$ meV, $\mu^*=0.2267$ (un-

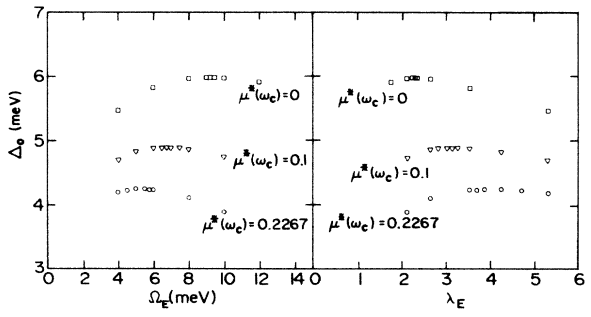

FIG. 1. The gap edge Δ_0 in meV for a δ-function spectrum $\alpha^2F(\Omega)=A\delta(\Omega-\Omega_E)$ with $A=10.652$ meV shown for three values of $\mu^*=0$, 0.1, and 0.2267 as a function of Ω_E in meV and again as a function of $\lambda_E=2A/\Omega_E$ (dimensionless). The ratio Δ_0/A is independent of A and the position of the maximum Ω_E^* proportional to A. The region of highest density of points is around the maximum.

changed) and $A=5.326$ meV which is exactly half the value previously used. For these parameters $\Delta_0=2.178$ meV and $\Delta_0/A=0.409$ which is to be compared with 0.397 when $A=10.672$ meV was used with $\Omega_E=6$ meV. The agreement is excellent (about 3%) and represents a numerical test of our scaling theorem.

The maximum observed in Fig. 1 for each value of μ^* considered represents the maximum value for the ratio of the gap to A that can be achieved for any shape of $\alpha^2F(\Omega)$ since the peak is assumed to occur when the phonon energy in the δ function (4) is placed at the maximum of its own functional derivative $\delta\Delta_0/\delta[\alpha^2F(\Omega)]$. If we determine the value of $\overline{\Omega}_E$ at maximum and denote it by $\overline{\Omega}_E^*$ we conclude that

$$\Delta_0^*=Ag(\overline{\Omega}_E^*,\mu^*)\equiv Ab(\mu^*) \tag{9}$$

since $\overline{\Omega}_E^*$ is a well-defined dimensionless number. In Table I we show the results obtained for $b(\mu^*)$. We see that $b(\mu^*)$ is reduced as μ^* increases which is as expected. For any other spectrum with the same μ^* we expect

$$\Delta_0\le Ab(\mu^*)=\Delta_0^* . \tag{10}$$

In a recent paper Mitrović, Zarate, and Carbotte[8] have calculated Δ_0 and the ratio $2\Delta_0/k_BT_c$ for a large number of materials for which $\alpha^2F(\Omega)$ is known through inversion of tunneling data. These results can be used here to test the inequality (10). This is shown in Fig. 2 where we show the line $b(\mu^*)$ versus μ^* and also place on the same figure the ratio Δ_0/A for the superconductors considered in Ref. 8 as well as for a few others, La,[10] V,[11] and various models for Nb_3Sn, Nb_3Al, Nb_3Ge, and V_3Ga.[12] The solid dots, unidentified individually, are for PbTlBi alloys and the crosses for InTl alloys. Note that the inequality (10) on the gap is well satisfied. The system falling closest to the $b(\mu^*)$ versus μ^* curve is the alloy $Pb_{0.65}Bi_{0.35}$ for which $\mu^*=0.0996$ and $\Delta_0/A=0.43$. This is to be compared with the value of $b(\mu^*=1)$ given in Table I which is 0.46 and represents the maximum possible value. The difference with $Pb_{0.65}Bi_{0.35}$ is only 10%. This shows that some real materials can very nearly exhibit the maximum possible gap value for their particular spectral weight $A=\int\alpha^2F(\Omega)d\Omega$.

To end this section we consider the value of $\overline{\Omega}_E^*$ at optimum, i.e., where $\overline{\Delta}_0$ peaks for a given value of μ^* in Fig. 1. Denoting this quantity by $c(\mu^*)$, we have

$$\overline{\Omega}_E^*=c(\mu^*)\quad\text{or}\quad\Omega_E^*=c(\mu^*)A \tag{11}$$

with the value of c entered in Table I. We note that c varies considerably with μ^*, decreasing with increasing Coulomb pseudopotential.

TABLE I. The variation of $b(\mu^*)$ and $c(\mu^*)$ with Coulomb pseudopotential. The quantities $b(\mu^*)$ and $c(\mu^*)$ give, respectively, the value of Δ_0/A and Ω_E^*/A at maximum (see Fig. 1).

	$\mu^*=0$	$\mu^*=0.1$	$\mu^*=0.2267$
$b(\mu^*)$	0.56	0.46	0.40
$c(\mu^*)$	0.87	0.63	0.52

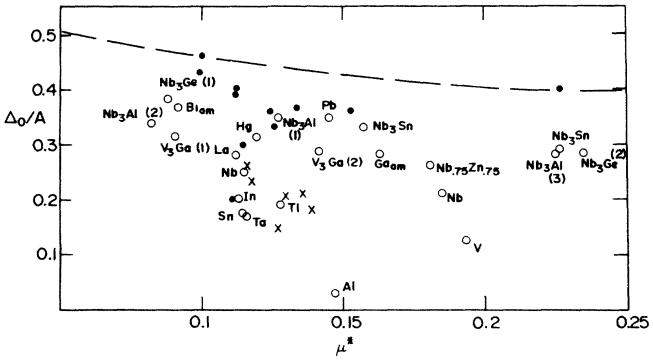

FIG. 2. The optimum line (— — —) giving $b(\mu^*)$ as a function of Coulomb pseudopotential. For any superconductor at all, Δ_0/A [with $A=\int_0^\infty\alpha F(\omega)d\omega$] must fall on or below the dashed curve which represents an upper bound on this ratio. This is well satisfied by all the points shown. The unidentified solid dots are for PbTlBi alloys while the crosses are for InTl alloys. In placing the points on the figure we have neglected the variations in Coulomb cutoff from case to case. This is not expected to be a large effect and could be corrected for.

III. THE RATIO $2\Delta_0/k_BT_c$

Equations (5) and (6) can also be solved at the critical temperature $\overline{T}_c$ in which case they can be linearized. When this is done and combined with the results of the previous section we can obtain the ratio $2\Delta_0/k_BT_c$ for our δ-function model. In Fig. 3 we present results for the case of $\mu^*=0.2267$ with $A=10.65$ meV. In Fig. 3(a) the results are plotted vs Ω_E while in (3b) we use

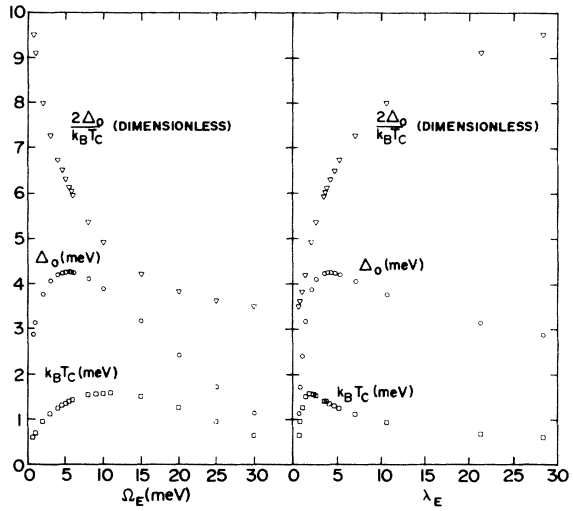

FIG. 3. For the case $\mu^*=0.2267$, $A=10.652$ meV we show the variation of the gap Δ_0, the critical temperature, and the ratio $2\Delta_0/k_BT_c$ as a function of Ω_E (a) and of $\lambda_E=2A/\Omega_E$ (b). A δ-function spectrum $\alpha^2F(\Omega)=A\delta(\Omega-\Omega_E)$ was used. Note that both Δ_0 and k_BT_c show clear maxima in the Ω region considered. This is not so for $2\Delta_0/k_BT_c$ which is still rising at the lowest frequency considered, namely $\Omega_E=0.75$ meV. When plotted against λ_E rather than Ω_E the same data show more of a tendency to level off.

$\lambda_E = 2A/\Omega_E = 2/\bar{\Omega}_E$. Also, shown for comparison are our results for T_c and for Δ_0 separately. The range of Ω_E considered has now been greatly expanded and spans the interval (30 to 0.75 meV). At the lower energy end $2\Delta_0/k_BT_c$ has reached a value of 9.5. This corresponds, of course, to a very unphysical situation in that $\Omega_E = 0.75$ meV means the the entire spectral weight would need to occur around 8 K. This will never be the case in real materials. For this reason we did not think it essential to proceed further with the numerical calculation. Our general Eliashberg programs were showing signs of numerical difficulties as the calculations cease to converge adequately. Instead of writing new programs to specially handle this region, we decided to examine analytically the limit $\Omega_E \to 0$. Before doing so, however, it is important to emphasize that we still have not reached a maximum for $2\Delta_0/k_BT_c$ although consideration of Fig. 3(b) indicates that we may not be far off.

The functional derivatives of $2\Delta_0/k_BT_c$ with $\alpha^2F(\omega)$ calculated by Mitrović *et al.*[6] show a sharp peak about $\Omega_E \cong \frac{4}{3}k_BT_c$. For the specific case $\Omega_E = 0.75$ the k_BT_c value was 0.6 meV. This means that we expect the functional derivative to peak around 0.8 meV. This is a further indication that we should be near the peak.

We now turn to an analytic proof that for $\Omega_E \to 0$, the ratio $2\Delta_0/k_BT_c$ must reach a finite value which we estimate to be approximately 7 in Sec. IV. While this last number is only a rough estimate it indicates again that the curve in Fig. 3(a) for $2\Delta_0/k_BT_c$ will need to peak in the interval $\Omega_E = (0.75$ meV to 10 meV) and then fall to a value below 9.5.

For convenience, only the case $\mu^* = 0$ will be considered. A finite μ^* can be introduced and the theorem will still remain approximately true since we need only neglect the effect of small changes in the Coulomb cutoff just as we have done in Sec. II. We will now show that for $\Omega_E \to 0$ the zero-temperature gap edge and the critical temperature both scale like $(A\Omega_E)^{1/2}$. This means that the ratio $2\Delta_0/k_BT_c$ will go towards a finite universal number. Substitution of Eq. (1) into (2), so as to eliminate the renormalization function Z, leads, after some rearrangement, to the single equation

$$\Delta(i\omega_n) = \pi k_BT \sum_{m\,(\neq n)} \lambda(m-n) \times \left[\frac{\Delta(i\omega_m) - (\omega_m/\omega_n)\Delta(i\omega_n)}{[(\omega_m^2 + \Delta^2(i\omega_m)]^{1/2}} \right], \tag{12}$$

where we have noted that the term $m \neq n$ does not enter the sum on the right-hand side of this last equation because for $n = m$ the quantity in large parentheses is zero. For $m \neq n$ and in the limit $\Omega_E \to 0$, the expression for $\lambda(m-n)$ reduces to

$$\lambda(m-n) = \frac{2\Omega_E A}{(\omega_n - \omega_m)^2} . \tag{13}$$

In arriving at this last result we are assuming that $\Omega_E \ll T$ (the temperature of interest). Note, from the form of Eq. (12), that $\Delta(i\omega_n)$ is an explicit function of T and also of $i\omega_n$ which, of course, contains another factor of temperature. To make these dependences explicit we will write $\Delta(T, i\omega_n)$ instead of the shorter notation $\Delta(i\omega_n)$. If both sides of Eq. (12) are divided by $(A\omega_E)^{1/2}$ and T is changed to T' through the transformation $T/(A\Omega_E)^{1/2} = T'$, we obtain a new equation which makes no explicit reference to material parameters. Writing

$$\bar{\Delta}(T', i\omega_n') \equiv \frac{\Delta[T'(A\Omega_E)^{1/2}, i\omega_n'(A\Omega_E)^{1/2}]}{(A\Omega_E)^{1/2}}$$

we obtain

$$\bar{\Delta}(T', i\omega_n') = \pi k_BT' \sum_{m\neq n} \frac{2}{(\omega_n' - \omega_m')^2} \times \left[\frac{\bar{\Delta}(T', i\omega_m') - \dfrac{\omega_m'}{\omega_n'}\bar{\Delta}(T', i\omega_n')}{[\omega_m'^2 + \bar{\Delta}(T', i\omega_m')^2]^{1/2}} \right], \tag{14}$$

where ω_n' denotes the Matsurbara frequency $T'\pi(2n-1)$. It is clear that the solution of the last equation depends in no way on ω_E and A and is therefore independent of any particular system. Solving this equation for $T' \to 0$ and performing an analytic continuation to the real ω' axis by setting $i\omega_n' \to \omega'$ leads to a function $\bar{\Delta}(\omega')$ independent of any material. It is related to $\Delta(T, \omega)$, the analytic continuation of $\Delta(T, i\omega_n)$, by

$$\Delta[T'(A\Omega_E)^{1/2}, \omega'(A\Omega_E)] = (A\Omega_E)^{1/2}\bar{\Delta}(T', \omega') . \tag{15}$$

Taking the limit of very small T' we find the gap edge Δ_0 from the equation

$$\Delta_0 = \mathrm{Re}\Delta(0, \Delta_0) = (A\Omega_E)^{1/2}\mathrm{Re}\bar{\Delta}\left[0, \frac{\Delta_0}{(\Omega_E A)^{1/2}}\right] . \tag{16}$$

or

$$\bar{\Delta}_0 = \mathrm{Re}\bar{\Delta}(0, \bar{\Delta}_0) \tag{17}$$

with $\bar{\Delta}_0 \equiv \Delta_0/(A\Omega_E)^{1/2}$. But $\bar{\Delta}_0$, the solution of Eq. (17), is a universal number which we denote by d, so that $\Delta_0 = d(A\Omega_E)^{1/2}$.

To get the critical temperature associated with Eq. (14) the equation needs to be linearized. From its form, it is clear that T_c' will be another universal number independent of all material parameters. Denote it by d' and hence $k_BT_c = d'(A\Omega_E)^{1/2}$. Therefore the ratio

$$\frac{2\Delta_0}{k_BT_c} = \frac{2d}{d'} \quad (\Omega_E \to 0) \tag{18}$$

is a universal finite number in the limit $\Omega_E \to 0$. This is what we wished to demonstrate. It is of interest to make a rough estimate of this limiting value of the gap to critical temperature ratio. We next turn to this problem.

IV. ROUGH ESTIMATE OF $2\Delta_0/k_BT_c$ FOR $\Omega_E \to 0$

We limit ourselves to the case $\mu^* = 0$ so as to keep the algebra as simple as possible. The generalization to finite

μ^* is straightforward but adds little to our discussion. We go back to Eqs. (1) and (2) and take the zero-temperature limit to get

$$Z(\omega)\Delta(\omega)=\tfrac{1}{2}\int_{-\infty}^{+\infty}d\omega'\frac{2\Omega_E A}{\Omega_E^2+(\omega-\omega')^2}\times\frac{\Delta(\omega')}{[(\omega')^2+\Delta^2(\omega')]^{1/2}} \tag{19}$$

and

$$Z(\omega)=1+\frac{1}{2\omega}\int_{-\infty}^{+\infty}d\omega'\frac{2\Omega_E A}{\Omega_E^2+(\omega-\omega')^2}\times\frac{\omega'}{[(\omega')^2+\Delta^2(\omega')]^{1/2}}\ . \tag{20}$$

In the previous section we established that for $\Omega_E\to 0$, Δ_0 and T_c are both proportional to $\sqrt{A\Omega_E}$. This means that Δ_0 will be much greater than the position of Ω_E so that we expect $\Delta(\omega)$ to be near Δ_0 up to $\omega=\Delta_0$ with phonon structure occurring in a very small range $\sim\Omega_E$ just above this value. This suggests a model for the gap

$$\Delta(\omega)=\begin{cases}\Delta_0 & \text{for } \omega<\Delta_0\\ 0 & \text{for } \omega>\Delta_0\ .\end{cases} \tag{21}$$

First, we treat the renormalization function which is only of interest for small ω. In this case

$$Z(\omega\to 0)=1+\int_{-\infty}^{+\infty}d\omega'\frac{\Omega_E A}{[\Omega_E^2+(\omega')^2]^2}\times\frac{2(\omega')^2}{[(\omega')^2+\Delta^2(\omega')]^{1/2}}\ . \tag{22}$$

Substitution of (21) into (22) leads to

$$Z(\omega\to 0)=1+2\Omega_E A\left[2I(\Omega_E,\Delta_0)+\frac{1}{\Delta_0^2+\Omega_E^2}\right] \tag{23}$$

with

$$I(\Omega_E,\Delta_0)=\int_0^{\Delta_0}d\omega'\frac{\omega'^2}{(\omega'^2+\Delta_0^2)^{1/2}}\frac{1}{(\Omega_E^2+\omega'^2)^2}\cong\frac{\pi}{4}\left[\frac{\Delta_0}{\Omega_E}\right]\frac{1}{\Delta_0^2}\left[1-\frac{4}{\pi}\sqrt{2}\frac{\Omega_E}{\Delta_0}\right] \tag{24}$$

so that

$$Z(\omega\sim 0)=1+\frac{\pi A}{\Delta_0}-\frac{4A\Omega_E}{\Delta_0^2}(\sqrt{2}-\tfrac{1}{2})\ . \tag{25}$$

Next we consider the gap equation (19) and substitute into it our ansatz (21) for the gap to get for $\omega<\Delta_0$

$$Z(\omega\sim 0)=2\Omega_E A J(\Omega_E,\Delta_0) \tag{26}$$

with

$$J(\Omega_E,\Delta_0)=\int_0^{\Delta_0}\frac{d\omega'}{(\Delta_0^2+\omega'^2)^{1/2}}\frac{1}{\Omega_E^2+\omega'^2}\cong\frac{\pi}{2\Omega_E\Delta_0}\left[1-\frac{2\sqrt{2}}{\pi}\frac{\Omega_E}{\Delta_0}\right]\ . \tag{27}$$

Combining (25) with (26) leads to

$$1+\frac{\pi A}{\Delta_0}-\frac{4A\Omega_E}{\Delta_0^2}(\sqrt{2}-\tfrac{1}{2})=\frac{\pi A}{\Delta_0}-2\sqrt{2}\frac{A\Omega_E}{\Delta_0^2}\ . \tag{28}$$

Note that the term $\pi A/\Delta_0$ cancels out of each side of this equation and that after rearrangement

$$\Delta_0=(A\Omega_E)^{1/2}[2(\sqrt{2}-1)]^{1/2}\cong 0.91(A\Omega_E)^{1/2}\ . \tag{29}$$

The solution for T_c in the limit $\Omega_E\to 0$ has already been obtained by Allen and Dynes[3] [their Eq. (24)] and is

$$T_c=0.18\sqrt{2}\sqrt{A\Omega_E}\ , \tag{30}$$

which yields a value for $2\Delta_0/k_BT_c$ of approximately 7.

A final point should be made. In our formal proof that T_c and Δ_0 both scale like $(A\Omega_E)^{1/2}$ we immediately dropped the Ω_E^2 factor in the denominator of $\lambda(n-m)$ while in this section we retain it. To understand why this is necessary it is important to realize that in Eq. (12) the $n\neq m$ term does not enter because the equation for Z has been substituted into that for Δ and the term involving

$$\lambda=2\int\frac{\alpha^2F(\Omega)}{\Omega}d\Omega$$

never enters. This is not so when both equations are treated separately. However, the term in $I(\Omega_E\Delta_0)$ in Eq. (24) that depends on Ω_E leads to the term $\pi A/\Delta_0$ in Z which was noted to cancel out of the final equation (28) against the term dependent on Ω_E coming from $J(\Omega_E,\Delta)$ [Eq. (27)]. These were the only terms which entered as a result of retaining the Ω_E^2 factor in this section.

V. CONCLUSIONS

We have established a new upper bound on the gap value for any electron-phonon superconductor characterized by an electron-phonon spectral density $\alpha^2F(\Omega)$ and Coulomb repulsion parameter μ^*. It is shown under certain assumptions that $\Delta_0\le b(\mu^*)A$ where A is the area under $\alpha^2F(\omega)$—a parameter first emphasized by Leavens and Carbotte. Values for $b(\mu^*)$ are given in Table I and depend only on the structure of the Eliashberg equations and not on any material parameter. The maximum value for $2\Delta_0/k_BT_c$ was found to be greater than 9.5 which occurs for the case of a very unrealistic spectrum, namely a δ function at $\Omega_E=0.75$ meV with $A=10.652$ meV and $\mu^*=0.2267$. While it is expected to rise even further as Ω_E is reduced, arguments are given that we are near maximum and that for $\Omega_E\to 0$ the ratio will drop to about 7. While this number is a rough estimate based on approximate analytic solutions of the Eliashberg equations for $\Omega_E\to 0$, it was shown quite generally that both Δ_0 and T_c scale like $\sqrt{\Omega_E A}$ in this region. This implies a finite limit for this ratio.

ACKNOWLEDGEMENT

This research was supported in part by the Natural Sciences and Engineering Research Council (NSERO) of Canada.

[1]C. R. Leavens and J. P. Carbotte, J. Low Temp. Phys. **14**, 195 (1974).
[2]W. L. McMillan, Phys. Rev. **167**, 331 (1968).
[3]P. B. Allen and R. C. Dynes, Phys. Rev. B **12**, 905 (1975).
[4]C. R. Leavens, Solid State Commun. **17**, 1499 (1975).
[5]C. Bergmann and D. Rainer, Z. Phys. **263**, 59 (1973).
[6]B. Mitrović, C. R. Leavens, and J. P. Carbotte, Phys. Rev. B **21**, 5048 (1980).
[7]J. M. Daams and J. P. Carbotte, J. Low Temp. Phys. **43**, 263 (1981).
[8]B. Mitrović, H. G. Zarate, and J. P. Carbotte, Phys. Rev. B **29**, 184 (1984).
[9]L. Y. L. Shen, Phys. Rev. Lett. **24**, 1104 (1970); **29**, 1082 (1972).
[10]R. Baquero and J. P. Carbotte, J. Low Temp. Phys. **51**, 135 (1983).
[11]J. M. Daams, J. P. Carbotte, M. Ashraf, and R. Baquero, J. Low Temp. Phys. **55**, 1 (1984).
[12]B. Mitrović, E. Schachinger, and J. P. Carbotte, Phys. Rev. B **29**, 6187 (1984).