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Superconducting and transport electron-phonon coupling constants in $YBa_2Cu_3O_7$: effect of the interband anisotropy.

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Using previously reported first-principle frozen-phonon LDA calculations we have calculated the effective superconducting and transport electron-phonon coupling constants. We have taken into account the anisotropy due to the difference between four bands crossing the Fermi level in $YBa_2Cu_3O_7$, and found that because the anisotropy influence both electron-phonon coupling constants, but *in the opposite direction*, the superconducting constant becomes larger than the transport one The absolute values of the effective coupling constants is close to 2. The superconducting gaps for the different bands vary by nearly an order of magnitude. We also discuss how various experiments might have been explained in terms of the interband anisotropy

It is well known that if a metal has several bands with different electron-phonon couplings crossing the Fermi level, such an anisotropy can increase the superconducting transition temperature [1, 2], and decrease the phonon-limited resistivity [3]. In the last years the first issue has been addressed several times in connection with the $YBa_2Cu_3O_7$ high-T_c superconductor (see, e.g., [4]), although no quantitative estimates have been done by now. However, the anisotropy effects on the electrical transport in this material have never been discussed, although in principle they are of the same order and should be treated on the same footing. Furthermore, LDA calculations of the Fermi surface of $YBa_2Cu_3O_7$, confirmed by several experiments, uncovered four different sheets of the Fermi surface, suggesting that instead of the usually used two-band model the four-band model should be used.

Recently very accurate LDA calculations for the coupling of the electrons with selected phonons in $YBa_2Cu_3O_7$ have been performed[5] which allow to put the problem on a more quantitative basis. In this paper, we make use of these calculations to estimate the effect of the interband anisotropy in $YBa_2Cu_3O_7$ on both the effective superconducting coupling constant λ_s and the effective transport coupling constant λ_{tr} (apparently, the effect is opposite in both cases)

The following notations are used (i and j label different bands, $E_F = 0$, $\epsilon_{\mathbf{k}}$ and $\mathbf{v}_k$ are electron energies and velocities, α is a Cartesian index):

$$
\begin{aligned}
&N = \sum_i N_i = \sum_i \sum_{\mathbf{k}} \delta(\epsilon_{i\mathbf{k}}) \\
&W^\alpha = \sum_i W_i^\alpha = \sum_{\mathbf{k}} (v_{i\mathbf{k}}^\alpha)^2 \delta(\epsilon_{i\mathbf{k}}) \\
&P_{\mathbf{k},\mathbf{k}'} = \sum_\nu 2(M_{\mathbf{k},\mathbf{k}'}^\nu)^2 / \Omega_{\mathbf{k}-\mathbf{k}',\nu} \\
&l_{ij} = \sum_{\mathbf{k}\mathbf{k}'} P_{\mathbf{k},\mathbf{k}'} \delta(\epsilon_{i\mathbf{k}}) \delta(\epsilon_{j\mathbf{k}'}) = U_{ij} N_i N_j \qquad (1) \\
&r_{ij}^\alpha = t_{ij}^\alpha / W_i W_j; \quad t_{ij}^\alpha = t_{ij}^{\alpha(out)} - t_{ij}^{\alpha(in)} \\
&= \delta_{ij} \sum_{\mathbf{k}\mathbf{k}'n} P_{\mathbf{k},\mathbf{k}'} (v_{i\mathbf{k}}^\alpha)^2 \delta(\epsilon_{i\mathbf{k}}) \delta(\epsilon_{n\mathbf{k}'}) \\
&- \sum_{\mathbf{k}\mathbf{k}'} P_{\mathbf{k},\mathbf{k}'} v_{i\mathbf{k}}^\alpha v_{j\mathbf{k}'}^\alpha \delta(\epsilon_{i\mathbf{k}}) \delta(\epsilon_{j\mathbf{k}'}).
\end{aligned}
$$

Here $M_{\mathbf{k}\mathbf{k}'}$ is the standard electron-phonon matrix element for the branch ν, corresponding phonon frequency being Ω. As usually, we shall neglect in a first approximation the "scattering-in" term, which reduces the last equation to

$$
t_{ij}^\alpha = t_{ii}^{\alpha(out)} \delta_{ij} = \sum_j \bar{U}_{ij} N_j W_i .
$$

Matrices l and t define the mass renormalization constants for each sheet:

$$
\lambda_i = \textstyle\sum_j l_{ij} / N_j
$$

and both isotropic coupling constants

$$
\lambda_s^0 = \sum_{ij} l_{ij} / N = \lambda_s^0 = \sum_i \lambda_i N_i / N
$$

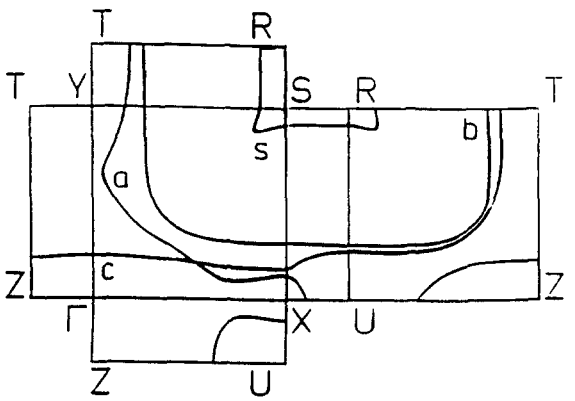

Figure 1 Fermi surface of $YBa_2Cu_3O_7$

$$\lambda^0_{tr} = \sum_{ij} t_{ij}/W$$

and the effective coupling constants with anisotropy being included [2, 3]

$$\begin{aligned} \lambda_s^{eff} &= \max[\text{eigenvalues}\{l_{ij}/N_j \equiv U_{ij}N_i\}] \\ \lambda_{tr}^{eff} &= W/\sum_{ij}(r^{-1})_{ij} \end{aligned} \qquad (2)$$

It is easy to show, and has already been shown in the Refs.[2, 3], that $\lambda_s^{eff} \geq \lambda_s^0$, while $\lambda_{tr}^{eff} \leq \lambda_{tr}^0$. The equalities hold when the average interactions U and $\bar{U}$ are isotropic, i.e., U_{ij} is the same for all ij. A useful illustration to this is provided by a realistic assumption that $\bar{U}_{ij} = U_{ij}$. In this case λ_s^0 is obtained by averaging λ_i with the weights N_i, λ_{tr}^0 by the same way with the weights W_i, and to obtain λ_{tr}^{eff} one has to average the inverse quantity, $1/\lambda_i$. A direct consequence is that if $\lambda_s^0 \approx \lambda_{tr}^0$, then always $\lambda_s^{eff} \geq \lambda_{tr}^{eff}$.

Let us now make contact with first-principle calculations for $YBa_2Cu_3O_7$ [5]. In the Refs.[5] frozen-phonon calculations of the electron-phonon coupling with 17 selected phonons were reported, which are essentially exact within the LDA. Furthermore, these phonons couple to different inter- and intraband transitions so one can get some hint about the average interaction matrix $\bar{U}$

Five of the phonons in questions are zone center (Γ) phonons. For those we have calculated [5] the

Table 1
Partial densities of states N_i and partial integrated Fermi velocities W_i

	s	b	a	c	total
N_i,st./Ry/spin	9 2	5.9	14.4	5.7	35.1
$W_{i,x}$, st Ry·a_B^2	0 02	0 75	0 46	0 04	1.28
$W_{i,y}$, st Ry·a_B^2	0.03	0 83	0.33	1 05	2.24
$W_{i,z}$, st Ry a_B^2	0.00	0 01	0 06	0 04	0 11

following quantity·

$$\lambda_\Gamma = \sum_{i\mathbf{k}} P_{i\mathbf{k},i\mathbf{k}}\delta(\epsilon_{i\mathbf{k}}) = \sum_i U_{ii}(0)N_i$$

The last equality defines of $U_{ii}(0)$, which are shown in Table 2. For 12 other phonons we have calculated λ's as follows·

$$\begin{aligned} \lambda(\mathbf{q}) &= \frac{1}{N}\sum_{ij\mathbf{k}} P_{i\mathbf{k},j\mathbf{k}+\mathbf{q}}\delta(\epsilon_{i\mathbf{k}})\delta(\epsilon_{j\mathbf{k}+\mathbf{q}}) \\ &= \sum_{ij} U_{ij}(\mathbf{q})\zeta_{ij}(\mathbf{q}), \end{aligned}$$

where $\zeta_{ij}(\mathbf{q})$, proportional to the electronic susceptibility, is defined in Ref.[5].

$$\zeta_{ij}(\mathbf{q}) = \lim_{\omega\to 0}\chi(\mathbf{q},\omega)/\omega = \sum_{\mathbf{k}}\delta(\epsilon_{i\mathbf{k}})\delta(\epsilon_{j\mathbf{k}+\mathbf{q}}).$$

The calculated values for $U_{ij}(\mathbf{q})$ are given in Table 2 In order to be able to use Eqs.1 we average the elements of the matrix $U_{ij}(\mathbf{q})$ over three, two or one phonon, and the 2 elements remained unknown, U_{sb} and U_{sa}, we approximate by U_{sc} (We use notations of Ref.5b. *S*tick, plane *B*onding, plane *A*ntibonding and *C*hain bands, with one important correction: Since the fourth and the third band interchange they character when k_x becomes larger than $\approx 0\ 58\pi/a$ we ascribed the parts of the fourth *and* the third band which have predominantly chain character to the *C*-band and the rest to the *A*-band). Then we come to the matrix $\langle U_{ij}\rangle$ which is also shown in Table 2, and calculate all four coupling constants discussed above, assuming that $\bar{U}_{ij} = U_{ij} = \langle U_{ij}\rangle$. The calculations give the following numbers

	λ_{sc}	λ_{tr-x}	λ_{tr-y}	λ_{tr-z}
λ^0	1.49	1.51	2.01	2 08
λ^{eff}	1.95	1 47	1 74	1 96

Table 2
Interaction matrix U_{ij} averaged over different phonons in Γ, Y and S points, and the total average

	U_{ij}, mRy			
ij	Γ	Y	S	total
ss	0.886	—	—	0.886
sa	—	0.046	—	0.046
sb	—	—	—	↓
sc	—	—	—	↓
aa	1.045	0.470	3.940	1.818
ab	—	0.793	0.043	0.418
ac	—	5.685	0 444	3.064
bb	0 608	0.381	2 330	1.106
bc	—	7.016	0.402	3.710
cc	0.328	—	—	0.328

Note that, first, the interband anisotropy increases the effective superconducting coupling constant by 31%, and reduces the transport coupling constant by 3–14%. Accidentally, the anisotropy of W cancels to large extent the anisotropy of U.

Lastly, we have used the BCS equation for the gaps [1]

$$\Delta_i = \sum_j U_{ij} N_j \Delta_j F(\Delta_j) \qquad (3)$$

$$F(\Delta) = \int_0^{\omega_D} dE \tanh\left(\frac{\sqrt{E^2+\Delta^2}}{2T}\right)/\sqrt{E^2+\Delta^2}$$

to calculate the ratios $\Delta_i/2\omega_{ph}$. The result is shown in Fig.2. Of course, one should not take these numbers too seriously, first of all due to uncertainty of U, but also because the strong-coupling effects on Δ cannot be neglected (contrary to the calculations of the effective λ's; cf. [2]). Nevertheless, if one believes that the qualitative picture is correct, it provides appealing explanation of several experimental facts:

1)If we assume the cut-off frequency in Eq.3 to be 350 cm^{-1}, then our largest (chain) gap (16% weight) will be 650 cm^{-1}, the plane gaps at 330 (A, 41%) and 170 (B, 17%), and the stick gap will be at 35 cm^{-1} with the weight 26%. Recent measurements of L. Genzel et al, [10]using highly accurate Fourier-interferometer technique, are consistent with a multiple gap structure where about 15% of the total weight is placed in a gap at 330 cm^{-1}, about 13% at 220 cm^{-1}, about 18% at 180 cm^{-1}, and the rest 56% are distributed between 70 and 140 cm^{-1} (and *not*consistent with any single gap). This is in partial agreement with our calculations, the main discrepancy being the misplacement of the chain gap (be it at 50-150 cm^{-1}, the agreement would be very good). Interestingly, the same measurements on Fe-substitited samples (Fe is known to go into chains) show no changes in the gap structure above 150 cm^{-1}, in accord with the above assumption that the chain gap is misplaced. A reason for such a misplacement may be that the *intra*chain pairing interaction is fairly weak, and the *induced* gap is so large only because the chain-plain interaction turns out to be so strong. The latter comes in our calculations only from Y-phonons, and it is likely that other phonons would not emphasize this interaction so drastically

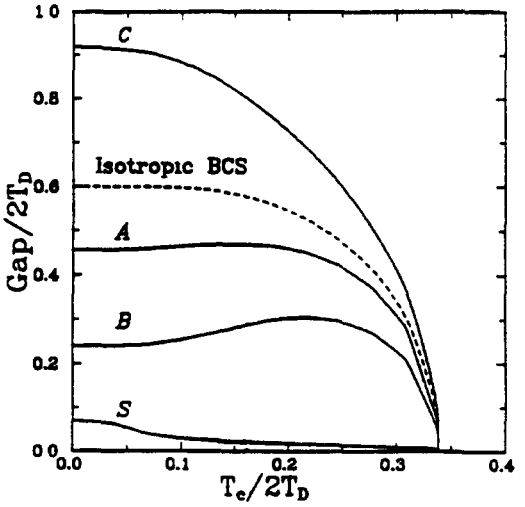

Figure 2. Temperature dependence of the superconducting gaps

2) The latest tunneling experiments show a finite density of states below gap at T~ 0. This can be explained easily by an anisotropic gap, like in d-pairing, or essentially in the same way by an interband anisotropy like that discussed above. Moreover, some experiments explicitely suggest a

multigap structure. Presumably, recent explanations of the temperature dependence of the NMR relaxation time in terms of d-pairing would also be valid in this case

3) Many experiments (optics, penetration depth, tunneling) give much slower T-dependence for the gap than in the BCS theory, but more like the 2-fluid model. It can be seen from Fig.2 that our plane gaps behave in the same way. Moreover, the fact that the stick gap comes out so small, brings an interesting analogy with the classical 2-fluid model. It would be interesting to revisit these experiment from such point of view

4) Without going into details, let us mention that there are indications that the critical field for the stick is much smaller than for the planes. This is in accord with our calculations.

It is interesting to compare our λ's with the experiment. All variety of experimental estimates can be found in the literature, from 0.3 to 8. We shall try to use the values obtained with the help of the same band structure that we exploit in this work Shulga et al [6] analyzed the specific heat measurements of Phillips et al [7] and got for λ (in our notations, for λ_s^0) ≈ 2. As the bare density of states they used that calculated in Ref.[5]. Mazin and Dolgov[8] used the plasma frequencies from the same calculations (i.e., the W's shown in Table 1) together with the resistivity coefficients measured by Friedmann et al [9] to get the effective transport constants of 1.8, 1.4 and 3.7 for x, y and z, respectively (the last value was very unsure because of experimental difficulties). Qualitatively, all these value compare favorably with the calculated λ's above. Note that taking into account such a correlation-induced renormalization in N and W would bring both estimates down. For instance, if one would assume a renormalization of about 2, in terms of the effective mass, as suggested by some photoemission experiments, our calculated λ's and W's would be twice smaller, and N's twice larger. Correspondingly, the specific heat λ would become $\lambda' = (1+\lambda)/2 - 1 \approx 0.5$, and the resistivity λ's would be $\lambda' = \lambda/2 \approx 0.9$, 0.7 and 1.8, still being reasonably consistent with the calculations.

To summarize, we report first microscopical estimations of the magnitude of the electron-phonon coupling in $YBa_2Cu_3O_7$, taking into account the interband anisotropy. We find rather large coupling, and also show how the superconducting coupling can be enhanced due to this anisotrpoy. The fact that the anisotropy effects turns out to be very important in $YBa_2Cu_3O_7$ suggest that the experimentaly observed transport electron-phonon coupling constants should not be uncautionally used in the context of the superconductivity, since the effective superconducting coupling constant can be much larger.

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