Asymptotic limit for the thermodynamics of a boson-exchange superconductor

F. Marsiglio,* P. J. Williams, and J. P. Carbotte
Physics Department, McMaster University, Hamilton, Ontario, Canada L8S 4M1
(Received 28 September 1988)

We establish formulas for the free-energy difference (ΔF) between the superconducting and normal states of an Eliashberg superconductor valid in the asymptotic limit $\lambda \rightarrow \infty$ where λ is the mass-renormalization parameter. It is shown that (ΔF) varies as $\lambda\omega_E^2$ times a universal function of the reduced temperature $t = T/T_c$. Here ω_E is the characteristic energy of the exchanged boson. The universal function is calculated numerically for finite $t>0$.

Stimulated by the discovery of superconductivity in the oxides[1] with values of the critical temperature T_c now as high as 125 K, Marsiglio, Akis, and Carbotte[2] considered the thermodynamics and other properties of an Eliashberg superconductor for values of T_c comparable in size or greater than the characteristic boson energy $\omega_{\ln}$. The parameter $\omega_{\ln}$ was first introduced by Allen and Dynes[3] and is well defined in terms of the electron-boson spectral density $\alpha^2F(\omega)$ which enters the kernels of the Eliashberg equations. In their work, Marsiglio, Akis, and Carbotte[2] carry out calculations somewhat beyond $T_c/\omega_{\ln}=1$. This corresponds to large cases, as compared with conventional cases, but still quite finite values of λ. Here we wish to consider the limit of $\lambda \rightarrow \infty$. While this regime is not likely to ever be reached in real materials, it gives particularly simple results which can help in understanding the large but finite λ region.

The work starts from the Eliashberg equations in the Matsubara representation[4,5] for the gap $\Delta(i\omega_n)$ and renormalization $Z(i\omega_n)$ at the Matsubara frequencies $i\omega_n = i\pi T(2n-1), n=0, \pm 1, \pm 2, \ldots$, with T the temperature. They are

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

and

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

where, for convenience, we have ignored the Coulomb pseudopotential μ^* and where $\lambda(m-n)$ contains the information on the spectral density $\alpha^2F(\omega)$ for boson exchange. While the form of Eqs. (1) and (2) were first derived for the electron-phonon interaction, they can still be used for the exchange of other more exotic low-energy bosons which restrict the Cooper-pair scattering to the Fermi surface. Thus, our asymptotic limit will be approximately valid in such cases as well. In terms of $\alpha^2F(\omega)$, we have

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

If we use for $\alpha^2F(\omega)$ a δ function centered at the Einstein energy ω_E and of weight A, we obtain

$$\lambda(m-n) = \frac{2\omega_E A}{\omega_E^2 + (\omega_n - \omega_m)^2}. \quad (4)$$

For $m=n$, the quantity given in Eq. (4) reduces to the electron-boson mass-renormalization factor $\lambda = 2A/\omega_E$. Here we will be interested only in the limit $\lambda \rightarrow \infty$ which can be achieved in many ways. For example, A can be fixed and ω_E taken to go to zero (as we do in our numerical work). Alternatively, ω_E can be fixed and A taken to infinity. Both alternatives are equivalent mathematically. In the limit $\lambda \rightarrow \infty$, it is justified to neglet the ω_E^2 term in the denominator of Eq. (4) for $n \neq m$, provided it is assumed that $\omega_E \ll 2\pi T$. We will return to this condition later when it will be fully explained. For the moment, we proceed. On substituting Eq. (2) into Eq. (1) to get a closed equation for the gap, we note that a term of the form

$$\pi T \lambda(0) \frac{\Delta(i\omega_n)}{[\omega_n^2 + \Delta^2(i\omega_n)]^{1/2}}$$

will occur on both right- and left-hand sides, and therefore cancel. Thus only terms with $m \neq n$ will remain in the single equation for the gap. Referring to Eq. (4) with $n \neq m$, neglecting ω_E^2 in the denominator, and dividing by $\sqrt{A\omega_E}$ we get a material-independent equation for the dimensionless gap $\bar{\Delta}(i\bar{\omega}_n)$:

$$\bar{\Delta}(i\bar{\omega}_n) = \pi t \bar{T}_c \sum_{m \neq n} \frac{2}{(\omega_m - \omega_n)^2} \times \left[\frac{\bar{\Delta}(i\omega_m) - (\bar{\omega}_m/\bar{\omega}_n)\bar{\Delta}(i\bar{\omega}_n)}{[\bar{\omega}_m^2 + \bar{\Delta}^2(i\bar{\omega}_m)]^{1/2}} \right], \quad (5)$$

where any $\bar{Q} = Q/\sqrt{A\omega_E}$ and the reduced temperature $t \equiv T/T_c$. On examination of Eq. (5), we see that all references to material parameters have dropped out so that $\bar{\Delta}(i\bar{\omega}_n)$ is simply a universal function ($f_n(t)$) of the reduced temperature t, i.e., $\bar{\Delta}(i\bar{\omega}_n) = f_n(t)$. In particular, iteration of the linearized version of (5) yields the critical temperature $\bar{T}_c = 0.2584$ which is a universal number first given by Allen and Dynes.[3] Thus, in the asymptotic limit the critical temperature is

$$T_c = 0.2584\sqrt{A\omega_E} = 0.183\omega_E\sqrt{\lambda}\,. \tag{6}$$

To calculate the thermodynamics in the asymptotic limit, we need to know the free-energy difference between superconducting and normal state $\Delta F(t)$, which is given in terms of the Δ's and Z's by the Bardeen-Stephen[6] formula

$$\frac{\Delta F}{N(0)} = -2\pi T \sum_{n=1}^{\infty} \omega_n \left[Z^S(i\omega_n) - \frac{Z^N(i\omega_n)}{[1+\Delta^2(i\omega_n)/\omega_n^2]^{1/2}} \right] \times \left[\left(1 + \frac{\Delta^2(i\omega_n)}{\omega_n^2} \right)^{1/2} - 1 \right], \tag{7}$$

where $N(0)$ is the single-spin electronic density of states at the Fermi energy. From Eq. (5), it is clear that the square-root factor in (7) is independent of λ as it depends only on $\bar{\Delta}(i\bar{\omega}_n)$. Further, the superconducting-state renormalization factor can be written as

$$Z^S(i\omega_n) = 1 + \frac{\pi \bar{T}}{[\bar{\omega}_n^2 + \bar{\Delta}^2(i\bar{\omega}_n)]^{1/2}}\lambda + \frac{\pi \bar{T}}{\bar{\omega}_n} \sum_{m \neq n} \frac{2}{(\bar{\omega}_m - \bar{\omega}_n)^2} \frac{\bar{\omega}_m}{[\bar{\omega}_m^2 + \bar{\Delta}^2(i\bar{\omega}_m)]^{1/2}}, \tag{8}$$

and its normal-state value Z^N is obtained from Eq. (8) by setting $\bar{\Delta}(i\bar{\omega}_m)$ equal to zero in the last two terms on the right-hand side. We note that for both Z^N and Z^S, the second term depends on λ and hence on material parameters, but the last term does not since $\bar{\Delta}(i\bar{\omega}_m)$ is universal. On inserting Eq. (8) into Eq. (7), it is clear that the λ dependence in Z^S and Z^N cancels so that the expression in the large parentheses is material independent, leaving us with a free energy that scales similar to T_c^2 because of the presence of an overall factor of T^2; and so[7]

$$\frac{\Delta F}{N(0)} = \frac{A^2}{\lambda} g(t) \equiv \tfrac{1}{4}\lambda \omega_E^2 g(t)\,, \tag{9}$$

where $g(t)$ is a universal function of reduced temperature T/T_c. This function, which is independent of material parameters, can be calculated from the universal equation (5) for $\bar{\Delta}(i\bar{\omega}_m)$ and from the free-energy difference (7) noting that λ, which still appears explicitly in both Z^S and Z^N, cancels in the combination needed in formula (7).

The thermodynamic critical magnetic field $H_c(T)$ follows from $\Delta F(T)$ as does the specific-heat difference $\Delta C(T)$. Thermodynamics yields

$$H_c(T) = \sqrt{8\pi \Delta F} \text{ and } \Delta C(T) = T\frac{d^2 F}{dT^2}\,. \tag{10}$$

Direct calculation of $g(t)$ as a function of reduced temperature yields $H_c(t)$ and $\Delta C(t)$. The results of our numerical calculations are given in Fig. 1. Instead of $g(t)$ itself, we have chosen to plot $h_c(t)$ (the reduced thermodynamic critical magnetic field) defined by

$$h_c(t) = \frac{H_c(t)}{|dH_c(t)/dt|_{t=1}} = \frac{\sqrt{g(t)}}{|[d\sqrt{g(t)}/dt]_{t=1}|}, \tag{11}$$

which is simply $\sqrt{g(t)}$ normalized to its slope at $t=1$, i.e.,

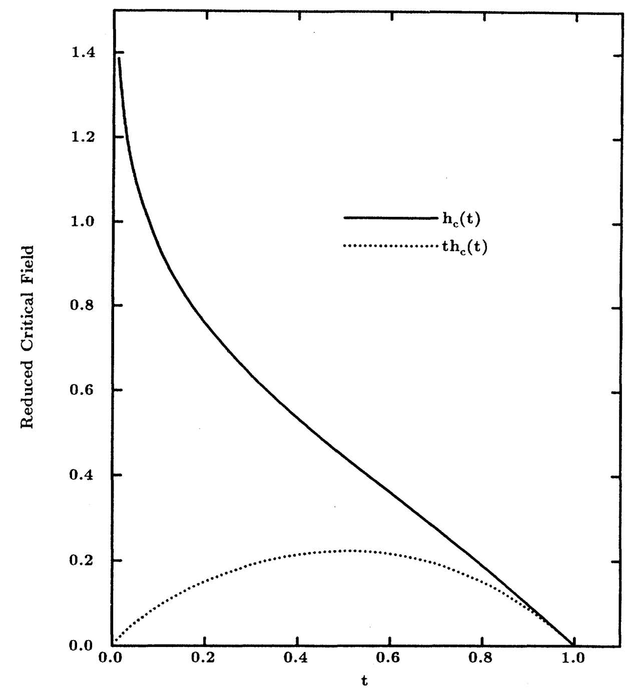

FIG. 1. The reduced critical thermodynamic magnetic field (solid curve) as a function of reduced temperature t in the limit $\lambda \to \infty$. The curve has pronounced positive curvature with the zero-temperature value unclear. The dotted curve is t times the reduced field $h_c(t)$ and shows a finite limit at $t \to 0$.

$T = T_c$. From the solid curve of Fig. 1, it is clear that in the asymptotic limit the reduced critical field looks very different from its value in BCS theory. For example, within BCS, the $h_c(t)$ curve has negative curvature at all temperatures and at $t=0$ $h_c(0)=0.576$. In contrast, in the asymptotic limit $h_c(t)$ exhibits a large region of near linear dependence below $t=1$ and then shows the opposite curvature bending upward as t decreases. It is still rising rapidly at $t=0.008$. This is the lowest reduced temperature we could handle in our numerical work due to computer time limitations. Consequently, we do not have information on its zero-temperature behavior. To understand that this is not a serious limitation, we return to the condition $\omega_E \ll 2\pi T$ introduced from the very beginning into our formalism. It can easily be changed, with the help of Eq. (6) for T_c valid in the asymptotic limit, into an inequality

$$\sqrt{\lambda} t \gg 1\,, \tag{12}$$

which is central to our work. We see now that for any fixed finite value of t, λ must be taken large enough so that Eq. (12) holds in order that the approximation $\omega_E \ll 2\pi T$ be valid. Recalling that

$$H_c(t) = \sqrt{2\pi N(0)\lambda}\,\omega_E \sqrt{g(t)} = \sqrt{2\pi N(0)\lambda}\,\omega_E \left| \left(\frac{d\sqrt{g(t)}}{dt} \right)_{t=1} \right| h_c(t)\,, \tag{13}$$

we rewrite it in the form

$$H_c(t)=\sqrt{2\pi N(0)}\lambda\left\{\frac{1}{\sqrt{\lambda t}}[th_c(t)]\right\}\left|\left(\frac{d\sqrt{g(t)}}{dt}\right)_{t=1}\right|\omega_E\,. \tag{14}$$

We see that condition (12) requires $1/\sqrt{\lambda t}\ll 1$. Also, we note that $th_c(t)$ shown in Fig. 1 (dotted curve) is well behaved even for $t\to 0$. Thus, the expression in the brackets of Eq. (14) is also well behaved in the range $\sqrt{\lambda t}\gg 1$. What we need to remember is that λ must go to ∞ before t goes to zero for the condition $\sqrt{\lambda t}\gg 1$ to be satisfied.

Our results for $h_c(t)$ or $th_c(t)$ cover the entire temperature dependence of the free-energy difference, and so the specific heat should follow as well [formula (10)]. Evaluation of the jump in $\Delta C(T)$ at T_c and its slope give, respectively,

$$\frac{\Delta C(T_c)}{\gamma(0)T_c}=\frac{19.9}{\lambda} \tag{15}$$

and

$$\frac{d}{dt}\left[\frac{\Delta C(T_c)}{\gamma(0)T_c}\right]_{t=1}=\frac{39.2}{\lambda}\,. \tag{16}$$

Rough estimates of the two universal numbers appearing above using a single Matsubara gap approximation yield 12 and 84, respectively, instead of 19.9 and 39.2. The values of jump and slope given by (15) and (16) cannot be compared directly with the universal BCS values of 1.43 and 3.77, respectively. BCS theory is the weak-coupling case which is the opposite limit to that considered here. It is clear, however, that for large λ's, both quantities fall below BCS values. This behavior, which can be taken to be a signature of the asymptotic limit, is very different from the conventional strong-coupling case for which the corrections to BCS theory tend to increase these coefficients over the BCS value. More specifically Marsiglio and Carbotte[8] find

$$\frac{\Delta C(T_c)}{\gamma(0)T_c}=1.43\left[1+53\left(\frac{T_c}{\omega_{\ln}}\right)^2\ln\left(\frac{\omega_{\ln}}{3T_c}\right)\right] \tag{17}$$

and

$$\frac{d}{dt}\left[\frac{\Delta C(T_c)}{\gamma(0)T_c}\right]=3.77\left[1+117\left(\frac{T_c}{\omega_{\ln}}\right)^2\ln\left(\frac{\omega_{\ln}}{2.9T_c}\right)\right], \tag{18}$$

where $T_c/\omega_{\ln}$ is the characteristic strong-coupling parameter and $\omega_{\ln}$ is the average boson energy of Allen and Dynes which is given by

$$\omega_{\ln}=\exp\left[+\frac{2}{\lambda}\int_0^\infty\frac{\alpha^2F(\omega)\ln(\omega)}{\omega}d\omega\right]. \tag{19}$$

Equations (17) and (18) apply only for $T_c/\omega_{\ln}\lesssim 0.25$.

While both the normalized jump and slope go to zero as $\lambda\to\infty$ their ratio remains constant. It is equal to 1.96, which is to be compared with a BCS value of 2.64. For conventional superconductors, it is found to be somewhat greater.

In conclusion, we have calculated the free-energy difference between normal and superconducting states at any finite reduced temperature t in the asymptotic limit $\lambda\to\infty$. The free energy is found to scale similar to $\lambda\omega_E^2$ times a universal function of t which is independent of any material parameter and which we have calculated numerically. The formula obtained holds only for $\sqrt{\lambda t}\gg 1$ so that very large values of λ are needed if the low-temperature region is to be investigated. Our calculations are based on equations that are independent of λ and therefore, universal. The normalized jump and slope at T_c of the specific heat were also computed and found to be proportional to $1/\lambda$ with material independent constants of proportionality. While the asymptotic limit is not likely to be reached in real systems, it nevertheless gives information on how a very-strong-coupling superconductor is likely to behave.

This research was supported in part by the Natural Sciences and Engineering Research Council of Canada (NSERC). J.P.C. is also supported by the Canadian Institute for Advanced Research (CIAR).

*Present address: University of California at San Diego, La Jolla, CA 92093.

[1]See, for example, *Novel Superconductivity*, edited by S. A. Wolf and V. Z. Kresin (Plenum, New York, 1987).
[2]F. Marsiglio, R. Akis, and J. P. Carbotte, Phys. Rev. B **36**, 5245 (1987).
[3]P. B. Allen and R. C. Dynes, Phys. Rev. B **12**, 905 (1975).
[4]J. M. Daams and J. P. Carbotte, J. Low Temp. Phys. **43**, 263 (1981).
[5]D. Rainer and G. Bergmann, J. Low Temp. Phys. **14**, 50 (1974).
[6]J. Bardeen and M. Stephen, Phys. Rev. **136**, A1485 (1964).
[7]L. N. Bulaevskii, O. V. Dolgov, and M. O. Ptitsyn, Phys. Rev. B **38**, 11290 (1988).
[8]F. Marsiglio and J. P. Carbotte, Phys. Rev. B **33**, 6141 (1986).