The Optical conductivity resonance from an exact description of the electronic states around the Fermi energy.

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Abstract

In this paper we show that the optical conductivity can be calculated to agree with experiment if the details of the electronic states around the Fermi level are taken into account with some care. More precisely, we present a calculation of the optical conductivity in YBa$_2$Cu$_3$O$_7$ on the basis of an exact (ab initio) three dimensional electronic band structure calculation from which we extract the information on the bands near the Fermi energy that can be associated to the CuO$_2$ plane-carrier states. To simulate the superconducting state we superimpose a gap to these bands alone. On these basis, we calculate from the known Kubo-Greenwood formula, the optical conductivity in the normal and in the superconducting state. Our calculation agrees with the experimental result even in the higher part of the frequency spectrum. Our way of calculating the resonance suggests a model of evolution for the bands under the effect of doping consistent with the recent experimental findings that the optical resonance can disappear while the sample remains superconducting. An important conclusion of this paper is that the resonance depends mostly on the details of the electronic band structure. It is enough to take into account the effect of the superconducting transition through a single parameter (the gap). No details on the mechanism are needed so no mechanism can be tested on this basis. Our calculation suggests a model of evolution for the bands around the Fermi energy under doping that gives some microscopic foundations to the the recent experiments that show unambiguously that the optical resonance cannot be the cause of superconductivity. Most importantly, it indicates how the background is built up and depends on the electronic excitations accessible through values of the energy transfer on a wider interval than those causing the resonance. These electronic excitations determine the allowed optical transitions. From this point of view, it is an obvious consequence that the background is with small differences, common to all the cuprates having a CuO$_2$ plane. But the most important conclusion is that the background contains essentially the same physics as the resonance does and so does not have any detailed information on the superconducting mechanism as well, contrary to the conclusions of recent work.
I. INTRODUCTION.

In a recent publication, J. Hwang, T. Timusk and G. D. Gu [1] have reported an infrared spectroscopy study of the optical conductivity as a function of doping in various samples of Bi-2212. The effect of doping into Bi-2212 is to lower both the critical temperature, $T_c$, and the intensity of the resonance peak that appears in the superconducting state. This fact represents a unique opportunity to dissociate the resonance from the mechanism of superconductivity by means of a direct experiment. These authors have reported the fabrication of several superconducting samples of Bi-2212 with different doping content up to a particular one with 0.23 holes per Cu atom that did not show the resonance anymore. Its high critical temperature ($T_c=55K$) demonstrates that superconductivity in this sample is still robust. This experimental fact leads to the sharp conclusion that the resonance cannot be taken as the cause of superconductivity. Nevertheless, since the resonance appears in the superconducting and only in the superconducting state, it should be somehow tightly bound to the phase transition itself.

A resonance peak [2, 3] appears also in the spin polarized magnetic susceptibility, $\chi_s(\omega)$, at a frequency, $\omega_{res}$, that is characteristic of the specific sample. The magnetic resonance peak appears as a common excitation to the superconducting state of all high-Tc superconductors investigated by Inelastic Neutron Scattering (INS) so far with a maximum $T_c \approx 90K$. The existence of the excitation does not depend on the number of CuO$_2$ planes per unit cell: one for Tl$_2$Ba$_2$CuO$_{6+\delta}$, two for YBa$_2$Cu$_3$O$_{6+\delta}$ and Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$. It has never been observed in the monolayer system La$_{2-x}$Sr$_x$CuO$_4$ with maximum $T_c \approx 40K$ [4]. Although, there are several proposals in the literature [4] to trace the origin of the resonance to a mode of magnetic origin, we want to point to a direct and simple relation between the effect that the superconducting phase transition has on the electronic band structure, and the resonance itself.

J. Hwang, T. Timusk and G. D. Gu present in their quoted paper the optical single-particle self-energy which is directly related to the optical conductivity. They call the resonance that they find "the resonance optical mode". This resonance optical mode in the optical conductivity, $\sigma_{opt}(\omega)$, is produced at the same characteristic frequency, $\omega_{res}$, as in the susceptibility. Both resonances differ on details though. It is important to notice that the two thermodynamic functions can be considered mutually excluding each other in the sense that while
the non-zero contributions to the matrix elements in the spin polarized susceptibility are intra-band, in the optical conductivity these are inter-band transitions. In that sense it might appear at first sight surprising that the two resonances have the same origin. Carbotte et al. assumed that the resonance in $\chi_s(\omega)$ can be related to the effective spectrum of the spin fluctuations and used it to construct the Eliashberg function of the conventional theory of superconductivity from which all the information on the thermodynamics follows. They have used this knowledge to calculate the resonance in the optical conductivity, $\sigma_{opt}(\omega)$, in the superconducting state. Their result agrees with experiment. They further used an inversion procedure that allows to extract information about the Eliashberg function from the optical conductivity. In this way they got back their assumed Eliashberg function (directly related to $\chi_s(\omega)$ in their work). The procedure used by Carbotte et al. establishes an essentially common origin to the resonance in both thermodynamic functions (not to the functions themselves). Since the experiments by J. Hwang et al. neatly show that the resonance in the optical conductivity is not responsible for superconductivity, it is natural to expect that the resonance in the susceptibility will not be responsible for superconductivity as well and therefore cannot be directly related to the real Eliashberg function. But an important point is that Carbotte et al. show explicitly that the resonances in both functions have a common origin. The resonance has been the object of a substantial amount of work in the last years.

ARPES experiments by Lanzara et al. have shown that a "kink" in the kinetic energy spectra of several cuprate superconductors reveals a coupling of the carriers to the intermediate boson that causes the superconducting transition. They have attributed it to phonons. Other researchers have attributed it rather to a coupling to a magnetic mode. A more recent paper by Lanzara et al. emphasizes the same previous conclusion: the intermediate boson is a phonon. It is clear that the optical self-energy as measured by infrared is somehow related to the quasiparticle self-energy as measured in ARPES experiments but they are not identical and there are important differences in the two quantities.

To calculate the optical conductivity in YBa$_2$Cu$_3$O$_7$, we start from an ab initio LAPW three dimensional (3D) calculation of the electronic band structure. When we compared the band structure calculations in the literature among themselves, we found that there is a certain disagreement on the exact description of the bands around the Fermi level,
E_F. To improve our results according to experiments and to the accepted information on the bands around the Fermi level, we found it useful to fit our 3D \textit{ab initio} bands to a tight-binding Hamiltonian. This allows us to slightly fine-tune our bands around the Fermi level (see below).

We, next, calculate the optical conductivity, $\sigma_{\text{opt}}(\omega)$, in the normal state for YBa$_2$Cu$_3$O$_7$ from the known Kubo-Greenwood formula \[29\] and compare our result to experiment \[28\]. For that purpose, we have identified the electronic bands of the carriers associated to the CuO$_2$ plane. We then perform the same calculation in the superconducting state. To simulate the superconducting state, we have introduced into the electronic band structure a superconducting gap to the bands that describe the carriers on the CuO$_2$ plane and only to them. We perform the calculation using the same formula and our built up ”superconducting band structure”. The resonance appears in the superconducting and only in the superconducting state, at $\omega_{\text{res}} = 2\Delta = 38\text{meV}$ ($\Delta$ is the gap that we used for the CuO$_2$-plane carrier-bands). So we argue that the superconducting phase transition modifies effectively the electronic bands around the Fermi level and that this feature opens several new channels for allowed transitions with energy transfer $\omega_{\text{res}} = 2\Delta$ and thus produces the experimentally observed effect. We will show below how both the intra- and inter- band transitions are projected by the superconducting phase transition to the same energy $2\Delta$ a fact that explains the common origin of the resonance in both thermodynamic functions.

The model that we present here has the advantage that, on exactly the same footing, accounts for several experimental results of different character \[30\]. We will comment on this further below. We deal in this paper with YBa$_2$Cu$_3$O$_7$. Our model separates sharply the cause of the resonance from the cause of superconductivity as the infrared experiments \[1\] indicate. The resonance arises from the effect that the superconducting transition (the gap) has on the electronic band structure but superconductivity (the gap itself) can arise by whatever mechanism. Further, to the extend in which we can account for the resonance by taking only the gap value as the information on the superconducting state, it is clear that no information on the specific mechanism can be obtained from it. It appears that the resonance does not contain enough information on the superconducting mechanism to be useful to decide on it.

The background is built up from the allowed transitions at energies different from $\omega_{\text{res}}$. The physics that it contains is essentially the same. No information on the mechanism
can be extracted from the background as well, since it appears that the main contribution to the optical conductivity comes from the optical allowed transitions determined by the electronic states around the Fermi energy and by the influence that the superconducting phase transition (solely through the gap value) has on them. The background as a source of information on the mechanism has been suggested by Hwang et al. [1] solely on the basis that it is common to all HTSC. It has been further emphasized by Norman [31]. As it appears to us, neither the resonance nor the background in the optical conductivity can be used effectively to decide on the mechanism of HTSC.

The situation seems not to be the same with the "kink" in the self-energy found in the ARPES experiments [20]. The kink does reveal a coupling and most probably is the key to the superconducting mechanism. Carbotte et al. [25] have argued that the ARPES experiments can be interpreted as supporting either spin-fluctuations or the phonon-mediated mechanism. They eliminate the possibility of a phonon-mediated mechanism on the basis that their own calculation of the optical conductivity assuming this mechanism gives a wrong dependence of this function at high frequencies. As we shall see below, our model gives the right high-frequency dependence of the optical conductivity. We do not assume any mechanism, we only introduce a detailed description of the electronic bands. It is far from being clear whether or not the phonons plays a role in HTSC. Nevertheless, in a recent work on the isotope effect, Gweon et al. [32] suggest that the singlet pairing of electrons and the electron-lattice coupling mutually enhance each other. On the basis of our work as it stands no mechanism can be analysed. We go backwards in a certain sense. We want to show how far one can go in describing the thermodynamics of YBa$_2$Cu$_3$O$_7$ by taking the attitude that the carriers have to be described in detail while superconductivity itself is described just by the gap value. In conventional superconductivity the details of the phonon spectrum are crucial while the descrition of the electrons enter just through the density of states at the Fermi energy. We deal here with a particular experiment and with a particular HTSC.

The rest of the paper is organized as follows. In the next section 2, we present our electronic band structure and compare it with other work in literature. We also include at this point our description of the superconducting state. In section 3, we calculate the optical conductivity for YBa$_2$Cu$_3$O$_7$ in the normal and in the superconducting state and analyze our result. In section 4, we show that our model leads directly to a suggestion for the approximate way in which the electronic band structure might develop around the Fermi Energy under
doping for the observed property to emerge quite naturally (the resonance disappears while superconductivity remains). In a last section 5, we put our model in perspective and draw our conclusions. We make at this point some experimental suggestions that might contribute to prove the usefulness of our model. In particular, we suggest that there is no reason for the two resonances to disappear at the same doping concentration. The "kink" in the ARPES experiments should remain as long as the sample remains superconducting irrespective to whether it presents one, two or no-resonance at all would it be the key experiment to reveal the mechanism.

II. THE NORMAL AND THE SUPERCONDUCTING STATE OF YBA$_2$Cu$_3$O$_7$

A. The Electronic Band Structure.

The 3D-electronic band structure of YBa$_2$Cu$_3$O$_7$ has been calculated by different \textit{ab initio} methods and by the tight-binding method \cite{26, 27, 33, 34, 35, 36, 37, 38, 39, 40, 41}. When we compare the different results in the literature, we find that there are differences. The exact position of the bands can differ in as much as 100 meV. These are important differences on the scale of meV which is the proper scale to describe the effect of the superconducting gap.

We have first perform an \textit{ab initio} LAPW calculation of the normal-state electronic band structure using the WIEN97 code and the parameters of reference \cite{39}. We found useful to fit further our calculation to a tight-binding description as well to analyze some details of it \cite{?}. We have put special attention to the description of the band near the Fermi energy. Some features of our final result are that we find the extended van Hove singularity around the high symmetry point Y \cite{42} at 14 meV below the Fermi energy in agreement with experiment \cite{43}. Below the Fermi level, we also found a van Hove singularity at about -200 meV at $k = (0.42\pi/a, 0.13\pi/b, 0)$ which has been reported in ref. \cite{27}. The overall features of our calculation coincide well with the rest of the other works in the literature. We reproduce our result for the bands around the Fermi energy in Fig. \ref{fig:bands}. In this figure, the bands labelled 1 and 4 belong to in-CuO-chain states while the 2 and 3 ones describe in-CuO$_2$-plane states. Notice that bands 2 and 3 that belong to the planes do not show a significantly different dispersion from S-X than they do from S-Y, while bands 1 and 4
that belong to the chains do have a different dispersion. In the upper part of Fig. ??, we present the total density of states (DOS) that we get from our band structure. We have obtained a very similar result by calculating it through the Green’s function or using the tetrahedral method of integration. In the lower part of the same figure, we present the DOS discriminated for each scenario (planes, chains and c-axis). At the Fermi level, their relative contribution is 74% (planes), 15% (chains) and 10% (c-axis). The most important contribution comes by far from the CuO$_2$-plane states as it is well known.

B. Description of the superconducting state.

By whatever mechanism, the superconducting transition has the effect of introducing a gap at the Fermi energy, $E_F$, on the electronic states of the carriers affected by it. To simulate the superconducting phase transition, we have introduced by hand a constant gap, $\Delta$, into our normal-state electronic band structure to the bands near $E_F$ that can be associated to electronic states that belong to the CuO$_2$ plane. It is important to say at this point that this model allows us to reproduce right away the optical conductivity and the spin polarized susceptibility on exactly the same basis both in the superconducting and normal state ($\Delta = 0$). This point is important since, as we have already recall, these thermodynamic functions seem to exclude each other in the sense that the contributing transitions to their corresponding matrix elements are inter-band in the first case and intra-band in the second. We present the calculation of the spin magnetic susceptibility in detail elsewhere as well as the calculation of the tunnelling characteristics. Here we merely want to say that these two results other results agree with the known experiments.

We have introduced the gap into the electronic band structure in the way that is familiar in BCS theory. So, we have removed the bands that can be associated to the CuO$_2$ plane from the energy interval ($E_F-\Delta, E_F+\Delta$). The states above $E_F$ accumulate at the upper edge of the interval and the ones below at the bottom. Would we introduce the gap in another way (d-symmetry, for example) the result would differ noticeably from the experimental result. We discuss this point in detail elsewhere. We emphasize that we introduced a gap only to the bands formed by electronic states that can be associated with the atoms belonging to the CuO$_2$ plane. In this way we obtained what we call the ”superconducting electronic band structure” for the CuO$_2$ plane. In what follows we make use of our tight-binding fit.
to our own ab initio calculation to calculate the optical conductivity.

III. CALCULATION OF THE OPTICAL CONDUCTIVITY.

The dielectric function, \( \epsilon = \epsilon_1(\omega) + i\epsilon_2(\omega) \) characterizes the optical properties of a material. Experimentally it can be obtained from the reflectance spectrum. The real and imaginary part of it are related through the Krammers-Kronig relations. The imaginary part of the dielectric function is directly related to the optical conductivity as

\[
\epsilon_2(\omega) = \frac{4\pi\sigma_{\text{opt}}(\omega)}{\omega}.
\]

For inter-band transitions, we can calculate the optical conductivity from the Kubo-Greenwood formula [29]

\[
\sigma(\omega) = -\frac{\pi e^2 h^2}{m^2 \omega \Omega} \sum l,n \int dk P_{ln}^{i} P_{nl}^{j} f_n(k)[1 - f_l(k)]\delta(E_l(k) - E_n(k) - \hbar\omega)
\]

where

\[
P_{ln}^{i} = <\Psi_l(k)|\frac{\partial}{\partial x_i}|\Psi_n(k)>
\]

is the optical transition matrix. \( |\Psi_n(k)\rangle \) is the Bloch function for the n-band and \( k \) is the wave vector defined in the first Brillouin zone. \( E_n(k) \) is the corresponding band energy, \( f_n(k) \) is the Fermi-Dirac distribution function, \( \omega \) is the frequency of the radiation and \( \Omega \) is the volume of the unit cell. The rest are known constants. Now we expand the Bloch function in term of orbital functions as

\[
|\Psi_n(k)\rangle = \frac{1}{\sqrt{N}} \sum_{\alpha,j} u_{n,\alpha} e^{i k \cdot r_j} |\varphi_\alpha(r - r_j)\rangle.
\]

where \( N \) is the number of unit cells, \( \varphi_\alpha(r - r_j) \) is the orbital wave function with quantum numbers \( \alpha \) and \( r_j \) is the origin of the j-th unit cell. The \( u_{n,\alpha} \) are the coefficients of the expansion. Substituting Eq. 3 into Eq. 2 we get

\[
P_{ln}^{i} = \sum_{\alpha,\beta} u_{l,\alpha} u_{n,\beta} \sum_{m,j} M_{ijm}^{\alpha,\beta} e^{i k \cdot (r_j - r_m)}
\]

with

\[
M_{ijm}^{\alpha,\beta} = <\varphi_\alpha(r - r_m)\left|\frac{\partial}{\partial x_i}\right|\varphi_\beta(r - r_j)>
\]
The matrix element, Eq. 5, is zero except for in-site and first nearest neighbors transitions. $M_{ijm}^{\alpha,\beta}$ can be calculated from our tight-binding fit if we use an approximation suggested by Harrison [51]. Within this approximation, for inter-site transitions (atom at $r_j$ with atom at $r_i$), $M_{ijm}^{\alpha,\beta}$ can be cast proportional to $x_m^2$, where $x_m$ is the m-component of the vector $r_j - r_i$ and $d = |r_j - r_i|$. For intra-site transitions due to symmetry considerations, $M_{ijm}^{\alpha,\beta}$ is zero whenever the difference between the angular momentum projections $l_{\alpha} - l_{\beta}$ is even and different from zero otherwise.

### A. The normal state

We have calculated Eq. 1 in 1/8 of the first Brillouin zone (FBZ) at $T = 0K$ therefore the Fermi functions were put equal to 1 for energies below or equal to the Fermi energy, $E_F$, and 0 otherwise. We show in the next Fig. ?? three components of the optical conductivity tensor (Eq. 1) namely $\sigma_{xx}$, $\sigma_{yy}$, and $\sigma_{zz}$ so that we can compare our results with the ones in the literature. Fig. ?? (top) shows our results for an energy interval from 1-10 eV. Fig ?? (bottom) gives low-energy details (0-0.5 eV) of the three tensors. There is a clear anisotropy at low energies between $\sigma_{xx}$ and $\sigma_{yy}$. This is due to transitions that take place on the chains ($y$-direction) that contribute to $\sigma_{yy}$ but not to $\sigma_{xx}$. Garriga et al. [52] report measurements on $\varepsilon_2(\omega)$ which show a maximum around $\omega = 8eV$, a peak at $4 - 5eV$ and a minimum around $2 - 3eV$. Tajima et al. [53] report similar results at high energies and a minimum around $6eV$. Our calculation agrees well with these experimental results and with theoretical calculations at low energy ?? and at medium and high energies [55, 56].

### B. The superconducting state

We have calculated the optical conductivity from Eq. 1 in 1/8 of the FBZ with 64 points per axis. We have used our electronic band structure where a gap was inserted in the way described above. We allow only inter-band transitions on the in-CuO$_2$-plane states. Our result for $\sigma(\omega)$ in the normal and in the superconducting state appears in the next Fig. ??.

As we can see in this figure, the effect of the transition is to shift the spectral weight of the almost featureless $\sigma(\omega)$ function to higher energies, namely above 30 meV, producing the sharp resonance at 38 meV. This occurs because all the allowed transitions within bands
(one below and one above the Fermi level) that differ in the normal state by less than $2\Delta$
are projected in the superconducting state to the gap edges (above and below $E_F$) and the
transition will take place at $2\Delta$ irrespective to the energy at which it occurs in the normal
state. We have used $\Delta_{plane}=19$ meV for YBa$_2$Cu$_3$O$_7$. Both, the calculation in the normal
state and the one in the superconducting state, reproduce the experimental results. Our
model does not assume any mechanism whatsoever. Therefore an interesting point that
arises is that on quite general grounds, namely that the phase transition introduces a gap to
the electronic band structure, the resonance can be reproduced. This fact casts some doubts
on whether at all the optical conductivity has enough information to allow a sharp decision
on the mechanism (neither in the resonance nor in the background).

IV. SUPERCONDUCTIVITY WITH AND WITHOUT THE RESONANCE

A suggestion based on our model on how the effect of doping can cause the total disap-
pearance of the resonance while the sample remains superconducting is sketched on Fig. 5.
Let the band (a) contains a possible initial state (i) below the Fermi energy, $E_F$ (dash-dot
line). The energy difference between state (i) and $E_F$ let it be less than the gap associated
to the plane, $\Delta_{plane}$ (dashed line). As the contributing transitions are inter-band, the final
state has to lie on a different band (b) above the Fermi level. The transitions are direct (no
momentum transfer). In the normal state this transition contributes to the resonance at a
frequency equal to the energy difference between the final and the initial state. In the super-
conducting state, this and several similar events will contribute as well but at an energy $2\Delta$
due to the effect that the superconducting transition has on the bands. It is enough that,
upon doping, the bands evolve so that their energy difference in the normal state gets higher
than $2\Delta$ at this particular point of the FBZ where the transition occurs for this particular
event to cease to contribute to the resonance. It will contribute at a higher energy and,
consequently, the resonance will have one less event that contributes and its spectral weight
diminishes. Eventually the resonance disappears. It is obvious, on the other hand, that
bands at certain doping that did not contribute at a previous one can contribute, but the
net effect can be a lost of contributing events due to doping. The exact issue depends on
the details of the bands and on the specific influence of the doping on them and on the value
of the gap for each family of compounds and it has to be calculated in detail. We suggest
that this is what happens in the Bi-family \[1\] where experiment shows the disappearance of the resonance with doping. Under doping, the gap shrinks at a slower pace than the number of events contributing to the resonance and, consequently, the resonance disappears but superconductivity remains.

V. CONCLUSIONS

We have shown in this paper that the resonance in the optical conductivity that appears in the superconducting and only in the superconducting state can be obtained from an ab initio three dimensional calculation just by introducing to the electronic bands that can be associated to the CuO$_2$ plane a gap, $\Delta$. The actual calculation of the optical conductivity is two-dimensional (in-plane). The model produces the resonance at $2\Delta$ and therefore we have consequently introduced into the calculation $\Delta = 19\text{meV}$ to reproduce the resonance at the right experimental frequency. The curves agree very well with experiment in the normal and the superconducting state. It is interesting that we get the experimental trend of the function at high frequency both in the normal and in the superconducting state. We do not assume any mechanism in our calculation. We have further suggested a way in which this model can account for the experimental results on the effect of doping on the intensity of the resonance \[1\].

It is important to say that using exactly the same model, we have calculate the spin polarized susceptibility in the normal and in the superconducting state and reproduce the experimental results. We obtain that this resonance could disappear as well but that there is no reason for it to disappear at the same doping level than the one in the optical conductivity \[47\]. The model does not reproduce the experimental results for the tunneling experiments unless it is extended to three dimensions. If we impose further to the 3D bands obtained from our ab initio calculation, an additional gap to the states that can be associated to the chains ($\Delta_{\text{chains}} = 7\text{meV}$) and keep $\Delta = 0$ for the bands that can be associated to the c-axis, we reproduce the tunnelling characteristics in agreement with experiment \[48\]. A somehow similar approach in the sense that they used a different value for the gap on each scenario (planes, chains and c-axis) has been used before \[57\] to simulate successfully experimental results on tunnelling, specific heat and ultrasonic attenuation. On that basis we expect to reproduce these two last results as well from our more detailed model.
A more delicate point is to reproduce the temperature behavior of the resonance. The resonance frequency hardly changes in the range from zero to the superconducting temperature but, on the contrary, its intensity is very sensitive to it, decreases with increasing temperature and vanishes steeply at $T_c$ \[4\]. We will suggest that this is a combined effect of the behavior of the superconducting gap with temperature and the separate effect of the increasing temperature on the electronic band structure itself. The effect of temperature on the electronic bands itself has never been considered before in this context but within the critical temperature range ($\approx 100 \text{ K} \approx 10 \text{ meV}$) also the temperature itself could have a non-negligible effect on the electronic band structure at the meV scale. Calculations of this effect in metals like Cu and Ni have been made in the past by Delgadillo et al. \[58\]. They find that the electronic bands around the Fermi level do displace themselves as an effect of temperature in the meV scale. This fact and the known temperature dependence of the superconducting gap itself might explain (always within the same model) the behavior of the resonance with temperature. Notice that 10 meV is of the order of $\Delta/2$, where $\Delta$ is the superconducting gap associated to the CuO$_2$ plane \[59\].

The goal of the work presented in this and some other papers is to show how far one can go in describing the experimental results starting from what could be said “the result” of a theory of superconductivity for high-Tc superconductors. One possible conclusion is that the detailed description of the carriers plays an important role in HTSC a fact that is in sharp contrast with conventional superconductivity where the electronic band structure characteristics enter merely through the density of states at the Fermi energy. as we atated above.

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FIGURE CAPTIONS

Fig.1 3D-electronic band structure of YBa$_2$Cu$_3$O$_7$ near the Fermi level. Bands 2 and 3 are in-CuO$_2$-plane states; bands 1 and 4 belong to in-CuO-chain states. Notice that the dispersion in the interval S-X is not very different from the one in the interval S-Y for the bands labelled 2 and 3 (the in-CuO$_2$-plane states). This is not true for bands labelled 1 and 4 that are in-CuO-chain states. The X-Y symmetry is not expected on this scenario.

Fig.2 The total density of states (a) and the contribution of each scenario (b).

Fig.3 In the upper part (a), we show the optical conductivity-tensor components $\sigma_{xx}$, $\sigma_{yy}$, and $\sigma_{zz}$ in the normal state in a scale 0-10 meV. In the lower part (b), we show the same functions in more detail below 0.5 eV so that our results can be compared easily with the ones in the literature (see text).

Fig. 4 The optical conductivity function, $\sigma(\omega)$, in the normal (full line) and in the superconducting state (dots). Notice that at higher energies, $\sigma(\omega)$, increases with energy in the superconducting state.

Fig. 5 The dash-dot line is the Fermi energy and the dash-lines above and below it are the gap edge in the superconducting state. Let us consider allowed transitions in the normal state. In the band (a) we have selected a possible initial state (i) and on the band (b) a possible final state. In the normal state, this transition contributes to the resonance at a frequency equal to the energy difference between (f) and (i). In the superconducting state, both (f) and (i) will be projected to the gap edge so that this and several other low-lying similar transitions will contribute all at the same energy $2\Delta$ due to the effect of the superconducting transition on the bands. Upon doping, it is enough that the bands evolve so that their energy difference in the normal state gets higher than $2\Delta$ at this point of the FBZ (dot-line) for this particular event to cease to contribute to the resonance (see text).
band b upon doping

Energy

band a

gap edge

(final state)

(initial state)