Nature of the pseudogap in the optical conductivity of oxygen-deficient $YBa_2Cu_3O_x$

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The pseudogap in the c-axis optical conductivity of oxygen-deficient $YBa_2Cu_3O_x$ is explained on the basis of the resonant tunneling through the barrier between the CuO_2 planes with the use of localized centers formed on place of the CuO chains. The conductivity as a function of frequency has a maximum, and its location and magnitude depend only on the spectrum of resonant levels, and hence do not depend on temperature. In the case of a fully oxygenated substance the chains are complete, and no resonance centers are formed. These features were observed in experiment. Comparison is done with existing data. Other possible mechanisms of the pseudogap formation are briefly discussed. [S0163-1829(96)02942-6]

I. INTRODUCTION

The pseudogaps in the normal state of high-temperature superconductors have a long history. A broad variety of ideas has been proposed (see references in Refs. 1 and 2 and the end of this paper). We will be concerned here with the pseudogap appearing above T_c in the c-axis optical conductivity of the oxygen-deficient $YBa_2Cu_3O_x$, where it is well pronounced.[1,2] The phenomenon consists of a depression in the frequency-dependent conductivity at low frequencies. With increasing frequency the conductivity starts to rise and after a maximum has a trend to decrease. One of the important properties of this pseudogap is that it appears only in oxygen-deficient samples, and it is absent in fully oxygenated $YBa_2Cu_3O_{6.95}$ (see Refs. 1 and 2); it is also almost absent in $YBa_2Cu_4O_8$ (Refs. 3 and 4) (the small depression of the conductivity at temperatures slightly above T_c can be explained by fluctuations[5]). Another important point is that neither the location nor the height of the maximum depend on temperature.

Our explanation is based on the idea of resonant tunneling through localized states formed in place of broken chains between the CuO_2 bilayers in the oxygen-deficient $YBa_2Cu_3O_x$. Since these states do not exist in fully oxygenated samples with $x\approx 7$ and in $YBa_2Cu_4O_8$, there is no well pronounced pseudogap in such samples (we do not consider temperatures below T_c where some sort of gap exists but it is most probably due to superconductivity). The resonant tunneling idea permitted to get a reasonable fit to experimental data for the resistivity ratio ρ_c/ρ_{ab}.[6,7] As we will see, this approach permits to explain the pseudogap, which, actually, proves to be a misleading notation for the description of the behavior of $\sigma(\omega)$; it is more adequate to speak about the threshold behavior of this function. The location of this threshold depends only on the lower edge of the resonant localized states, and although this edge varies slightly with the oxygen concentration, it does not depend on temperature.

II. DERIVATION OF THE OPTICAL CONDUCTIVITY

We will start with Eq. (6), derived in Refs. 6 and 7, and expressing the current in the c direction under the influence of an electric field represented by its vector potential. Previously we used the limit $\omega_0\rightarrow 0$, and now we consider the general case. If we write this equation as $j=-QA$, the real part of the conductivity can be obtained as

$$\begin{aligned}\mathrm{Re}\sigma(\omega_0)&=-c\,\mathrm{Im}Q(\omega_0)/\omega_0\\&=(2/\omega_0)(etn_id)^2\nu_e\frac{1}{2\pi}\int_{-\infty}^{\infty}d\omega\int_{E-\varepsilon}^{E+\varepsilon}dE_j\left(\tanh\frac{\omega+\omega_0}{2T}-\tanh\frac{\omega}{2T}\right)\mathrm{Im}G_R(\omega,E_j)\mathrm{Im}G_R(\omega+\omega_0,E_j),\end{aligned}\tag{1}$$

where the notations are the same as in Refs. 6 and 7, and particularly,

$$-\mathrm{Im}G_R(\omega,E_j)=\frac{1/2\tau}{(\omega-E_j)^2+(1/2\tau)^2}\tag{2}$$

(τ is the scattering time in the plane). This function is close to $\pi\delta(\omega-E_j)$, and, if we assume that its width $1/2\tau\ll\omega_0$, then both delta functions in Eq. (1) will be well separated (this limit is opposite to the one assumed in Refs. 6 and 7 for static conductivity). Performing the integration over ω, we obtain

$$\mathrm{Re}\sigma(\omega_0)=\frac{(etn_id)^2\nu_e}{2\tau\omega_0^3}\int_{E-\varepsilon}^{E+\varepsilon}dE_j\left(\tanh\frac{E_j+\omega_0}{2T}-\tanh\frac{E_j-\omega_0}{2T}\right).\tag{3}$$

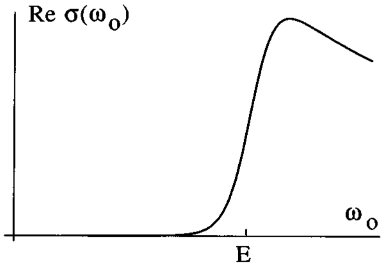

FIG. 1. Schematic presentation of the normal state c-axis optical conductivity at very low temperatures in the case if all resonant states have the same energy E.

The integration over dE_j takes into account the distribution of the resonant levels in the tunneling barrier. If all these states had the same energy, say E, and the temperature would be much less than E, the optical conductivity would be proportional to $n_F(E-\omega_0)$, n_F being the Fermi function, i.e., it would be exponentially small at $\omega_0<E$, and increase rather steeply around $\omega_0=E$. At larger values of ω_0 it would decrease due to the factor in front of the integral in (3) (the scattering probability $1/\tau$ can be also frequency dependent at $\omega_0 \geqslant T$), and hence there will be a maximum in the vicinity of $\omega_0=E$ (schematic plot at Fig. 1). The location of this maximum as well as its value do not depend on temperature and are defined only by the energy of the resonant states. In a fully oxygenated substance there are regular CuO chains, whose bands are hybridized with the bands of CuO_2 planes, and hence no such behavior can be expected.

This picture is a very rough reproduction of the pseudogap but it describes all its major properties. Therefore, it seems very likely that the proposed explanation of the pseudogap is a true one. At least, the author is unaware of any other one, accounting for all essential features of this phenomenon.

III. RESONANT LEVEL DISTRIBUTION AND EXPERIMENTAL DATA

The result (3) corresponds to the same assumption about the level distribution, which was made in Refs. 6 and 7, namely that the resonant levels are located within a stripe $(E-\varepsilon, E+\varepsilon)$ with a constant density. If in reality the distribution is described by some more general function $f(E_j)$, then at low temperatures the integral in Eq. (3) must be replaced by

$$2\int_{E_{\min}}^{\omega_0} f(E_j)dE_j. \qquad (4)$$

Differentiating this function, we get the resonant level distribution. The main obstacle is superconductivity. In order to have a normal metal at low temperatures T_c must be low, and hence the oxygen concentration must be not far from the metal-insulator transition. In order to avoid guesses about the frequency dependence of τ, it is necessary to measure simultaneously the optical conductivity in the ab plane and to take the ratio σ_c/σ_{ab}, as we did for the static conductivity in Refs. 6 and 7 (the static σ_{ab} will be divided by $\omega_0^2\tau^2$).

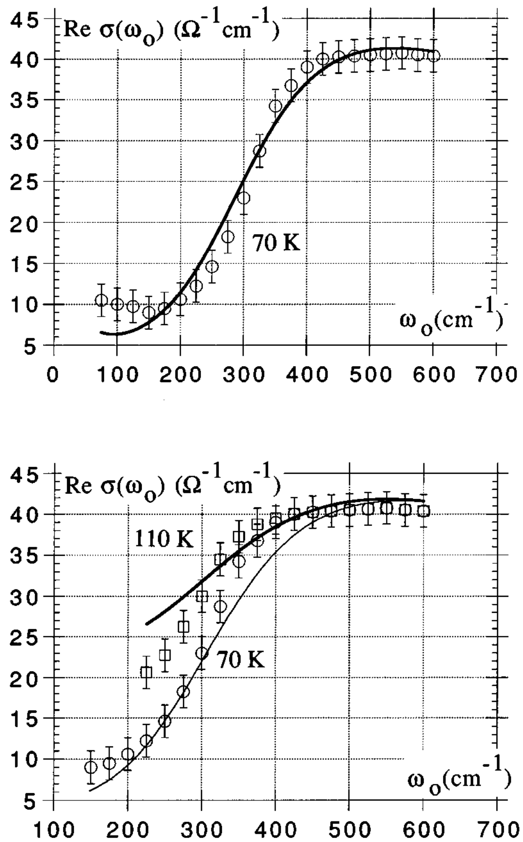

FIG. 2. Fitting of the theoretical curve to experimental data for the c-axis optical conductivity of $YBa_2Cu_3O_{6.7}$ ($T_c=63$ K): (a) Best fit for the data at 70 K ($E-\varepsilon=271$ cm^{-1}) and (b) fit for data taken at two temperatures, 70 and 110 K ($E-\varepsilon=286$ cm^{-1}); only data at frequencies $\omega_0 \geqslant 3$ T were used for this fit. The bars represent not the experimental error but the ''wiggling'' of the experimental curve, which is possibly due to an uneven distribution of resonant levels.

Unfortunately these data are absent, and we have to use what is available. The curves for optical conductivity as a function of frequency at several temperatures were obtained for $YBa_2Cu_3O_{6.7}$ ($T_c=63$ K) by Homes *et al.* in Refs. 1 and 2. Performing the integration in (3), we obtain

$$\mathrm{Re}\sigma(\omega_0)=(etn_id)^2\nu_e(T/\tau\omega_0^3)\times\ln\left[\frac{\cosh(E+\varepsilon+\omega_0)\cosh(E-\varepsilon-\omega_0)}{\cosh(E-\varepsilon+\omega_0)\cosh(E+\varepsilon-\omega_0)}\right].$$

Using the estimates obtained in Refs. 6 and 7: $E\approx 1250$ K ≈ 870 cm^{-1}, $\varepsilon>800$ K ≈ 550 cm^{-1} (the correspondence factor is 0.695 cm^{-1}/K), we come to the conclusion that for all temperatures and frequencies in question (the pseudogap was observed at $T\leqslant 150$ K and $\omega_0 \leqslant 500$ cm^{-1}) we can assume $\exp[-(E+\varepsilon\pm\omega_0)]\ll 1$. We are left with the result

$$\mathrm{Re}\sigma(\omega_0)=(etn_id)^2\nu_e(T/\tau\omega_0^3)[\ln\{1+\exp[-(E-\varepsilon-\omega_0)/T]\}-\exp[-(E-\varepsilon+\omega_0)/T]]. \qquad (5)$$

In order to apply this formula we have to know $1/\tau$, the scattering probability in the plane, as a function of temperature and frequency, and this has not been definitely established by now. At the lowest temperature $T=70$ K the assumption $1/\tau=\mathrm{const}\times\omega_0$ ($\mathrm{const}\ll 1$) gives a good agreement [Fig. 2(a)]. The error bars at this plot represent the ''wiggling'' of the experimental curve which can reflect the uneven distribution of resonance levels. The deviation at lower frequencies can be ascribed to a failure of the assumed form for $1/\tau$ at small ω_0 due to the influence of a finite temperature. The value $E-\varepsilon=271$ cm^{-1}, obtained from fitting, does not contradict the data resulting from static conductivity.

The fitting is worse for data taken at higher temperatures, particularly at low frequencies. An example of this is presented in Fig. 2(b), where we tried to get the fit of Eq. (5) with the same coefficients (particularly, $E-\varepsilon=286$ cm^{-1}) to data taken at two different temperatures, although we took into account only data starting from frequencies $\omega_0\geqslant 3$ T. Another possible cause of discrepancies is the condition $1/\tau\ll\omega_0$, which can be also violated at higher temperatures.

IV. DISCUSSION

Although the goal of this paper was confined to the description of optical properties within the resonant tunneling model proposed for underdoped $YBa_2Cu_3O_x$, it should be mentioned that similar phenomena were observed in other materials. The exponential growth of the ratio of static resistivities ρ_c/ρ_{ab} with decreasing temperature was observed in $Bi_2Sr_2CaCuO_{8+\delta}$,[8,9] in $Tl_2Ba_2CuO_{6+\delta}$,[10,11] and recently in the underdoped ($x<0.12$) $La_{2-x}Sr_xCuO_4$.[12] In the latter work a pseudogap in the optical c conductivity was also observed, although it was definitely weaker than in $YBa_2Cu_3O_x$, where the decrease of the conductivity was four times at the lowest temperature above T_c. In principle, the mechanism could be the same, i.e., some resonant centers between the CuO_2 planes, although the fluctuational explanation[5] leading to a shallow minimum, as in $YBa_2Cu_4O_8$,[3,4] is not excluded.

The authors of the work[12] prefer another explanation of the pseudogap based on the RVB idea of spin-charge separation and formation of spinon pairs, i.e., a gap in the spinon density of states.[13,14] Since the current in the c direction requires recombination of spinons and holons,[15,16] the c-axis conductivity would have an activation behavior. In principle this idea could also provide an explanation, the more so that it can explain also the ''spin gap,''[17] i.e., the decrease of the electron spin susceptibility in the underdoped $YBa_2Cu_3O_x$ with decreasing temperature far above T_c. The general problem with this concept is that it is strictly two dimensional (actually it was proven only in one dimension) and does not permit a crossover to three dimensions, which actually happens in many of the layered cuprates including $La_{2-x}Sr_xCuO_4$.[12]

An alternative explanation of the spin gap is based on the idea of ''preformed pairs'' of electrons in the case of strong attraction (see, e.g., Ref. 18). This idea could give an explanation also to the pseudogap in angle resolved photoemission spectra.[19,20] What concerns the pseudogap in the optical conductivity, so it could be attributed to the fact that tunneling of pairs between the CuO_2 planes is prohibited due to their double charge. It seems, however, that this is not the proper explanation, since in this case the c-axis conductivity should have the same temperature dependence as the sin susceptibility, and this is not the case.

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