Estimation of the electron-phonon coupling in $YBa_2Cu_3O_7$ from the resistivity

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Recent data on the single-domain resistivity of $YBa_2Cu_3O_7$ are analyzed using the local-density-approximation calculations of the plasma frequencies and Fermi velocities. It is shown that the transport coupling constants λ_{tr} for all three directions come out to be of the same order, namely about 1.5. The corresponding mean free path $l=11$ Å at $T=300$ K, which dispels the popular notion that the local-density-approximation band structure yields unreasonably large λ and small l values. The possibility of an anisotropy in λ_{tr} and of a difference between λ and λ_{tr} is discussed with the help of results from rigid-muffin-tin calculations of the Hopfield factors η.

$YBa_2Cu_3O_7$ appears to be, at the moment, the best studied high-T_c material. Now twin-free single crystals have become available for experiments. In particular, several experimental estimates of the plasma frequencies are available.[1,2] Highly accurate band-structure calculations have been recently performed[3,4] (note that the recent angle-resolved photoemission experiments[5] prove the validity of conventional band-structure calculations for $YBa_2Cu_3O_7$). Finally, resistivity anisotropy has been measured.[6] These data, if used together, provide a unique possibility to estimate the electron-phonon coupling constants. In fact, there already were some attempts of this kind.[7,8] However, they used much less reliable data—collected on twinned or even ceramic samples—and also referred to band-structure calculations less accurate than those presently available, which is especially important with regards to the mean-free-path estimation. The goal of this paper is to reconsider the subject with these more appropriate tools.

We recall that the phonon-limited resistivity in the linear region ($T \gtrsim \Theta_D/4$) may be written as

$$\rho(T)=8\pi^2\hbar\omega_p^{-2}k_B T\lambda_{tr} , \tag{1}$$

where $(\hbar\omega_p)^2$ is proportional to the electron velocity averaged over the Fermi surface (FS):

$$\langle N(0)v^2\rangle=\sum_{\mathbf{k},\alpha}\delta(\varepsilon_{\mathbf{k}\alpha})\mathbf{v}_{k\alpha}^2 \tag{2}$$

($\varepsilon_{\mathbf{k}\alpha}$ and $\mathbf{v}_{\mathbf{k}\alpha}$ are the energy and the velocity of an electron with the wave vector $\mathbf{k}$ in band α), and transport coupling constant λ_{tr} is defined by

$$\lambda_{tr}=2\sum_{\nu}\sum_{k,\alpha}\sum_{q,\beta}\delta(\varepsilon_{k\alpha})\delta(\varepsilon_{q\beta})(\mathbf{v}_{k\alpha}-\mathbf{v}_{q\beta})^2 \times M^{v2}_{\mathbf{k}\alpha,q\beta}/2\langle N(0)v^2\rangle , \tag{3}$$

where $M^{\nu}_{\mathbf{k}\alpha,q\beta}=\sum_t\langle\mathbf{k}\alpha|(\delta V/\delta\mathbf{R}_t)\mathbf{e}_{\nu t}|k\beta\rangle/\sqrt{2m_t\Omega_{\nu,\mathbf{k}-\mathbf{q}}}$ is the electron-phonon matrix element. Here $\mathbf{e}$ and Ω are the polarization vector and the frequency of the corresponding phonon. The superconducting coupling constant is defined in an analogous way:

$$\lambda=2\sum_{\mathbf{k},\alpha}\sum_{\mathbf{q},\beta}\delta(\varepsilon_{\mathbf{k}\alpha})\delta(\varepsilon_{q\beta})M^2_{\mathbf{k}\alpha,q\beta}/N(0) . \tag{4}$$

A standard assumption, used, for instance, in Refs. 7 and 8, is that $\lambda\cong\lambda_{tr}$. Using this assumption, together with Eq. (1), one can extract λ from the resistivity measurement, as it was done in Refs. 7 and 8. However, at that time there were no reliable single-crystal resistivity data. Instead, the polycrystal line data were used which led to the conclusion[8] that $\lambda=2.8$, which was considered unphysically large. As an estimate for $\hbar\omega_p$ the value 3.6 eV, calculated by Mattheis and Weber, was used. Then subsequently the authors made the further assumption that the mean free path $l=\langle v_F\rangle\tau_{e-ph}=\hbar\langle v_F\rangle/2\pi T\lambda$, where $\langle v_F\rangle$ may be estimated as $\sqrt{\langle N(0)v^2\rangle/N(0)}$. This led to the conclusion that $l=1.7$ Å, which is unphysically small. In fact, v_F varies greatly over the FS, and because of that l was severely underestimated in Ref. 8 (see below). Thus the conclusion[8] was that the true value of $\hbar\omega_p$ is 1.1 eV and that λ is about 0.3. This conclusion was in line with the then popularly held notion that band theory was irrelevant to the study of the high-T_c superconductors, and that the electron-phonon interaction plays a secondary role. However, in the three years since then, more evidence that the electron-phonon interaction is strong (see, for instance, Ref. 9 for a list) has been accumulated and it is beginning to be realized that the calculated band structures are not very far from reality. To the last point we can mention the recent photoemission experiments[5] and the fact that the discrepancy between the estimations of $\hbar\omega_p$ from the optical spectroscopy and the band-structure calculations is getting smaller. Indeed, the analysis below shows that the latest single-domain resistivity data can be easily reconciled with the band-structure calculations and that the corresponding electron-phonon coupling also is very reasonable.

Friedman *et al.*[6] give, for the resistivity slope $d\rho/dT$,

the values of 0.6, 0.25, and 12.5 $\mu\Omega$ cm/K for the x, y and z directions, respectively, with the z value claimed to be less reliable than the other two. In Fig. 1 we have plotted λ_{tr} as a function of $\hbar\omega_p$ for the three directions, taking the values above (the y axis is parallel to the chains). We have marked $\hbar\omega_p$ corresponding to the LDA band-structure calculations. There exist only a few optical experiments for single crystals.[1,2] In these two works, only the values of the *screened* $\hbar\omega_p$ are given, namely 0.86 and 1.03 eV in the x direction and 1.49 and 1.58 eV in the y direction in Refs. 1 and 2, respectively. Note that the unscreened $\hbar\omega_p$ is larger by the factor $\sqrt{\epsilon_\infty}$, where ϵ_∞ is at least 4. This shows that calculated and measured $\hbar\omega_p$ agree qualitatively, but it is not clear yet which data are more reliable. It is worth mentioning that the penetration depth, often used for estimating $\hbar\omega_p$, in fact gives $\hbar\omega_p$ renormalized by the electron-phonon coupling, which makes such estimates even less reliable. In the following discussion we shall use always the calculated $\hbar\omega_p$, keeping in mind that some overestimation of $\hbar\omega_p$ is still possible.

As seen from Fig. 1, despite the enormous anisotropy of the resistivity, all three values of λ_{tr} agree very well. In fact, use of the calculated $\hbar\omega_p$ yields λ_{tr} values of 1.4, 1.8, and 3.7, in the x, y, and z direction, respectively. One should keep in mind that both the experiment and the calculations are less accurate in the z than in the x and y directions, the former due to additional scattering mechanisms for the z-axis current, and the latter due to smallness of the v_{kz}. In fact, many groups are convinced that the conductivity in the z direction is nonmetallic. So, the value that we give for $\lambda_{tr}(z)$ is included more for completeness, as in Ref. 6, and should not be taken too seriously. However, the x-y anisotropy is a reliable quantity. The fact that ϵ_∞ is unknown makes it difficult to obtain experimental values for $\hbar\omega_{px}$ and $\hbar\omega_{py}$. Assuming ϵ_∞ is the same in the x and y direction, we obtain an anisotropy of $\hbar\omega_p$ slightly less than the calculated ones, so that $\lambda_{tr}(x)/\lambda_{tr}(y) \simeq 1$.

The reasoning above suggests that λ_{tr} for all three directions is about the same, 1.5–1.7, and most probably the superconducting λ is also of the same magnitude. However, it may also be that the x-y asymmetry of λ_{tr} according to the calculated $\hbar\omega_p$ is not an artifact. It is instructive to look at the electronic structure in order to understand possible causes for such an anisotropy.

The standard method for calculating electron-phonon coupling in the framework of the conventional band-structure calculation is due to the so-called rigid-muffin-tin approximation (RMTA),[10] which may be readily generalized to the case of phonon-limited resistivity.[11] This approximation is well understood for classical superconductors; however, its accuracy for the high-T_c materials is unclear. It has been used for them, nevertheless,[9,12] and we believe that it is reasonable for qualitative analysis, while one should refrain from making quantitative conclusions.

Equation (1) for λ_{tr} may be decomposed into two parts: λ_{20} and λ_{11}, where the first part includes v_k^2 and the second $v_k \cdot v_q$. A difference between λ and λ_{tr}, as well as an anisotropy of λ_{tr}, may come from both parts. However, for transition metals it is known that $\lambda_{11} \ll \lambda_{20}$.[11] There are two reasons for that: First, it may be shown that in the RMTA a small numerical factor appears before the corresponding expression (see Ref. 11 for details) and, second, averaging of the vector quantity v_k over the FS introduces generally a smaller result than averaging the scalar expression v_k^2, independent of the way of averaging. So we shall concentrate on λ_{20}. Then, we shall use instead of λ the corresponding Hopfield factors

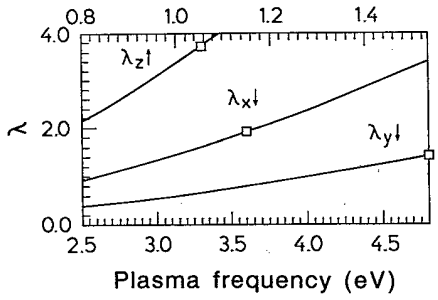

FIG. 1. Transport electron-phonon coupling constant as a function of the plasma frequencies $\hbar\omega_p$, as derived from the experimental resistivity slopes (Ref. 5). The markers correspond to the $\hbar\omega_p$ calculated from the LDA band structure (Ref. 3).

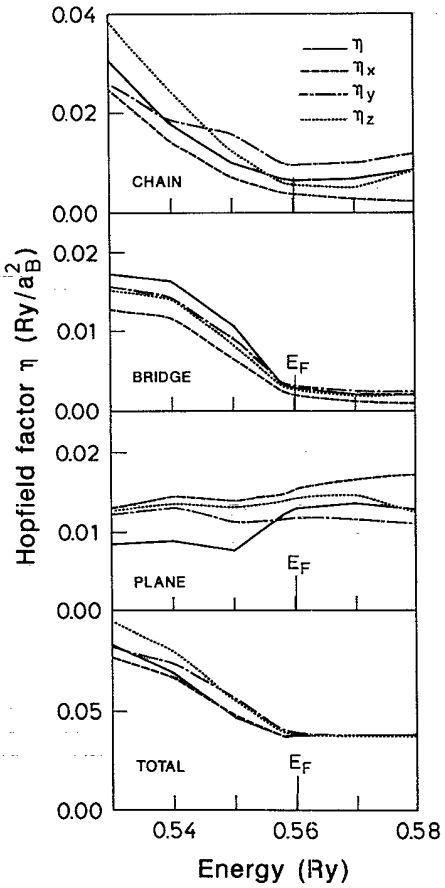

FIG. 2. Transport and superconducting Hopfield factors as calculated in the RMT approximation.

η, which differ from λ's in a sense that the phonon dependence is excluded:

$$\eta = \sum \eta_t = \sum_t \sum_{k,\alpha} \sum_{q,\beta} \delta(\epsilon_{k\alpha})\delta(\epsilon_{q\beta}) \times \langle \mathbf{k}\alpha|\delta V/\delta \mathbf{R}_t|\mathbf{q}\beta\rangle|N(0)\,, \quad (5)$$

and $\eta_{\rm tr}$ is defined in the same way. In the RMTA this can be rewritten as

$$\eta_t = \sum_{L,L_1,L_2,L_3} N^t_{LL_1} W^t_{L_1L_2} N^t_{L_2L_3} W^t_{L_3L}/N(0)\,, \quad (6)$$

where W is the muffin-tin potential matrix element and N is the density matrix in the angular representation. For η_{20} one should substitute N_{LL_1} in (6) by $\langle Nv^2\rangle_{LL_1}$ and $N(0)$ by $\langle N(0)v^2\rangle$. A standard approximation is to "cancel out" the factor v^2 and to neglect the difference between η and $\eta_{\rm tr}$. However, it is incorrect when the electron velocity changes too much over the Fermi surface.[11] To check this, we have made the calculations of η's according to the algorithm described in Ref. 11. The results are shown in Fig. 2. We see that the total η's do not show significant anisotropy, or any difference between η and $\eta_{\rm tr}$. The same is true for the partial Hopfield factors of the "bridging" atoms (bridging O and Ba). However, the plane atoms' η shows a considerable anisotropy of the same sign as that extracted from the experiment (Fig. 1). The anisotropy of chains' η is opposite. The cancellation occurs only if the hardness of the chain phonon is the same as for plane ones, which is not necessarily so. This provides an explanation of the possible ρ_x/ρ_y anisotropy from the band-structure point of view.

The last point is due to the mean free path l. There are parts of the FS with a small v_F and a large density of states, and other parts with a much larger v_F. The transport occurs by scattering of the *fast* electrons into regions of the FS with large densities of states. Thus the v_F to be used in estimating l must be taken from the "fast" parts of the FS where it is about 5.5 eV a_B, and not as an average over the whole FS, as has been done in Ref. 8. At $T=300$ K, it gives $l \approx 11$ Å, which is reasonable in that it does not contradict the fact that $YBa_2Cu_3O_7$ is, presumably, a clean-limit superconductor. On the other hand, some corrections to the clean-limit results are possible, for instance, to H_{c2} (cf. Ref. 13).

To conclude, we have used the unscreened plasma frequencies from conventional band-structure calculations to extract the values of the transport electron-phonon coupling constant and found that they are close to each other: All three of them have values around 1.5–2. This suggests that the superconducting coupling constant λ should be of the same order of magnitude. The corresponding room-temperature mean free path is about 11 Å. The difference from the earlier estimations[8] comes mainly from the following two factors: better data on the resistivity and more accurate Fermi velocities. We have also investigated the corresponding Hopfield factors (the electronic part of λ) in the rigid-muffin-tin approximation and discussed possible sources of the anisotropy in $\lambda_{\rm tr}$, if any, as well as of the difference between λ and $\lambda_{\rm tr}$.

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