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Electron–phonon coupling and specific heat in $YBa_2Cu_3O_7$

S.V. Shulga [a], O.V. Dolgov [b,1] and I.I. Mazin [c,1]

[a] *Institute of Spectroscopy, Troitsk, Russia*
[b] *Institut für Festkörperforschung, Forschungszentrum Jülich, W-5170 Jülich, Germany*
[c] *Max-Planck-Institut für Festkörperforschung, W-7000 Stuttgart-80, Germany*

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We have calculated the renormalization of the specific heat in the normal state and the specific heat jump at T_c, using a realistic Eliashberg function, extracted from tunneling spectroscopy. The magnitude of the Eliashberg function was scaled so as to have the total coupling constant λ from 1.5 to 2.5. Using these calculations, we have analyzed recent measurements of the specific heat and have found that they can be reconciled with the band structure calculations, if $\lambda \approx 2$.

1. Introduction

After the discovery of the high-temperature superconductors (HTSC) great-interest has been attached to the thermodynamical properties of these compound. Nevertheless, reliable measurements of the low-temperature specific heat and of the specific heat jump at T_c have appeared only recently [1–3]. However, the interpretation of the data is difficult, since even assuming a conventional boson-exchange mechanism for the superconductivity one cannot use simple BCS formulas. The reason is that, as we shall show below, the experimental data are consistent with a moderate to strong coupling regime and in this case a numerical solution of the Eliashberg equation is unavoidable. Moreover, there are now various other experimental indications of the strong coupling, first of all tunneling, photoemission and optical measurements of the gap.

In this paper we solve numerically the Eliashberg equations for different strengths of the electron–phonon coupling, with a natural model for the shape of the Eliashberg function $\alpha^2F(\omega)$. We also use the same Eliashberg function to find the temperature dependent renormalization of the electronic specific heat in the normal state. Then we show that the experimental results can be reconciled with the band-structure-derived density of states if the electron–phonon coupling constant λ is taken to be about 2. In particular, we show that the low-temperature results of Phillips et al. [1] can be naturally interpreted in the strong-coupling theory with the same λ.

2. Normal state

Electron specific heat, including electron–phonon interaction effects, is given by the following equation [4,5]:

$$C_{el}(T) = \frac{2\pi^2}{3} N_b(0) k_B^2 T \times \left[1 + \frac{6}{\pi k_B T} \int_0^\infty f\left(\frac{\omega}{2\pi k_B T}\right) \alpha^2F(\omega)\, d\omega\right], \quad (1)$$

where $N_b(0)$ is the bare density of states per spin at the Fermi level, $\alpha^2F(\omega)$ is the Eliashberg function, which characterizes the frequency dependence of the electron–phonon coupling, and

$$f(x) = -x - 2x^2 \operatorname{Im} \psi'(ix) - x^3 \operatorname{Re} \psi''(ix), \quad (2)$$

[1] On leave from the P N Lebedev Physical Institute Moscow, Russia.

is the universal function defined via the digamma function, $\psi(x)=\Gamma'(x)/(x)$. The physical meaning of this function is that it defines the variational derivative of $C_{el}(T)$ with respect to the Eliashberg function:

$$\delta C_{el}(T)/\delta\alpha^2F(\omega) = 4\pi N_b(0)k_B f(\omega/2\pi k_B T)\,. \quad (3)$$

The function $f(x)$ is shown in fig. 1. It changes sign at $\omega/\pi k_B T\approx 1$. This means that phonons with frequency $\omega\gtrsim\pi k_B T$ enhance the electronic specific heat and those with $\omega\lesssim\pi k_B T$ have the opposite effect. At $T\to 0$ all phonons are of the first kind and $f(x)\approx 1/6x$, so that

$$C_{el}(T\to 0)=(1+\lambda)\gamma_0 T\,, \quad (4)$$

where $\lambda=2\int_0^\infty d\omega\,\omega^{-1}\alpha^2F(\omega)$ is the electron–phonon coupling constant (see ref. [6]). In the opposite limit, $\langle\omega_{ph}^2\rangle\ll(2\pi k_B T)^2$, we have $f(x)=-x$ and

$$C_{el}(T\to\infty) = \gamma_0 T[1-6\lambda\langle\omega_{ph}^2\rangle/(2\pi k_B T)^2]\,, \quad (5)$$

where $\langle\omega_{ph}^2\rangle=2\lambda^{-1}\int_0^\infty d\omega\,\omega\alpha^2F(\omega)$. According to the neutron scattering experiments, in $YBa_2Cu_3O_7$ $\langle\omega_{ph}^2\rangle\approx(2\pi k_B T_c)^2$, which means that $C_{el}(T\approx T_c)/T$ is considerably different both from γ_0 and from $(1+\lambda)\gamma_0$.

Fig. 2(a) shows the temperature dependence of $C_{el}(T)$, calculated according to eq. (1) and using the spectral function $\alpha^2F(\omega)$, restored from the tunneling density of states of Bi–Sr–Ca–Cu–O [17] and normalized to $\lambda=2$. We believe that this spectral function is also relevant to $YBa_2Cu_3O_7$, since the main role in the electron–phonon interaction is played by the CuO-plane phonons. Furthermore, it has been successfully used for a description of the optical properties of $YBa_2Cu_3O_7$ [7]. For comparison, we also show in fig. 2(a) $C_{el}(T)$ for an Einstein spectrum with $\omega_{ph}=500\ cm^{-1}$ and $\lambda=2$.

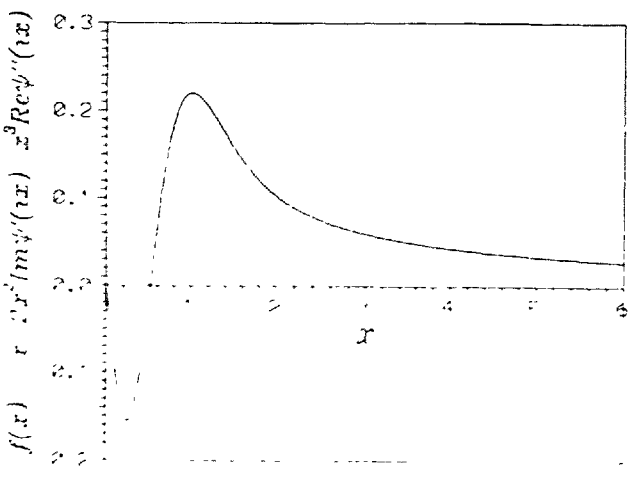

Fig. 1. The universal function $f(x)$ which appears in eq. (1).

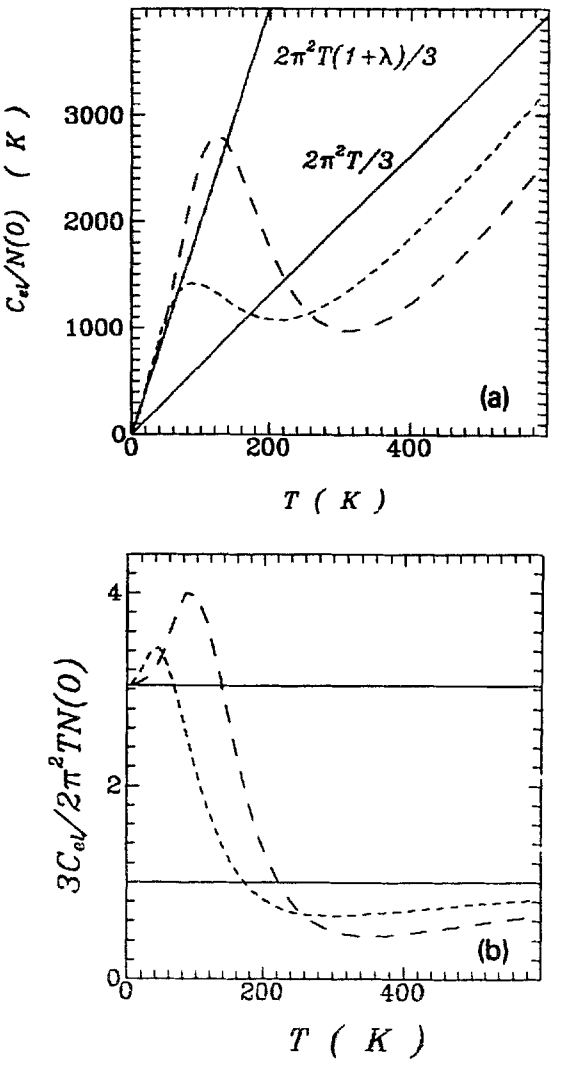

Fig. 2. (a) The temperature dependence of the electronic specific heat $C_{el}(T)$ calculated for the spectrum reconstructed from the tunneling data (long-dash line) and the Einstein model (short-dashed line) with $\lambda=2$. The straight lines correspond to the free particle limit and to $\gamma(0)T$. (b) The same as in (a) but for the normalized function $\gamma(T)/\gamma_0=3C_{el}/2\pi^2TN_b(0)$.

One can introduce the specific heat coefficient $\gamma(T)$ as

$$C_{el}(T)=\gamma(T)T, \tag{6}$$

where $\gamma(\infty)=\gamma_0=\frac{2}{3}\pi^2 k_B^2 N_b(0)$ is defined by the bare electron density of states at the Fermi level, and $\gamma(0)=(1+\lambda)\gamma_0$. The function $\gamma(T)$ is compared with γ_0 and $\gamma(0)$ in fig. 2(b). Apparently, $\gamma(T\approx T_c)$ is substantially different from both γ_0 and $\gamma(0)$. In table 1 we show the values of T_c (obtained by the numerical solution of the Eliashberg equation with $\mu^*=0.1$) and $\gamma(T_c)/\gamma_0$ for the spectral function of the same shape but with the different magnitudes (characterized by λ).

3. Superconducting state

In the Bardeen–Cooper–Schrieffer model the order parameter (the energy gap Δ) depends only on temperature, but not on the frequency. The fact that the interaction is retarded manifests itself only via the cut-off frequency. However, in the case of a strong retarded electron–electron interaction (as, for instance, for strong electron–phonon coupling) two complex functions are needed to describe the superconducting state. They are the renormalization function $Z(\omega,T)$ and the gap function $\Phi(\omega,T)$. The thermodynamics of a superconductor is defined by the values of these functions at Matsubara frequencies $i\hbar\omega_n=i\pi k_B T(2n+1)$. $\Phi_n\equiv\Phi(i\omega_n)$ and $Z_n\equiv Z(i\omega_n)$ are related to each other by the nonlinear Eliashberg equations, which are obtained by maximizing the free energy difference of the normal and the superconducting states [8,9]:

$$\frac{F_N-F_S}{N_b(0)}=2\pi T\sum_n \omega_n\left(\frac{Z_n\omega_n}{\sqrt{Z_n^2\omega_n^2+\Phi_n^2}}-\operatorname{sign}\omega_n\right)$$
$$+\pi^2T^2\sum_{n,m}\left\{\left[\frac{Z_n\omega_n}{\sqrt{Z_n^2\omega_n^2+\Phi_n^2}}\frac{Z_m\omega_m}{\sqrt{Z_m^2\omega_m^2+\Phi_m^2}}\right.\right.$$
$$\left.-\operatorname{sign}(\omega_n\omega_m)\right]\lambda(\omega_n-\omega_m)$$
$$+\frac{\Phi_n}{\sqrt{Z_n^2\omega_n^2+\Phi_n^2}}\frac{\Phi_m}{\sqrt{Z_m^2\omega_m^2+\Phi_m^2}}[\lambda(\omega_n$$
$$\left.-\omega_m)-\mu^*]\right\}, \tag{7}$$

where

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

The specific heat jump at $T=T_c$ is defined by the second term in eq. (7):

$$\Delta C_{el}(T_c)=T_c\partial^2(F_N-F_S)/\partial T^2|_{T=T_c}. \tag{9}$$

We have solved the Eliashberg equations for Φ and Z using the spectral functions $\alpha^2F(\omega)$ described in the previous section and the results are shown in table 1. In the weak coupling limit, $\lambda\ll 1$, the specific heat jump is $[\Delta C_{el}(T_c)/\gamma T_c]_{BCS}=1.43$. A strong retarded interaction makes $\Delta C_{el}(T_c)$ to depend both on the total coupling strength λ and on the shape of the spectral function. However, the specific heat jump *relative to the specific heat value at* T_c is relatively independent on the shape of $\alpha^2F(\omega)$, as illustrated by the calculations with the Einstein model and with

Table 1
Results of the numerical solution of the Eliashberg equation with $\alpha^2F(\omega)$ extracted from the tunneling data and scaled to get given coupling constants λ. The critical temperature, T_c, the specific heat renormalization, $C_{el}(T_c)/\gamma_0 T_c$, and the relative specific heat jump are shown. In the last row γ_0 are shown, calculated from $\Delta C(T_c)/\gamma_0 T_c$ and assuming $\Delta C(T_c)/T_c=77$ mJ/(mol f.u. K^2)

	$\lambda=1.5$	$\lambda=2$	$\lambda=2.5$	$\lambda=2$ [a]
T_c (K)	62.4	82.5	100.0	87.0
$C_{el}(T_c)/\gamma_0 T_c$	2.62	2.58	2.42	3.15
$\Delta C(T_c)/\gamma_0 T_c$	5.13	7.45	9.13	8.96
$\Delta C(T_c)/\gamma(T_c)T_c$	1.95	2.88	3.77	2.84
γ_0	15.0	10.3	8.4	8.6

[a] For a δ-function shape of $\alpha^2F(\omega)$

realistic spectral functions (table 1). A more detailed discussion of the influence of the shape of $\alpha^2F(\omega)$ on the thermodynamics of a superconductor can be found in the review in ref. [10].

It is interesting to compare the exact results of table 1 with the so-called α-model [11], often used by experimentalists (e.g., ref. [1]). This model assumes a single phenomenological parameter α, defined as $\alpha=\Delta(0)/k_BT_c$, and $\alpha_{BCS}=1.76$. Then

$$C_{el}(T)/\gamma(T)T=-t(\mathrm{d}/\mathrm{d}t)\{3\alpha\pi^2 \times \int_0^\infty \mathrm{d}x\,[f_x\log f_x+(1-f_x)\log(1-f_x)]\}, \quad (10)$$

where $t=T/T_c$, $f_x\equiv[1+\exp(\alpha/t)\sqrt{x^2+\delta^2(t)}]$, and $\delta(t)=[\Delta(T)/\Delta(0)]_{BCS}=3.06\sqrt{1-t^2}$. At $T=T_c$ the direct evaluation of the integral in eq. (10) gives

$$\Delta C_{el}(T_c)/\gamma(T)T_c=1.43(\alpha/\alpha_{BCS})^2. \quad (11)$$

The α-model assumes a finite gap at all $T<T_c$. In fact, for a strong coupling the excitation spectrum is gapless at $T\approx T_c$ [12], and it is not clear a priori how reliable this model is near T_c. We have checked this by comparing the results of the α-model with the exact solution for our model spectral function. For instance, a numerical solution of the Eliashberg equations for $\lambda=2$ gives $\alpha=2.55$. Substituting this into (11) gives $\Delta C_{el}(T_c)/\gamma(T_c)/T_c=2.99$, in good agreement with our value (table 1). What is important is that one should use in eq. (10) $\gamma(T=T_c)$ and not γ_0. Actually, in the original paper [11] it was assumed that $\gamma(T_c)\approx\gamma_0$, which, as shown above, is a very poor approximation. Unfortunately there is no simple equation for $\gamma(T_c)/\gamma_0$ so in practice the α-model, despite of its tempting simplicity, is not very useful.

4. Analysis of the experimental data

The electronic specific heat in the high-T_c superconductors seemed very mysterious in the first years after they had been discovered. The most important point was that a linear term in $C(T)$ below T_c had been observed. This fact was understood as a strong argument in favor of exotic superconductivity, but later the linear coefficient was shown to be very sample-dependent. Now the consensus among the experimentalists is that this term is not associated with the superconducting phase (see review in ref. [3]). Moreover, there are already many experimental attempts to separate the electronic contribution from the total specific heat at $T>T_c$. They give estimates for $\gamma(T_c)$ from 20 to 35 mJ/(mol f.u. K^2) [3]. Also, the jump at T_c, although again sample-dependent, is estimated for a fully superconducting sample to be 60–80 mJ/(mol f.u. K^2) [3]. It is tempting to use these values together with the band-structure calculations for γ_0 to estimate the electron–phonon coupling, and that was actually done in several experimental papers. However, leaving aside even the great uncertainty of the experimental data, a reliable estimate of the electron–phonon coupling strength cannot be made with the help of a simple theoretical model, as long as the coupling is strong.

Results of the numerical solution of the Eliashberg equation, presented above, allow, in principle, to perform this task. To do that, we shall make use of the experimental data of Phillips et al. [1], which give a unique possibility to determine the specific heat coefficient of $YBa_2Cu_3O_7$ at $T\approx0$. In this work the so-called "metallurgical model" was adopted [3], which assumes the existence of non-superconducting regions comparable to or larger than the superconducting coherence length. It was furthermore assumed that such regions are formed around the localized Cu^{2+} magnetic moments residing on some bulk defects in $YBa_2Cu_3O_7$, and that in addition there are inclusions of another chemical phase. Their concentrations (n_2 and n_1, respectively) were independently determined. It was shown that the experimentally observed coefficient $\gamma^*(0)$ can be excellently fitted by the following relation:

$$\gamma^*(0)=\gamma_1 n_1+\gamma_2 n_2. \quad (12)$$

Here γ_1 characterizes the impurity phase, and $\gamma_2=\gamma(0)V_2/V_0$, where $\gamma(0)$ corresponds to the ideal $YBa_2Cu_3O_7$, V_0 is the cell volume and V_2 is the volume around a Cu^{2+} moment transformed into the normal state. Also, a clear correlation with n_2 has been found for the specific heat jump at T_c, and for $\mathrm{d}\gamma/\mathrm{d}H$ at $T=0$ (H is the magnetic field). These data, in principle, provide a possibility to find not only $\gamma(0)$, but also $\gamma(T_c)$ and the coupling constant λ. Such an attempt was actually made in the original paper [1], but we believe (see the discussion below)

that the analysis of the measured data, though qualitatively right, was quantitatively incorrect, and has led to a substantial underestimate of $\gamma(0)$ and of λ. Since we believe that the experiment of ref. [1] is at the moment the most promising one, we shall here re-analyze these data.

As already mentioned, it was shown in ref. [1] that $\gamma^*(0)=\gamma_1 n_1+\gamma_2 n_2$. The numerical values are $\gamma_1=107$ and $\gamma_2=1470$ mJ/(mol f.u. K^2). Furthermore, it was shown that $\Delta C/T_c$ also depends linearly on n_2, $\Delta C^*(T_c)/T_c=\Delta C(T_c)/T_c\,(1-n_2/n_2^*)$, where $n_2^*=0.012$ and $\Delta C(T_c)/T_c=77$ mJ/(mol f.u. K^2). The measured $d\gamma/dH$ is proportional to the superconductivity fraction: $d\gamma^*/dH=h\Delta C^*(T_c)/T_c$, where $h=0.0035$ T^{-1}. One firm fact that follows from the measurements is that for the ideal $YBa_2Cu_3O_7$ the specific heat jump at T_c is 77 mJ/(mol f.u. K^2) and $d\gamma(0)/dH=0.27$ mJ/(mol f.u. K^{2}T). This does not mean, however, that $\gamma(0)$ is given by hH_{c2}, as assumed in ref. [1]. Strictly speaking, even if $d\gamma(0)/dH$ is determined by the Abrikosov vortices only, the simple relation $\gamma(0)\approx(d\gamma(0)/dH)H_{c2}$ holds only for a weak-coupled dirty superconductor. Since $YBa_2Cu_3O_7$ is closer to the clean limit, and most probably to the strong coupling, and since a good theory for $d\gamma(0)/dH$ in such a case is missing, we prefer to abandon this way of estimating $\gamma(0)$.

$\Delta C(T_c)/T_c$ is more useful, as long as we have the results shown in table 1, and adopt some value for the bare density of states at the Fermi level. The best available band structure calculations [13,14] give $N_b(0)=2.5$ states/eV, corresponding to $\gamma_0=11.8$ mJ/(mol f.u. K^2). The last row of table 1 shows γ_0 calculated from $\Delta C(T_c)/\gamma_0 T_c$ and assuming $\Delta C(T_c)/T_c=77$ mJ/(mol f.u. K^2) [18]. A good agreement is achieved of $\lambda=2$ and the shape of the Eliashberg function extracted from the tunneling experiment [17]. (Note that the calculated T_c in this case is also close to the experiment.)

In ref. [1] yet another way to estimate $\gamma(0)$ was suggested: to extrapolate $\gamma^*=\gamma_2 n_2$ to $n_2=n_2^*$, that is, to the value of n_2 where the extrapolated $\Delta C(T_c)$ is zero. An assumption which was indirectly used was that the superconductivity fraction for a given concentration of the localized moments n_2 is the same at $T=0$ and n_2^* at T about 5 K below T_c (the measurements of γ are taken at $T\approx 0$ and those of ΔC close to T_c). Such a procedure gives 16 mJ/(mol f.u. K^2), which should be corrected for the possible increase of the superconductivity fraction at $T\to 0$. To estimate this correction theoretically is hardly possible. An interesting option is provided by recent optical experiments [15,16], where it was found that the optical conductivity can be fitted accurately by a sum of a normal (Drude) and a superconducting (Bardeen–Mattis) contribution. From ref. [16], for instance, the normal fraction at T_c-5 K is about 2.4 times larger than that at 0 K. Thus we obtain $\gamma(0)\simeq 35$–40 mJ/(mol f.u. K^2), which is close to that estimated from $\Delta C(T_c)$ for $\lambda=2$. On the other hand, this value of λ is close to $\lambda_{tr}\approx 1.5$ which was recently extracted from the measured resistivity slopes [19].

5. Conclusions

The first conclusion is that for a quantitative analysis of the specific heat data in the normal and superconducting state in a metal with a strong electron–phonon (or any other electron–boson) coupling it is necessary to use a realistic model for the Eliashberg function and to solve numerically the relevant equations. We have performed this task for $YBa_2Cu_3O_7$, using the Eliashberg function extracted from the tunneling experiments, and have re-analyzed the recent experimental results from this point of view. The value for the electron–phonon (electron–boson) coupling λ that we have extracted from the experiment is close to 2.

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