Strong-coupling μ^*/λ corrections for superconducting properties

C. L. Sammer and J. P. Carbotte

Physics Department, McMaster University, Hamilton, Ontario, Canada L8S4MI

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We have studied how large repulsive Coulomb pseudopotential μ^* values might affect various superconducting thermodynamic properties and the upper critical magnetic field in the clean and dirty limit. Existing approximate analytical expressions for these properties derived from Eliashberg theory were generalized to include a μ^*/λ correction term. The μ^*/λ corrections for the various superconducting properties were found to enhance rather than diminish strong-coupling effects.

I. INTRODUCTION

Isotope-effect measurements, which successfully pinpointed the phonon-mediated electron-pairing mechanism responsible for superconductivity in the conventional superconductors, have been performed by various groups¹⁻⁴ on the high- T_c superconductors and in particular Y-Ba-Cu-O. The results were quite unexpected. A measure of the isotope effect is given by the isotope effect coefficient β . By definition $T_c \sim M^{-\beta}$, where T_c is the critical temperature of the particular superconductor and M is the isotropic mass of the material, or equivalently the phonon frequency. The value of β for conventional superconductors according to BCS theory is β =0.5. Observations from the various groups demonstrate conclusively that there exists a very small, but measurable total isotope effect in Y-Ba-Cu-O of order β ~ 0.05.

A most natural explanation for the small isotope effect in Y-Ba-Cu-0 is to suggest that an electron-phonon interaction is not the dominant contribution to the pairing potential causing superconductivity in this high- T_c material and that there is an additional nonphononmediated coupling between the electrons which is independent of the mass of the ions in the lattice and which dominates over the phonons.

Another way, however, to achieve a small isotope effect in the oxide superconductors such as Y-Ba-Cu-0 is to consider large values of μ^* . This possibility is supported by the following argument: it is well known that the doping in the oxides is small. Small doping leads to a dilute electron gas within the material, and consequently, a reduction in the screening between the electrons. Since the Coulomb pseudopotential μ^* is a measure of the repulsion between the electrons, reduced screening suggests that μ^* is larger in the oxides than it is in the conventional superconductors for which $\mu^* \approx 0.1$.

The group at $\mathrm{Berkeley}^{2,5,6}$ considered the effect of large μ^* values on the isotope effect and the critical temperature T_c of Y-Ba-Cu-O. Their work is based directly on the phonon spectrum of Y-Ba-Cu-O and leads to the finding that reproduction of the experimental results of $\beta \approx 0$ and $T_c \sim 100$ K gives unphysically large values of μ^* and electron-phonon mass renormalization λ , which is a measure of the attractive interaction between the electron and the lattice.

The work performed by Akis and Carbotte⁷ is more general and less restrictive. Their approach was to find μ^* and λ by solving the Eliashberg equations numerically. In considering the very small isotope effect and large $T_c \sim 100$ K for Y-Ba-Cu-O, they found that if μ^* was as large as 0.5, than $\lambda \sim 5$, 6, or 7. Although large, these values for μ^* and λ are not completely unphysical. To compare, for the conventional superconductors $\mu^* \approx 0.1$ and the approximate range for λ is 0.5 < λ < 2.5. Values of $\mu^* \approx 0.1$ do not give the small isotope effect and large value for T_c . Of course, the high- T_c oxides are complex materials and there are other more materials-oriented possible explanations for the isotope effect results as well as the other observed properties.

The work of Akis and Carbotte suggested that large μ^* and λ values might effect other superconducting properties. This paper presents an extension of their work to other superconducting properties. The superconducting properties investigated were the specific heat jump and its slope, the gap, the critical magnetic field for type-I superconductors and its reduced form, and the upper critical magnetic field for type-II superconductors in the clean and dirty limit. Rather than follow the numerical but rigorous approach of Akis and Carbotte, it was decided that the approximate analytical work of Marsiglio, Carbotte, and Blezius^{$11-13$} would be generalized to include a μ^*/λ correction term.

When a superconducting property is expressed as a BCS ratio, the BCS theory of superconductivity¹⁴ predicts a universal value for that property. For conventional superconducting materials these BCS predictions are only qualitatively correct. Eliashberg theory, however, produces values to these BCS ratios which agree with experimental results to within 5%. While direct evaluation of BCS ratios using Eliashberg theory¹⁵ can only be found numerically due to the complexity of the equation, approximate analytic expressions have been determined by Marsiglio and Carbotte by the reduction of the Eliashberg equations using a number of a carefully chosen approximations. The result is the BCS constant value for the property plus a strong-coupling correction term. Higher-order terms are ignored, since they are negligible in comparison to the first-order term. In the work of Marsiglio and Carbotte the correction term is a function of the strong-coupling parameter T_c / ω_{ln} . Here ω_{ln} is the Allen-Dynes parameter,¹⁶ an appropriate moment of the electron-phonon spectral density $\alpha^2 F(\omega)$ and a measure of the average phonon energy involved. The strongcoupling term for the properties calculated in this paper is a function of the strong-coupling parameters T_c / ω_{ln} and μ^*/λ .

The approximate analytical expressions for all the superconducting properties Marsiglio and Carbotte studied have the same general form:

$$
(\text{BCS ratio}) = (\text{BCS const}) \left[1 + a \left(\frac{T_c}{\omega_{\text{ln}}} \right)^2 \ln \left(\frac{\omega_{\text{ln}}}{b T_c} \right) \right],
$$
\n(1)

where a and b are fitted parameters determined by fitting the curve to the exact numerical solutions to the Eliasberg equations corresponding to real materials.

In Sec. II the calculation of the μ^*/λ correction to the specific heat jump ratio is outlined. In Sec. III we present the results without derivation for the other thermodynamic properties and for the upper critical magnetic field in the clean and dirty limit. Conclusions are given in Sec. IV.

II. μ^* / λ STRONG-COUPLING CORRECTION TO $\Delta C(T_c)/\gamma T_c$

Thermodynamic properties depend on the free energy difference $\Delta F = F_S - F_N$ between the superconducting and normal state. The subscript $S(N)$ refers to the superconducting (normal) state.

As an example, the specific heat difference between the normal and superconducting state ΔC is related to ΔF by

$$
\Delta C(T) = C_S - C_N = -T \frac{d^2 \Delta F}{dT^2} \tag{2}
$$

where T is the temperature. The normalized specific heat jump ratio

$$
\frac{\Delta C(T_c)}{\gamma T_c} = \frac{C_S - C_N}{C_N} \tag{3}
$$

where $\gamma = \frac{2}{3}\pi^2 N(0)(1+\lambda)$ is the Sommerfield constant can be modified to an expression in ΔF :

$$
\frac{\Delta C(T)}{\gamma T_c} = -\frac{N(0)}{\gamma} \left[1 + \frac{(T - T_c)}{T_c} \right] \frac{d^2[\Delta F/N(0)]}{dT^2},
$$
\n(4)

where $N(0)$ is the single-spin electronic density of states at the Fermi surface.

The Bardeen-Stephen formula¹⁷ for the free energy difference is

$$
\frac{\Delta F}{N(0)} = -\pi T \sum_{m=-\infty}^{\infty} \left[\sqrt{\Delta_m^2 + \omega_m^2} - |\omega_m| \right]
$$

$$
\times \left[Z_S(m) - Z_N(m) \frac{|\omega_m|}{\sqrt{\Delta_m^2 + \omega_m^2}} \right].
$$
\n(5)

For notational brevity the energy gap function

 $\Delta(i\omega_m) = \Delta(m) = \Delta_m$ and similarly for the normalization function $Z(i\omega_m)$. Actually, an expansion of this free energy difference formula (5) either for near T_c or $T=0$, depending on what the property being calculated requires, is always used.

From Eq. (4) it is clear that the specific heat requires $\Delta F/N$ (0) to be expanded near T_c . Near T_c , the energy gap Δ_m approaches a very small value. Thus, since the Matsubara frequencies are proportional to temperature by $\omega_m = \pi T(2m - 1)$ for $m = 0, \pm 1, \pm 2, \ldots, \Delta_m / \omega_m$ and Δ_m /T also have very small values. This allows Eq. (5) for $\Delta F/N(0)$ to be expressed as a Taylor series in powers of Δ_m/ω_m .

All the terms in expansion of $\Delta F/N(0)$ are found using the two Eliashberg equations on the imaginary frequency axis. The Eliashberg equations are

$$
\Delta_n Z_n = \pi T \sum_{m=-\infty}^{\infty} \left[\lambda (m-n) - \mu^* \right] \frac{\Delta_m}{\sqrt{\omega_m^2 + \Delta_m^2}} \qquad (6)
$$

$$
\omega_n Z_n = \omega_n + \pi T \sum_{m=-\infty}^{\infty} \lambda(m-n) \frac{\omega_m}{\sqrt{\omega_m^2 + \Delta_m^2}} , \quad (7)
$$

where $\omega_n = \pi T(2n - 1)$ for $n = 0, \pm 1, \pm 2, \ldots$. $\lambda(m - n)$ is related to the electron-phonon spectral density function $\alpha^2 F(\omega)$ by

$$
\lambda(m-n) = \int_0^\infty \frac{2\nu \alpha^2 F(\nu) d\nu}{\nu^2 + (\omega_m - \omega_n)^2} \ . \tag{8}
$$

To ensure that the sum over m in Eq. (6) converges properly, the Coulomb pseudopotential μ^* has been given a cutoff ω_c , where ω_c is the largest energy in the problem.

The following two step-function approximations on the imaginary frequency axis¹⁸ are needed to make the Eliashberg equations analytic.

(1) The two-gap model:

$$
\Delta(m) = \begin{cases} \Delta_0(T) , & |\omega_m| \le \omega_0 \\ \Delta_\infty(T) , & |\omega_m| > \omega_0 \end{cases}
$$
(9)

where $\omega_0 = \pi T(2n - 1)$ is a rough cutoff taken to be the maximum phonon frequency found in the system.

(2) The two-step renormalization model:

$$
Z_S(m) = \begin{cases} Z_0(T), & |\omega_m| \le \omega_0 \\ 1, & |\omega_m| > \omega_0 \end{cases}
$$
 (10)

A number of other approximations are also made. Essential to the step-function approximations made are the requirements that $\omega_0 \gg \omega_{\ln}$ and $\omega_{\ln} \gg T_c$.

Following the procedure detailed in the work by Marsiglio, Carbotte, and Blezius^{11,1} '³ the utilization of the second Eliashberg equation, Eq. (7), modifies $\Delta F/N(0)$ to

$$
\frac{\Delta F}{N(0)} = \frac{1}{2} \frac{(1+\lambda)^2}{\lambda + \mu^*} [K(T)\Delta_0^4 + \frac{4}{3}L(T)\Delta_0^6] \ . \tag{11}
$$

 $F(T)$, $G(T)$, and $J(T)$ are defined in Ref. 8. Δ_0^4 and Δ_0^6 are found using the first Eliashberg equation, Eq. (6), which has been converted into the following form:

$$
1 = F(T) + \Delta_0^2 G(T) + \Delta_0^4 J(T) \tag{12}
$$

Expansion of Eq. (12) as a Taylor series about T_c produces an expression for Δ_0^2 which is squared and cubed to produce expressions for Δ_0^4 and Δ_0^6 . The second derivative of the resulting $\Delta F/N(0)$ expression is then found and evaluated at T_c as prescribed by the $\Delta C(T)/\gamma T_c$ Eq. (4). The normalized specific heat jump can be rewritten **as**

$$
\Delta C(T)/\gamma T_c = f + (1 - t)g \text{ , where } t = T/T_c \text{ , (13)}
$$

where

$$
f = \frac{-N(0)}{\gamma} \frac{(1+\lambda)^2}{\lambda - u^*} \frac{KF'^2}{G^2} \,,
$$
 (14)

$$
g = -f3T_c \left[\frac{1}{3T_c} + \frac{F''}{F} - \frac{2G'}{G} + \frac{2JF'}{G} + \frac{K'}{K} - \frac{4}{3} \frac{LK'}{KG} \right].
$$
\n(15)

 $K(T)$ and $L(T)$ are defined in Ref. 8 along with F, G, and J. Physically, f is the normalized specific heat jump at T_c and g is the normalized slope of the specific heat jump at T_c .

Up to this point the calculation of the correction terms to the normalized specific heat jump ratio $\Delta C(T)/\gamma T_c$ has been identical to the calculation performed by Marsiglio and Carbotte.¹¹ We now divert by continuing to retain μ^* explicitly.

At this point f and g are now expressed in terms of the variables $\bar{a}(T)$, \bar{b} , and $\bar{c}(T)$ defined by Mitrović Zarate, and Carbotte,¹⁹ retaining the μ^* explicitly. The T_c equation found from $1 = f(T_c)$ with μ^*/λ included,

$$
\frac{1+\lambda}{\lambda-\mu^*} = \ln\left[\frac{1.13\omega_{\rm ln}}{k_B T_c} \left(\frac{\omega_0}{\omega_{\rm ln}}\right)^{-\mu^*/\lambda}\right],\tag{16}
$$

and the approximation $\lambda \gg \mu^*$ which allows

$$
\frac{\lambda}{\lambda - \mu^*} \simeq 1 + \frac{\mu^*}{\lambda} + \cdots \tag{17}
$$

are also used to simplify the f and g expressions.

The resulting expressions for f and g with the μ^*/λ strong-coupling correction terms included are

$$
f = \frac{\Delta C(T_c)}{\gamma T_c}
$$

= 1.43 $\left[1 + \left[1 + \frac{\mu^*}{\lambda}\right] a_1 \left(\frac{T_c}{\omega_{\text{ln}}}\right)^2 \ln \left(\frac{\omega_{\text{ln}}}{b_1 T_c}\right)\right]$ (18)

and

$$
g = T_c \frac{d\Delta C/dT}{\Delta C(T)} \Big|_{T=T_c}
$$

= -3.77 $\Bigg[1 + \Bigg[1 + \frac{\mu^*}{\lambda} \Bigg] a_2 \Bigg[\frac{T_c}{\omega_{\text{ln}}} \Bigg]^2 \ln \Bigg[\frac{\omega_{\text{ln}}}{b_2 T_c} \Bigg] \Bigg]$. (19)

 a_1 , b_1 , a_2 , and b_2 are constants.

Figure 1 shows the normalized specific heat jump ratio result Eq. (18) as a function of increasing T_c / ω_{ln} for various μ^*/λ . The data points represent exact numerical solutions of the Eliashberg equations for the specific heat jump for various superconducting materials. The numerical solutions agree with experiment to within 5%. The superconducting materials have been grouped into various ranges of μ^*/λ . The curves represent the best fit lines through these sets of μ^*/λ ranges.

The values of the coefficients a_1 and b_1 in Eq. (18) producing the fit given in Fig. 1 are $a_1 = 39$ and $b_1 = 2.5$. Each curve has the μ^*/λ value indicated in the figure.

As can be seen from Fig. 1, all the curves for the various μ^*/λ values begin $(T_c/\omega_{\text{ln}} \rightarrow 0)$ at the BCS value of the specific heat 1.43. With increasing T_c/ω_{ln} , $\Delta C/\gamma T_c$ gets larger than the BCS value. This occurs for all the curves of different μ^*/λ values. In addition, the larger the μ^*/λ value of the curve, the larger $\Delta C/\gamma T_c$ becomes.

FIG. 1. Specific heat jump ratio $f \equiv \Delta C(T_c)/\gamma T_c$ as a function of T_c/ω_{ln} for different μ^*/λ values. The data points are exact numerical solutions to Eliashberg theory for the property to specific heat for various superconducting materials. These solutions agree with experiment to within 5%. Based on its μ^*/λ value, each superconducting material has been grouped into ranges of μ^*/λ . In increasing order of $\Delta C(T)/\gamma T_c$, the data points correspond to the following materials: for the $\mu^*/\lambda = 0$ range La and $Pb_{0.65}Bi_{0.35}$, for the $\mu^*/\lambda = 0.1$ range $Tl_{0.9}Bi_{0.1}$, In, Nb (Rowell), Mo, V₃Si-1, V₂Si (Kihl), Pb_{0.4}Tl_{0.6}, V₃Ga, Nb₃Al (2), Hg, Pb_{0.6}Tl_{0.4}, Nb₃Al (3), Nb₃Ge (1), Nb₃Al (1), Nb₃Ge (2), Nb₃Sn, Pb_{0.8}Tl_{0.2}, Pb, Pb_{0.9}Bi_{0.1}, Pb_{0.8}Bi_{0.2}, and Pb_{0.7}Bi_{0.3}, for the $\mu^*/\lambda = 0.2$ range Ta, Sn, Tl, and Nb (Arnold), for the μ^*/λ =0.3 range Al, V, and Nb (Butler). The curves correspond to Eq. (18) in the text. The coefficients a_1 and b_1 for each curve are $a_1 = 39$ and $b_1 = 2.5$. The value of μ^* / λ has been varied as indicated for each group of superconductors.

Even though there is some scatter in the points, a general trend is clearly shown in Fig. 1: the μ^*/λ correction enhances rather than diminishes the superconducting property. In other words, the strong-coupling parameter μ^* / λ acts to enhance the strong-coupling effect rather than diminish it, although for small values of this parameter the effects are not large.

The coefficients a_1 and b_1 used here have different
lues than those used by Marsiglio and Carbotte.¹¹ The values than those used by Marsiglio and Carbotte.¹¹ The Marsiglio and Carbotte expression corresponds to μ^*/λ =0. The values of the coefficients they used were a_1 =53 and b_1 =3.0 corresponding to the best fit line
through the exact numerical data points. These through the exact numerical data points. coefficient values do not consider the μ^*/λ values of those data points which may vary from 0.¹ to 0.3 between one point and the next. Their fit was intended to demonstrate that their approximate analytical solutions show general trends in the properties as a function of the strong-coupling parameter T_c/ω_{ln} . Only if the Eliashberg equations could be solved analytically could a curve be found that encompassed all the data points.

III. RESULTS FOR THE OTHER SUPERCONDUCTING PROPERTIES STUDIED

Calculations to determine the μ^*/λ strong-coupling corrections for the specific heat jump and its slope, the gap, the critical magnetic field for type-I superconductors and its reduced form, and the upper critical magnetic field for type-II superconductors in the clean and dirty limit were performed by generalizing the work by Marsiglio and Carbotte to include a μ^*/λ strong-coupling correction term. The calculation of the correction term for each of the superconducting thermodynamic properties studied in similar to the specific heat calculation described in Sec. II. However, the μ^*/λ correction terms for the upper critical magnetic field for type-II superconductors in the clean and dirty limit were determined by using the equations and approach found in Ref. 9, with μ^* again retained explicitly.

The resulting expressions with the μ^*/λ corrections for all the superconducting properties studied were found to follow the general form:

$$
\text{(BCS ratio)} = \text{(BCS const)} \left\{ 1 + \left[1 + \frac{\mu^*}{\lambda} \right] \left[c \frac{T_c}{\omega_{\text{ln}}} + a \left[\frac{T_c}{\omega_{\text{ln}}} \right]^2 \ln \left[\frac{\omega_{\text{ln}}}{b T_c} \right] \right] \right\},\tag{20}
$$

where a , b , and c are fitted constant parameters. Only the upper critical magnetic field for type-II superconductors in the dirty limit requires the linear term, i.e., the only property for which $c\neq 0$. Although the μ^*/λ correction terms found for the various superconducting properties were small, they suggested that strongcoupling effects are enhanced further by the introduction of a finite value of μ^* .

TABLE I. Values of the coefticients used by Marsiglio and Carbotte.

^aThe considerable scatter in the data for $h_{\rm q}^{\rm divy}(0)$ does not allow a single curve to describe the data. Two curves with difFerent sets of parameters are considered giving the upper (solid) and lower (dotted) curves shown in Fig. ¹ of Ref. 12.

As discussed in Sec. II, the coefficients a, b , and c for the normalized specific heat jump ratio $\Delta C(T)/\gamma T_c$ have been changed from the original values used by Marsiglio and Carbotte. While the values used by Marsiglio and Carbotte are a good first approximation, fine tuning of the coefficients, as demonstrated for the specific heat, gives a better fit to the data when μ^*/λ are considered. We have not carried out a new fit for the other quantities considered. Table I, however, gives the values of the coefficients used by Marsiglio and Carbotte for the various properties considered, which can be used as a first approximation to Eq. (20).

IV. CONCLUSIONS

Motivated by the possibility of reduced low electron density screening in the high- T_c oxides, we have studied the effect that a large value for the Coulomb pseudopotential μ^* might have on dimensionless ratios for superconducting properties. We have generalized recent calculations for strong-coupling corrections to BCS ratios

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which have appeared in the literature to include a finite value of μ^*/λ . Here, λ is the mass renormalization.

Several general features are seen in the results. All the curves begin at the BCS constant value at $T_c / \omega_{\text{ln}} = 0$ and then increase (or decrease) in magnitude as T_c / ω_{in} , or the strong coupling increases (or decreases) and a further enhancement (or reduction) to each of the properties is also seen as μ^*/λ is increased. Thus μ^*/λ strongcoupling corrections act in the same direction for any given superconducting property. In all cases considered, we find that at low values of T_c / ω_{ln} , variations in μ^* / λ have little effect on the properties. At higher values of T_c / ω_{ln} , the μ^* / λ corrections become more significant. In summary, μ^*/λ corrections invariably enhance strong-coupling effects, although the corrections are small for modest values of μ^*/λ . While such effects certainly do not provide an explanation for the anomalous superconducting properties observed in the oxides, they may be of importance in some systems such as the C_{60} superconductors.

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