Slope of specific-heat jump at T_c in a very-strong-coupling superconductor

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We have calculated the normalized slope of the specific heat at the critical temperature T_c as a function of coupling strength. As the coupling is increased the slope first increases rapidly from its Bardeen-Cooper-Schrieffer value of 2.63, reaches a maximum, and then decreases as we reach the very-strong-coupling regime. Using a δ-function spectral density, a local maximum is established which must be satisfied by any Eliashberg superconductor. Comparison with a recent experiment indicates a serious violation of this bound which, if confirmed, implies that some important modification of the theory is required.

The specific heat in the oxides superconductors La-Sr-Cu-O and Y-Ba-Cu-O has been measured by many authors.[1-20] At present, there is some agreement among various experiments as to the size of the jump $\Delta C(T)$ at T_c (the critical temperature) with some significant variation off the average value. This can be seen from Table I where we have compiled some of the data.[1-20] To make a comparison with results of Eliashberg theory,[21-23] it is necessary to form the dimensionless ratio $\Delta C(T_c)/\gamma_0 T_c$ where γ_0 is the Sommerfeld constant. This normalization is necessary to cancel out an electronic density of states at the Fermi energy factor which appears in both ΔC and γ_0. Unfortunately, γ_0 is, at present, not well known for the oxides. This introduces additional uncertainties and makes any comparison between theory and experiment of the ratio $\Delta C(T_c)/\gamma_0 T_c$ inconclusive. It is clear that it would be useful to seek a comparison which does not depend on our knowledge of γ_0.

Recently, Junod *et al.*[24] have given results for the difference in specific heat between superconducting and normal-state $\Delta C(T)$ at any temperature T below T_c and have compared their results with Bardeen-Cooper-Schrieffer (BCS) theory. They find that the initial decrease in $\Delta C(T)$ near T_c is much steeper than predicted by BCS theory. There is, of course, some uncertainty in their analyses related to their method of subtracting out the normal-state specific heat which they take to be approximated by that of a normal sample with Fe substitution. This straightforward procedure cannot be accurate as it leads to a violation of the entropy sum rule noted and stressed by the authors. Still, the data in the region immediately near T_c should suffer less from these limitations. If we normalize the slope of $\Delta C(T)$ at T_c, namely, $T_c[d\Delta C(T)/dT]_{T_c}$ to the jump at T_c [$\Delta C(T_c)$], this ratio will be independent of γ_0 and can be compared directly with theory. The normalized slope

$$T_c\left[\frac{d\Delta C(T)}{dT}\right]_{T_c}\Bigg/\Delta C(T_c)\equiv R, \qquad (1)$$

which we denote by R, depends only on the electron-boson exchange spectral density $\alpha^2 F(\Omega)$ and on the Coulomb pseudopotential μ^*.

In this work, we calculate R as a function of the strong-coupling parameter $T_c/\omega_{\ln}$ where[25]

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

This quantity sets the energy scale associated with the bosons that are being exchanged in the pairing process. The BCS limit results for $T_c/\omega_{\ln}\to 0.0$, the usual conventional strong-coupling regime ends around $\lesssim 0.20$ (Refs. 26 and 27) and the very-strong-coupling regime applies for $T_c/\omega_{\ln}\sim 1.0$.[28,29] A first calculation is based on the La-Sr-Cu-O spectrum $\alpha^2 F(\Omega)$ calculated by Weber[30] which we scale so as to get any desired value of $T_c/\omega_{\ln}$. The proposed scaling is a simple constant multiplicative factor on vertical and horizontal axis[31]

$$\alpha^2 F_M(\Omega)=B\alpha^2_{\text{La-Sr-Cu-O}}F(\Omega b), \qquad (3)$$

where the subscript M stands for model and B and b are the scaling factors. The factor B can be adjusted to get a T_c of 96 K or, for that matter, any value that might be of interest, and b is then varied to change $\omega_{\ln}$. It is a simple matter to verify that[28,31]

$$\omega_{\ln}^M=\frac{1}{b}\omega_{\ln}^{\text{La-Sr-Cu-O}}. \qquad (4)$$

TABLE I. Some representative experimental values for the specific-heat jump at $T_c[\Delta C(T_c)]$ divided by T_c in La-Sr-Cu-O and Y-Ba-Cu-O. This table does not represent an exhaustive survey of the literature nor does it include values known to us only in unpublished form.

$\Delta C(T_c)/T_c$ in mJ/mol K^2	
La-Sr-Cu-O	Y-Ba-Cu-O
7.6±1.8 (Ref. 1)	18 (Ref. 10)
20±5 (Ref. 2)	15.5 (Ref. 11)
16.8 (Ref. 3)	13 (Ref. 12)
8.8 (Ref. 4)	1.3 (Ref. 13)
22–26 (Ref. 5)	16 (Ref. 14)
11 (Ref. 6)	7 (Ref. 15)
9.9 (Ref. 7)	11±2 (Ref. 16)
10±2 (Ref. 8)	23±5 (Ref. 17)
6.5 (Ref. 9)	13 (Ref. 18)
	11.3 (Ref. 19)
	20 (Ref. 20)

The solid line of Fig. 1 gives our results for R as a function of increasing $T_c/\omega_{\ln}$ up to a value of 1.2. The solid curve starts at 2.63 for $T_c/\omega_{\ln}=0$ and initially increases as $T_c/\omega_{\ln}$ increases until a maximum slightly above 4.0 is reached around $T_c/\omega_{\ln}=0.12$ after which the normalized slope decreases somewhat. As we go beyond the conventional strong-coupling region $(T_c/\omega_{\ln}\lesssim0.20)$ the results are fairly flat and the value at $T_c/\omega_{\ln}=1.2$ is about 3.7. It is important to realize that these results are independent of the Sommerfeld constant γ_0 and depend only on spectral density $\alpha_M^2F(\Omega)$ and Coulomb pseudopotential μ^* which we fixed, for convenience, at the typical value of 0.09.

The results of Fig. 1 were obtained on solution of the Eliashberg gap equations at finite temperature and the evaluation of the free-energy difference formula. Details of these equations can be found elsewhere[21,22] and need not be repeated here. While we have used a model electron-phonon spectral density, any boson exchange mechanism can be treated in the same way by making use of the appropriate kernel (at least in a first approximation).

It is of interest to know the dependence of the solid curve for R given in Fig. 1 on the shape of the assumed spectral density $\alpha_M^2F(\Omega)$. Many other shapes could have been used. If this is done, we find no qualitative change, although there are significant quantitative differences. A case which is particularly different from the solid curve is the dashed curve labeled as a δ function.[32] This case will be of particular interest below and corresponds to a δ-function spectral density $\alpha_M^2F(\Omega)=A\delta(\Omega-\omega_E)$ of area A, positioned at the Einstein frequency $\omega_{\ln}=\Omega_E$. As this

Einstein frequency is varied, we see that we get a curve which is qualitatively the same as the solid curve but with much more pronounced features. At $T_c/\omega_{\ln}=0$ it starts at the BCS value as it must, then increases rapidly exhibiting a maximum slightly before $T_c/\omega_{\ln}=0.2$ of value approximately 4.76, and then decreases to take on a value of about 3.25 at $T_c/\omega_{\ln}=1.2$. As we have done in previous work,[32,33] we can show that the curve obtained is independent of the area A. Thus, the dashed curve of Fig. 1 is universal and shows, that for any δ-function shaped spectral density, the normalized slope R will take on a maximum at a definite optimum energy Ω_E^* given by

$$T_c/\Omega_E^*\cong0.16 \tag{5}$$

for $\mu^*=0.09$. As the value of the Coulomb pseudopotential is changed, the position of the optimum frequency changes as does the value at maximum. We can, in fact, show that the δ function gives a local maximum[33] and that the use of any other shape reduces the value of R. This is illustrated in Fig. 2 for the case $\mu^*=0.09$ and for a reduced temperature of $t=T/T_c=0.9$. We show this case because we could get more accurate numerical values for this functional derivative than we could exactly at T_c. What is plotted in Fig. 2 is[34]

$$\frac{\delta}{\delta\alpha^2F(\omega)}\left[\left[\frac{d\Delta C(t)}{dt}\right]_{t=0.9}\Big/\Delta C(T_c)\right], \tag{6}$$

which gives the change in the normalized slope at $t=0.9$ when an infinitesimal addition is made to the spectral weight $\alpha^2F(\Omega)$ at a particular frequency ω. The dashed
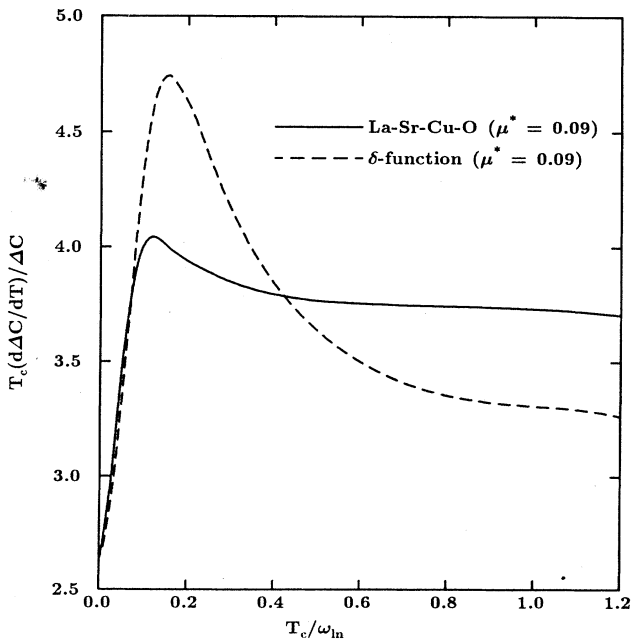

FIG. 1. The normalized specific-heat slope at $T_c\{[d\Delta C(T)]/dT\}_{T_c}/\Delta C(T_c)$ as a function of the strong-coupling index $T_c/\omega_{\ln}$ for the La-Sr-Cu-O spectrum (solid line) and for a δ function (dashed line).
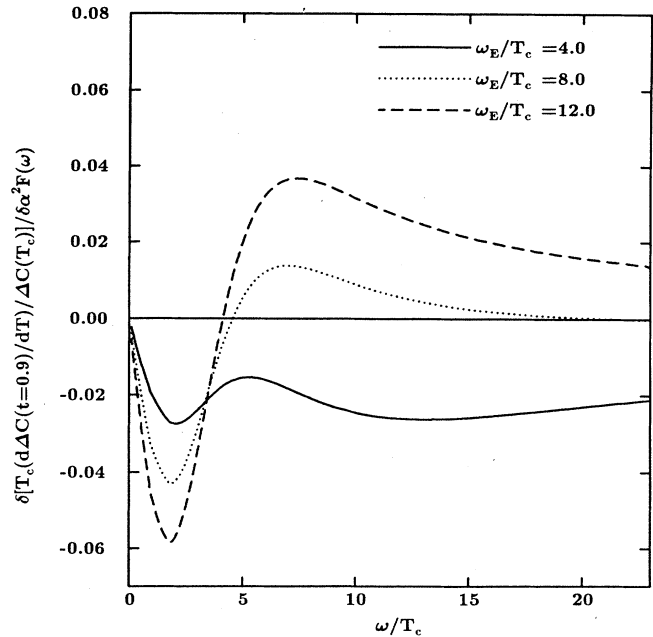

FIG. 2. The functional derivative of the normalized jump $\delta/\delta\alpha^2F(\omega)\{[d/dt\Delta C(t)]_{t=0.9}[1/\Delta C(T_c)]\}$ as a function of ω/T_c for the case $\mu^*=0.09$ and a base δ function with Einstein frequency $\omega_E=12.0T_c$ (dashed curve), $\omega_E=8.0T_c$ (dotted curve), $\omega_E=4.0T_c$ (solid curve).

line is for a base δ-function spectrum with Einstein frequency placed at $\omega_E = 12 T_c$ which is well beyond the maximum in the curve of

$$T_c \frac{d\Delta C(t=0.9)}{dT} \Big/ \Delta C(T_c) \qquad (7)$$

shown in Fig. 3 for a base δ function as a function of the position of ω_E. We see that adding spectral weight at low energies reduces the normalized slope (7) while an addition at high energies increases it. This is also true for the dotted curve with $\omega_E = 8.0 T_c$, although now we are closer to the maximum at $\omega_E = 6.1 T_c$ of Fig. 3 and the amplitude of the functional derivative is reduced. As we go through the maximum of Fig. 3, the functional derivative becomes negative definite as seen in Fig. 2 solid curve for $\omega_E = 4.0 T_c$. In this case, adding weight at any energy reduces the slope given by expression (7). Right at the maximum in the vase δ-function curve of Fig. 3, which identifies the optimum frequency ω_E^*, the functional derivative is negative everywhere but it is also exactly zero right at the optimum frequency $\omega_E^* = 6.1 T_c$. Thus, adding weight to the optimum spectral function

$$\alpha_M^2 F(\Omega) = A\delta(\Omega - \omega_E^*) \qquad (8)$$

for $\mu^* = 0.09$ right at the optimum ω_E^* leaves the slope unchanged and adding weight anywhere else reduces the slope. We have thus obtained a maximum normalized slope. Comparing this maximum normalized slope with the maximum in the δ-function curve of Fig. 1, we find it to be substantially less— 3.67 as opposed to 4.76. Thus, it should be emphasized that this quantity is sensitive to how it is taken.

It is of interest to compare our maximum normalized slope R with that found experimentally by Junod et al.[24] From Fig. 7 of Ref. 24 we find a slope of 8–14 depending on the temperature interval used in the determination. This is much larger than our maximum value of ~ 4.76. While this theoretical estimate will change a little with different values of μ^*, this difference cannot account for the large discrepancy between theory and this experiment. We should keep in mind that the experiments themselves have some uncertainty, as pointed out by the authors, and that the experiment of Loram and Mirza[35] gives a smaller value around 5. Nevertheless, it is important to realize
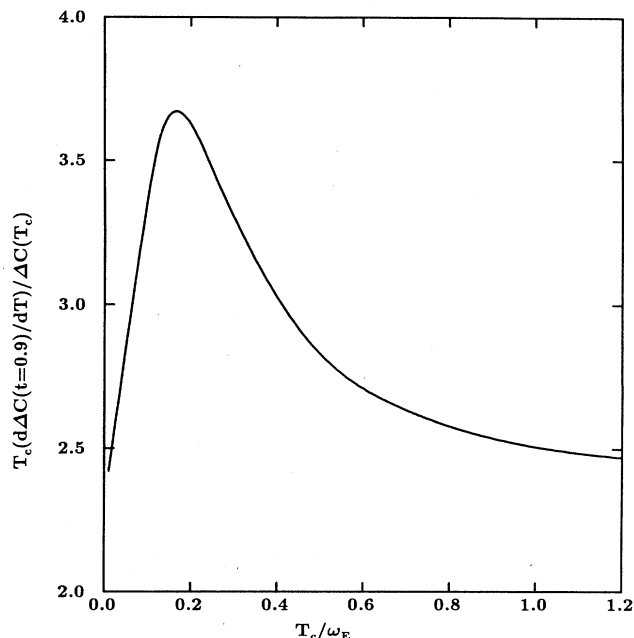

FIG. 3. The normalized specific-heat slope taken at the reduced temperature $t = 0.9[d/dt\Delta C(t)]_{t=0.9}/\Delta C(T_c)$ as a function of ω_E for a δ-function spectral density $\alpha^2 F(\Omega) = A\delta(\Omega - \omega_E)$.

that if the larger value is confirmed in other experiments, this would be the first clear indication that some essential modification of the isotropic Eliashberg equations are necessary to explain the data. This statement is quite independent of the choice of kernels in the Elishberg equations and does not depend on the preferred boson exchange mechanism provided it is assumed that the basic form of the equations remain valid, in a first approximation, for other nonphonon exchange mechanisms.

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