Formula for the Critical Temperature of Superconductors Based on the Electronic Density of States and the Effective Mass

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A formula for the superconducting transition temperature T_c is developed by comparing the total condensation energy contained within the coherence volume of a Cooper pair to the number of electronic states at the Fermi surface within the same coherence volume. It is found that T_c is proportional to the ratio of the condensation energy density and normal state charge carrier density. We find that this relation holds for over 2 orders of magnitude in temperature for numerous well-known superconducting compounds belonging to distinctly different classes.

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It has been suggested for some time that a new paradigm beyond that of the (enormously successful) BCS theory [1] is needed in order to advance our understanding of the phenomenon of superconductivity, particularly in the high-T_c cuprate superconductors. It would be ideal, should a new theory emerge, for this new perspective to be able to account for both the BCS-Eliashberg case [2] under well-defined conditions, as well as the mechanistic description of non-BCS superconductivity. In addition to providing an understanding of the physical mechanism responsible for superconductivity, one of the primary tests of any theory of superconductivity is its ability to accurately predict the critical temperature T_c below which the material enters the superconducting state. We present here an expression for the critical temperature, T_c, in terms of basic electronic and physical properties, providing insight into how fundamental properties of superconductors are interrelated. We find that $T_c \sim (1/n_n)H_c^2(0)$, where n_n is the normal state carrier density and $H_c(0)$ is the $(T = 0)$ thermodynamic critical field. By using data from the literature, we demonstrate that this relation holds for over 2 orders of magnitude in temperature for numerous well known superconducting compounds belonging to distinctly different classes. Being that no mechanism is invoked, this expression can be used generally as a potentially powerful tool by which to investigate the basic properties of superconductivity in a compound or system as the critical temperature evolves upon variation of a given parameter.

Recently [3], we arrived at a universal expression for the superconducting critical temperature, T_c, in terms of the $T = 0$ values of the penetration depth, λ_0, the superconducting coherence length, ξ_0, the anisotropy parameter, ϵ, and a characteristic parameter $\mathbb{C}_L$ which represents the fraction of the condensation energy, $H_c(0)^2/2\mu_0$, within a superconducting coherence volume that is associated with the binding of a Cooper pair. Using the Ginzburg Landau (GL) expression for the thermodynamic critical field $H_c(0)$, given by $H_c(0) = \Phi_0/2\sqrt{2}\pi\lambda_0\xi_0$ [4], it was found that

$$T_c = \frac{\mathbb{C}_L}{4\sqrt{2}\pi}\left[\frac{\Phi_0^2}{\mu_0 k_B}\right]\frac{\epsilon\xi_0}{\lambda_0^2}. \quad (1)$$

Equation (1) was arrived at in Ref. [3] by considering the $T \rightarrow 0$ limit of two related expressions for the vortex glass melting line, $H_g(T)$, and shown to hold for numerous high-T_c superconducting compounds. The expression for $\mathbb{C}_L$ found in Ref. [3] involves the Lindemann number, c_L, and an exponent, α, which characterizes the temperature dependence of $H_g(T)$. In this communication, we develop an expression for $\mathbb{C}_L$ that is independent of the nature of the vortex glass melting line. Subsequently, we arrive at an expression for T_c that is independent of the geometry of the Cooper pair coherence volume.

It was shown in Ref. [3] that the expression given in Eq. (1) above follows from the relation

$$k_B T_c = \mathbb{C}_L \frac{H_c^2}{2\mu_0} V_{\mathrm{coh}}. \quad (2)$$

where $\mathbb{C}_L$ is defined by $\mathbb{C}_L \equiv 8\pi\sqrt{2}(\pi^2 c_L^4)^\alpha$, $V_{\mathrm{coh}} \equiv V_\Phi = 2\sqrt{2}\pi\epsilon\xi_0^3$, and the definition of the geometry of V_Φ is based upon the structure of the core of a superconducting vortex flux line in which the superconducting order parameter is suppressed to zero.

As mentioned above, the value of $\mathbb{C}_L$ can be viewed as representing the fraction of the condensation energy within a given volume that is used in forming a single Cooper pair, or equivalently, it is the ratio of the energy density of a single Cooper pair (defined by its coherence volume) to the condensation energy density. Similar to this view, we could instead choose to count the number of one-electron states at the Fermi energy (for one direction of spin) contained in the coherence volume, V_Φ, with respect to the number used in the formation of the Cooper pair (2 electrons). In the simplest (flat band) approximation, this definition is then,

$$\mathbb{C}_L \equiv \frac{2}{N(0)E_F V_\Phi} = \frac{8}{3n_n V_\Phi} \tag{3}$$

where $N(0) = m^{*2}v_F/2\pi^2\hbar^3$ is the density of states at the Fermi level for a free electron gas, $E_F = m^* v_F^2/2$ is the Fermi energy, $n_n = \frac{k_F^3}{3\pi^2} = \frac{1}{3\pi^2}(\frac{m^* v_F}{\hbar})^3$ is the normal state carrier density, (m^* is the electron effective mass, and v_F is the Fermi velocity) [4].

We next define the effective penetration depth as, $\lambda_{\rm eff}(0) \equiv \lambda_L(0)/\sqrt{4\pi}$, where $\lambda_L(0)$ is the London penetration depth, given by $\lambda_L^2(0) = m_s^*/(\mu_0 n_s e^2)$ (in mks units) with n_s the superconducting carrier density and m_s^* the charge carrier effective mass in the superconducting state. The factor of $1/\sqrt{4\pi}$ was chosen as it was found to bring the measured values of T_c into close agreement with the T_c's expected from Eq. (4) below, *and was used for all data* in Fig. 1. We note that our definition of $\lambda_{\rm eff}(0)$ is a factor of $\sqrt{\pi}$ larger than that defined in Ref. [5], where the (effective) London penetration depth (as a function of doping concentration, p), is defined as $\lambda_L(p) \equiv 1/2\pi\omega_{ps}$, with $\omega_{ps} = \sqrt{\mu_0 n_s e^2/m^*}$. We further note that, as this approach to the definition of $\lambda_{\rm eff}(0)$ is heuristic in nature, we could have left the factor of $1/\sqrt{4\pi}$ (or $\sqrt{\pi}$) as a constant in Eq. (4) below to be determined by experiment. In this vein we have indicated in Fig. 1 by the dashed line the resulting shift of the data if we were to use the latter definition of the effective penetration depth given in Ref. [5] without any further adjustment. By inserting the above expression for

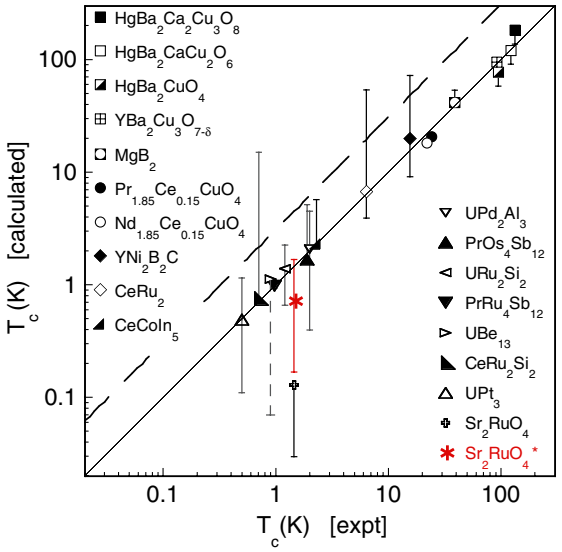

FIG. 1 (color online). Plot of the values of the superconducting critical temperature, T_c, calculated using the expression given in Eq. (4) vs the experimentally determined values of T_c. See Table (I) of the supplementary material for experimental values of the parameters used to calculate T_c and the references from which they are taken. See the text for an explanation of the meaning and determination of the error bars shown, the meaning of the long dashed line, and for discussion on the two shown calculated values of T_c for Sr_2RuO_4.

$\lambda_{\rm eff}(0)$ and Eq. (3) into Eq. (2) we arrive at,

$$T_c = \frac{2\pi}{3k_B}\left[\frac{n_s}{n_n}\right]\left(\frac{\hbar}{\xi_0}\right)^2 \frac{1}{m_s^*}, \tag{4}$$

which is *independent* of the geometrical definition of the Cooper pair coherence volume, $V_{\rm coh}$. For simplicity, at this time, we do not distinguish between the clean and dirty limit cases. Note also that since $\epsilon \equiv (m_{ab}^*/m_c^*)^{1/2} = \xi_c/\xi_{ab}$, then $m_{ab}^*\xi_{ab}^2 = m_c^*\xi_c^2$, so that Eq. (4) is invariant in the case of anisotropic materials.

From Eq. (4) we find a simple relationship between the superconducting critical temperature T_c and the upper critical field (of type-II superconductors) at $T = 0$, $H_{c2}(0)$, given by $H_{c2}(0) = \Phi_0/2\pi\xi_0^2$ [4]. Using this expression for $H_{c2}(0)$ and rearranging Eq. (4) gives,

$$H_{c2}(0) \approx (0.1776\ {\rm T/K})\left[\frac{m_s^*}{m_e}\right]\left[\frac{n_n}{n_s}\right]T_c. \tag{5}$$

In Fig. 1, we have plotted calculated values of the critical temperature, $T_c^{\rm calc}$, vs the experimentally determined values of T_c for a large number of compounds belonging to many of the known classes of superconductors. It can be seen that the relationship given by Eq. (4) holds for over two decades of T_c values, with the notable exception of Sr_2RuO_4, for which we show two different calculations of T_c. The meaning of the error bars is described below. We address the case of Sr_2RuO_4 in detail in the latter portion of this communication.

Of the three experimental parameters involved in calculating values of T_c via Eq. (4), n_s/n_n, m_s^*, and ξ_0 ($\xi_0[ab]$ for anisotropic compounds), the first two require special comment. With the exception of the hole-doped cuprate systems, the value of (n_s/n_n) is assumed equal to unity, in accordance with the result of Leggett for a simple one-component system with velocity independent forces [6]. For the hole-doped cuprate systems, we use the value found by Tanner *et al.* [7], $(n_s/n_n) \approx 1/4$ for samples at, or near, optimal doping. We also note that the calculated values of the superconducting critical temperature shown in Fig. 1, are obtained by using reported values of the effective electron mass obtained by either optical conductivity or de Haas–van Alphen (dHvA) measurements, denoted as $m_{\rm opt}^*$ and $m_{\rm cyc}^*$, respectively, where measurements of both mass values were taken with $H \parallel c$ for anisotropic compounds; i.e., we use $m_{\rm opt}^*[ab]$ or $m_{\rm cyc}^*[ab]$. Values of $m_{\rm opt}^*$ were used only for the cuprate-based superconductors. (An exception is the case of UBe_{13}, as indicated in Ref. [8]). The symbol shown for each compound is found using the reported mass value that gives the value of $T_c^{\rm calc}$ via Eq. (4) in closest agreement with the experimental value. (See Ref. [8]). The error bars represent the range of values of $T_c^{\rm calc}$ based upon the smallest and largest reported values of $m_{\rm cyc}^*[ab]$ or the respective error reported for $m_{\rm opt}^*[ab]$. The lower error bar for UBe_{13}, determined by the value of m^* extracted from specific heat measurements, is considered to significantly overestimate the lower bound of $T_c^{\rm calc}$.

As an example, in the case of the heavy-fermion (HF) system $PrOs_4Sb_{12}$, the effective mass $m^* \sim 50m_e$ has been estimated from measurement of the electronic specific heat coefficient [9]. However, dHvA measurements [10] yield values for the cyclotron effective mass $m^*_{\rm cyc}$, of $2.5m_e$, $4.1m_e$, and $7.6m_e$ for the α, β, and γ Fermi surface branches, respectively. As indicated in Table I of the supplementary material [8], the value of $T_c^{\rm calc}$ for $PrOs_4Sb_{12}$ shown in Fig. 1 is obtained by using the value $m^*_{\rm cyc} = 7.6m_e$ associated with the γ branch. However, as we point out below for $PrOs_4Sb_{12}$ and in the case of Sr_2RuO_4, the band associated with the symbol shown is not necessarily the sole superconducting band. A more complex calculation [see Eq. (6) below] may be appropriate with the result that the error bars shown in Fig. 1 would collapse when the relative contribution of charge carriers from all bands are experimentally determined. In this sense, these results would seem to indicate that because the dHvA effect gives individual band mass values it is possible to arrive at a more accurate determination of the combined superconducting effective mass m^*_s (which is directly measured by optical spectroscopy) than that obtained from measurements of the specific heat, particularly in the case of HF superconductors.

As implied above, there is evidence that some of these systems (e.g., $Pr[Os, Ru]_4Sb_{12}$, MgB_2), are multiband superconductors [11–14]. In these cases it may be appropriate to account for the condensation energy associated with each band separately by rewriting Eq. (4) as,

$$T_c = \frac{2\pi\hbar^2}{3k_B} \sum_i \frac{(n_s)_i}{n_n} \frac{1}{(m^*_s)_i} \frac{1}{(\xi_0^2)_i}, \tag{6}$$

with $\sum_i \frac{(n_s)_i}{n_n} = \frac{n_s}{n_n}$, where $i \in \{\alpha, \beta, \gamma, \ldots\}$.

For instance, in the case of $PrOs_4Sb_{12}$, (assuming two dominant superconducting bands) two possibilities are that the γ and β or γ and α branches become superconducting with an approximate allocation of charge carriers of 82% and 18% or 87% and 13%, respectively.

As mentioned above, we have shown two different calculated values of T_c for Sr_2RuO_4. The smaller value (black cross), which lies significantly off the solid line, is found using the reported values of the effective mass $m^*_{\rm cyc}$ and coherence length given in Ref. [15]. A simple explanation for this anomalous result is that our expression fails to fully or accurately account for all physical properties pertaining to the establishment of the critical temperature T_c in Sr_2RuO_4. We take a closer look here at relevant issues pertaining to Sr_2RuO_4, and suggest an alternative explanation for this discrepancy, upon which we base the second shown calculated value of T_c for Sr_2RuO_4 (red asterisk).

Of particular interest is the value of ξ_0 which has been extracted uniformly in the literature from measurements of $H_{c2}(0)$ [15,16]. However, if Sr_2RuO_4 is in fact a p-wave superconductor with a two-component order parameter, then it is possible that the physical structure and electronic properties of a vortex in Sr_2RuO_4 is significantly different than that of an Abrikosov vortex [17]—a topological defect in a superconductor with a one-component order parameter, and hence the intrinsic GL coherence length may differ significantly.

It has been found recently that the intrinsic GL coherence length in a noncentrosymmetric p-wave superconductor with a two-component order parameter can be expressed in terms of the superconducting gap [18], given by $\xi_0 = \hbar v_F/\sqrt{8}\Delta_0$. (This result can be generalized to the centrosymmetric case). The value of the GL coherence length calculated (below) by use of the above expression is 5 times smaller than that inferred from the relationship $H_{c2}(0) = \Phi_0/2\pi\xi_0^2$. It is difficult to ascribe this large of a discrepancy in the values of ξ_0 to an ambiguity of the definition of the GL coherence length. Rather, this would seem to indicate a real physical phenomenon at play. Following, the observation of Annett *et al.* [17], that similar vortex structures might be found in ^{3}He-A and Sr_2RuO_4, we suggest the existence of a ''composite vortex'' structure in Sr_2RuO_4 analogous to that found in the ABM phase of ^{3}He-A. If this were the case, then the length scale inferred from the relationship $H_{c2}(0) = \Phi_0/2\pi\xi_0^2$ is likely the outer soft core radius of the vortex. It is not clear, however, that bulk superconductivity would necessarily collapse when the boundaries of the soft core regions begin to overlap [19].

From measurements of the Knight shift, Murakawa *et al.* [20] find that the application of a very small magnetic field can cause the d vector (which determines the orientation of the spin wave function) to rotate away from the c-axis into a plane perpendicular to H. However, it is assumed that ℓ, (the angular momentum of the Cooper pair), remains locked to the c-axis direction due to electronic anisotropy. Thus, at sufficiently strong fields (well below $H_{c2}(0)$), in the region of a vortex beyond the hard core, the field is able to penetrate causing $\ell \nparallel d$, so that we now have a situation analogous to the ^{3}He-A ''composite vortex'' [21], wherein the vortex is comprised of both a ''hard core'' where the order parameter is suppressed, and a ''soft core'' where $\ell \nparallel d$ with a radius $\xi_d \approx$ (5–500)ξ_0 [22–24]. However, in this scenario, in the ''soft core'' region of the vortex, the orientation of d varies while ℓ stays fixed in direction. As in ^{3}He-A, as we move away from the center of the vortex, the strength of the penetrating field dies off, and eventually ℓ and d realign, leading to a similar ''healing length'' defining the radius of the ''soft core'' region. We also point out, that, for the other potential p-wave superconductors considered here, UPt_3 and $PrOs_4Sb_{12}$, experimental evidence indicate different symmetries of the order parameter, and, there is no evidence (to date) for a state where $\ell \nparallel d$. Hence the argument for a composite core vortex in Sr_2RuO_4 is not contradicted by these other likely p-wave cases.

Numerous studies (see Ref. [15] and references within) suggest that all three conduction bands in Sr_2RuO_4, α, β, and γ participate to some extent in superconductivity, with $\approx 57\%$ of the carriers on the γ band and 43% on the α and β bands [25] (Ref. [26] gives $>60\%$ on the γ band). Measurements and calculations of the ratio of the superconducting gap to the critical temperature give values of $\Delta_0 = 0.49$–1.54 meV, for $T_c = 1.435$ K, with 0.49 meV considered a lower limit [27–30]. We have calculated values of ξ_0 using the expression of Ref. [18], with the above values of Δ_0 and the reported values of the Fermi velocity, v_F for each band [15]. Then, using the calculated values of ξ_0 and the values of the effective masses given in [15,31], a value of T_c was calculated based on this 3-band picture using Eq. (6) and $(n_s)_{\alpha,\beta,\gamma}/n_n = 0.215, 0.215, 0.57$. An average value of $\Delta_0 = 1.02$ meV was used for all three bands and the error bars here are now defined by values of T_c calculated with $\Delta_0 = 0.49$ meV and 1.1 meV. As seen in Fig. 1, this result is in much closer agreement with that found for the other systems shown, with $T_c^{\mathrm{calc}} = 0.74$ K and upper and lower limits of 1.68 and 0.17 K. (If we use the values of m^*_{cyc} from Ref. [16] we obtain $T_c^{\mathrm{calc}} = 0.76$ K and upper and lower limits of 1.75 and 0.18 K). While this significant improvement of agreement between the calculated and experimental values of T_c in Sr_2RuO_4 is not necessarily proof of the above scenario, we are of the opinion that this coincidence is not accidental.

While Eq. (4) does not tell us how to make a superconductor, it does provide insight into how fundamental properties of superconductors are balanced against each other. In the context of high-T_c cuprate superconductors, this expression suggests that *if* it were possible to get all of the available electrons to participate in superconductivity, i.e., drive $(n_s/n_n) \rightarrow 1$, then the superconducting critical temperatures would, in some cases, exceed room temperature. This optimistic conclusion, however, runs up against the crux of the problem. By achieving $(n_s/n_n) = 1$, how does this effect the electron effective mass m_s^* and the energy scale that determines the coherence length ξ_0? We note also that Eq. (4) is consistent with the proposition of J. R. Schrieffer, wherein, (amongst other specified physical properties), a low effective mass is desired in order to achieve high superconducting critical temperatures [32].

In conclusion, we emphasize that the expression for the critical temperature found here is applicable to any kind or class of superconductor. The virtue of this simple approach is that it provides a general relationship to which any microscopic model of superconductivity, which also gives an explicit expression for T_c, can be compared, yielding further insight into how a specific mechanism of superconductivity is constrained by the balance between the characteristic quantities n_s/n_n, m_s^*, and ξ_0.

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