RAPID COMMUNICATIONS

PHYSICAL REVIEW B VOLUME 52, NUMBER 10 1 SEPTEMBER 1995-II

c-axis normal conductivity of $YBa_2Cu_3O_x$ as a function of x

A. A. Abrikosov

Materials Science Division, Argonne National Laboratory, 9700 South Cass Avenue, Argonne, Illinois 60439

(Received 22 May 1995)

A theory is presented of the static c-axis conductivity of $YBa_2Cu_3O_{7-\delta}$ in the normal state with varying oxygen concentration. The basis of the theory is an assumption that the hopping of electrons between the CuO_2 planes is due to resonant tunneling through localized centers between the planes. Comparison with recent systematic determinations of the temperature-dependent conductivity at different oxygen concentrations shows reasonable agreement.

The mechanism of conductivity, and hence superconductivity along the c axis in high-temperature superconductors (HTSC) was always somewhat mysterious. The long period in this direction means a large separation between CuO_2 single, double, or triple layers, and in absence of the CuO chains, which exist only in $YBa_2Cu_3O_7$ and $YBa_2Cu_4O_8$ (YBCO), the hopping between the CuO_2 layers should be negligible. Attempts to explain the conductivity along the c axis in the absence of chains led to many controversial assumptions. One of them was the universal existence of "normal metal layers" (see, e.g., Refs. 1–3); this hypothesis was not confirmed by angle-resolved photoemission experiments in $Bi_2Sr_2CaCu_2O_8$ (BiSCCO), which showed that there are no other Fermi surfaces, except that of CuO_2 planes (see Ref. 4). The other one was the RVB mechanism, associated with the existence of "spinons" and "holons"[5,6] (or, for superconductivity, "pair tunneling"[7]); however, in the presence of chains the angle-resolved photoemission spectroscopy (ARPES) experiments demonstrated a definite hybridization in the *one*-electron spectra of chains and planes, and this ruled out completely such a mechanism. There exist several attempts to connect the c-axis conductivity with "off-diagonal disorder," i.e., some sort of scattering by impurities, lying between planes (see Ref. 8). It is, however, difficult to understand the mechanism of such an enhancement unless some further assumptions are made, and this can alter substantially the picture.

At the same time there exists a very good check, namely, the recently performed systematic experimental determination of the temperature-dependent conductivity in $YBa_2Cu_3O_x$ with increasing x by Boyd Veal,[9] which show a crossover between "insulating" and "metallic" types of behavior as the chains are gradually formed. There exists another example of such a crossover, namely, the formation of impurity bands in semiconductors. It is well known that the disappearance of oxygen from the chains in YBCO happens randomly; this can be the basis of the similarity of these two cases.

On the other hand, in BiSCCO, as well as in tallium and mercury based superconductors, there is nothing like the CuO chains in YBCO, and hence there has to exist another mechanism for doping the CuO_2 planes with holes. It is generally believed that this doping is achieved by some sort of localized centers appearing as a result of intrinsic disorder in these substances. On the whole, the situation is very reminiscent of doped semiconductors.

In this paper we will consider a model where the hopping between the adjacent CuO_2 planes is achieved by resonant tunneling. The idea of resonant tunneling through localized states inside the barrier was proposed long ago by Lifshitz and Kirpichenkov.[10] They showed that in cases where such centers form a "resonant-percolational" path, the transparency along the path is of the order of unity. In the case where the path is short, as is most appropriate for the present case, it can contain only one resonant center, which must be located exactly in the middle of the barrier. The energy of the electron has to be equal to the energy of such a localized state. We will assume that these localized centers are located randomly along the median plane with a given concentration and some distribution of energies. The positions of these centers in different median planes (we consider a model with one CuO_2 plane per period) are assumed to be uncorrelated. The planes CuO_2 are metallic with some scattering of electrons from other agents (e.g., defects or other electrons belonging to the same plane) which are uncorrelated in different planes and are much more numerous than the resonant centers.

The Hamiltonian of the model is

$$H=\sum_n \left\{ \int \psi_n^\dagger(\rho)\xi\psi_n(\rho)d^2\rho+U_n+t\sum_j \left[\breve{\psi}_{n+1}^\dagger(\rho_j)\breve{\psi}_n(\rho_j)\exp\left(i\frac{e}{c}A_z d\right)+\breve{\psi}_n^\dagger(\rho_j)\breve{\psi}_{n+1}(\rho_j)\exp\left(-i\frac{e}{c}A_z d\right)\right]\right\}, \quad (1)$$

where the first term is the kinetic energy, the second corresponds to scattering within the plane leading to a finite lifetime, and the third, the resonant tunneling between the CuO_2 planes. Here ψ_n refers to the plane n, $\breve{\psi}$ means the part of the ψ operator

0163-1829/95/52(10)/7026(4)/$06.00

which corresponds to the energy of the resonant impurity E_j; ρ_j mean the planar coordinates of resonant impurities between the planes. The electric field along the c axis is represented by the vector potential A_z, d is the period along z, and we assume that A_z varies substantially at much larger distances than d.

In order to calculate the current we first define the contribution to the thermodynamic potential Ω having the second order in A_z and lowest in t. Since we have to take averages over electronic states, the correction in the first approximation is given by (see Ref. 11)

$$\Delta\Omega=-\frac{T}{2}\left(\frac{etd}{c}\right)^2\int_0^\beta d\tau\int_0^\beta d\tau'\sum_n\sum_{jj'}\check{G}_n(\rho_j-\rho_{j'},\tau-\tau')\check{G}_{n+1}(\rho_{j'}-\rho_j,\tau'-\tau)[A_z(\tau)A_z(\tau')-\tfrac{1}{2}A_z^2(\tau)-\tfrac{1}{2}A_z^2(\tau')]. \tag{2}$$

First we perform the summation over j,j'. Every impurity has its location and its energy level E_j (the energies are taken with respect to the chemical potential). We will assume that the resonant impurities are located randomly in the median plane between two adjacent $\mathrm{CuO_2}$ layers with some average concentration n_j, and the energy levels have a constant density within a stripe $(E-\varepsilon,E+\varepsilon)$. Resonant amplitudes involving different centers with the same energy are coherent. This is why the sum over impurity locations is performed in the amplitude (sum over j,j'). The tunneling through centers with different energies is incoherent. According to what was said, the sum over resonant impurities is transformed:

$$\sum_j \to n_j\int d^2\rho_j. \tag{3}$$

We have to take into account that the energies of both states j and j' must be equal.

From Eq. (2) we obtain the "thermodynamic" current

$$\begin{aligned}j_z(\tau)&=-c\,\frac{\delta\Delta\Omega}{\delta A_z(\tau)}\\&=\frac{4}{c}\,d(etn_j)^2\int_0^\beta d\tau'\int d^2\rho\check{G}_n(\rho,\tau-\tau')\check{G}_{n+1}(-\rho,\tau'-\tau)[A_z(\tau')-A_z(\tau)].\end{aligned} \tag{4}$$

Here in the $\check{G}$ functions the in-plane scattering is incorporated. According to our assumptions, this scattering is uncorrelated at different planes. Therefore, both functions are equal and depend only on coordinate differences. Passing to the Fourier representation in τ and ρ, we obtain

$$j_z(i\omega_0)=\frac{4}{c}\,d(etn_j)^2T\sum_m\int d^2k[\check{G}_n(k,i\omega_m+i\omega_0)\check{G}_{n+1}(k,i\omega_m)-\check{G}_n(k,i\omega_m)\check{G}_{n+1}(k,i\omega_m)]A_z(i\omega_0). \tag{5}$$

Now we perform two operations. First we find the analytical continuation to real frequencies. Then we pass from the k integration to the averaging over energies:

$$\int d^2k\to d(\nu_e/2)\int_{E-\varepsilon}^{E+\varepsilon}dE_j,$$

where ν_e is the three-dimensional electron density of states, including spins (i.e., the 2D density times $1/d$). For an isotropic model $\nu_e=m/(\pi d)$ and can be considered independent on energy. We obtain

$$\begin{aligned}j_z(\omega_0)=\frac{2}{c}(etn_jd)^2\nu_e\frac{1}{2\pi}\int_{-\infty}^{\infty}d\omega\int_{E-\varepsilon}^{E+\varepsilon}dE_j\biggl[&\tanh\left(\frac{\omega}{2T}\right)\mathrm{Im}G_R(\omega,E_j)G_R(\omega+\omega_0,E_j)\\&+\tanh\left(\frac{\omega+\omega_0}{2T}\right)G_A(\omega,E_j)\mathrm{Im}G_R(\omega+\omega_0,E_j)-\tanh\left(\frac{\omega}{2T}\right)\,\mathrm{Im}G_R^2(\omega,E_j)\biggr]A_z(\omega_0).\end{aligned} \tag{6}$$

The coefficient, connecting $j_z(\omega_0)$ and $A_z(\omega_0)$ (we denote it by $-Q$), vanishes at $\omega_0=0$.

The static conductivity is defined by the relation

$$\sigma=-ic\left(\frac{\partial Q(\omega_0)}{\partial\omega_0}\right)_{\omega_0=0}. \tag{7}$$

From this we obtain

$$\sigma=2(etn_jd)^2\nu_e\frac{1}{2\pi}\int_{-\infty}^{\infty}d\omega\int_{E-\varepsilon}^{E+\varepsilon}dE_j\frac{1}{2T}\cosh^{-2}\left(\frac{\omega}{2T}\right)[\,\mathrm{Im}G_R(\omega,E_j)]^2$$

$$=2(etn_jd)^2\nu_e\frac{1}{2\pi}\int_{-\infty}^{\infty}d\omega\int_{E-\varepsilon}^{E+\varepsilon}dE_j\frac{1}{2T}\cosh^{-2}\left(\frac{\omega}{2T}\right)\left[\frac{1/2\tau}{(\omega-E_j)^2+(1/2\tau)^2}\right]^2, \qquad (8)$$

where $1/\tau$ is the scattering probability entering the in-plane resistivity. The linear temperature dependence of this resistivity has still no final explanation. We will simply assume that $1/\tau=\alpha T$, and $\alpha\ll 1$, in order to keep the validity of the Fermi liquid model.

The integrand in Eq. (8) is a product of two δ-function-like factors. Since $1/2\tau$ we assume to be much less than T, the second factor we can replace by $\pi\tau\delta(\omega-E_j)$, and after that we obtain

$$\sigma_c=2(etn_jd)^2\nu_e\tau\left[n_F\left(\frac{E-\varepsilon}{T}\right)-n_F\left(\frac{E+\varepsilon}{T}\right)\right], \qquad (9)$$

where n_F is the Fermi function. Comparing this expression with the in-plane conductivity $\sigma_{ab}=(1/2)(ev)^2\nu_e\tau$, where v is the Fermi velocity, we obtain for the resistivity ratio

$$\frac{\rho_c}{\rho_{ab}}=\frac{1}{4}\left(\frac{v}{tn_jd}\right)^2\left[n_F\left(\frac{E-\varepsilon}{T}\right)-n_F\left(\frac{E+\varepsilon}{T}\right)\right]^{-1}$$

$$=\frac{1}{4}\left(\frac{v}{tn_jd}\right)^2\frac{\cosh(E/T)+\cosh(\varepsilon/T)}{\sinh(\varepsilon/T)}. \qquad (10)$$

The validity of this formula is based on the approximation of the second factor in the integrand of Eq. (8) by a δ function. In the case of $E\gg T$ this can fail. The necessary condition is (we substituted $1/\tau=\alpha T$)

$$(T/E)^4\exp(E/T)\ll T/(\varepsilon\alpha^3). \qquad (11)$$

We will assume that this is always fulfilled.

Comparison with experimental data[9] was performed on the basis of Eq. (10) written in the form

$$\frac{\rho_c}{\rho_{ab}}=A\,\frac{\cosh(T_0/T)+\cosh(T_1/T)}{\sinh(T_1/T)}, \qquad (12)$$

by choosing the optimal values of the constants A, T_0, and T_1. The fit is good for moderate oxygen concentrations, and somewhat worse in both limits: metallic and completely broken chains, hence in these limits our theory does not reflect all the details of the plain-chain relations. The fitting procedure is somewhat unstable, since slightly different sets of constants lead to the same quality of agreement. Fortunately the scatter is not too large, and therefore, some conclusions can be drawn. The constant T_0 remains essentially independent on oxygen concentration ($T_0\approx 1250$ K, or $E\approx 0.11$ eV) (it has to be remembered that the energy E is actually the difference $E-\mu$). The constant T_1 varies nonmonotonical being larger at large and small oxygen concentrations (≈ 1050 K) and smaller in between (≈ 700–800 K). If this variation reflecting the scatter of resonant levels is real, it can be explained by the idea that at small oxygen concentrations the total number of these localized states is small, and hence the fluctuations are large, whereas at large concentration the wave functions overlap, and a band of finite width is formed.

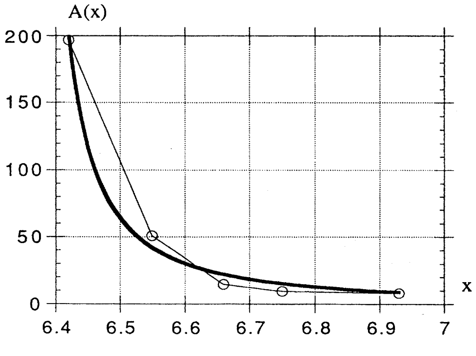

FIG. 1. Fit of the prefactor A in Eq. (12) obtained from experimental data of Ref. 9 with Eq. (14), describing its dependence on oxygen concentration.

On the basis of these data the condition (11) can be checked. We find that in all cases, if the constant α (we remind that $\tau^{-1}=\alpha T$) is less than unity, the condition (11) is fulfilled. We have to assume $\alpha\ll 1$ not only for this reason but also because otherwise the Fermi liquid concept fails.

Contrary to T_0 and T_1, the constant

$$A=\tfrac{1}{4}(v/tn_jd)^2 \qquad (13)$$

has a systematic dependence on oxygen concentration. If we try to fit it by the formula

$$A=a(x-b)^{-m}, \qquad (14)$$

where x is the amount of oxygen atoms per unit cell, we get the optimal values of the constants

$$a=3.94, \quad b=6.35, \quad m=1.46. \qquad (15)$$

The fit is presented in Fig. 1. It is surprisingly good, and the values (15) are very reasonable. The concentration $x=6.35$ corresponds to the metal-insulator transition. The Fermi velocity of the electrons can be expected to grow with x, and n_j is most likely approximately proportional to $(x-6.35)$. Therefore the exponent m must be somewhat less than 2, and it is really in this range.

This shows that the suggested model is reasonable, and being rather simple, it can nevertheless provide an explanation of experimental data.

I would like to express my deep gratitude to Boyd Veal for communicating his data to me prior to publication. This work was supported by the Department of Energy under Contract No. W-31-109-ENG-38.

[1] L. N. Bulaevskii and M. V. Zyskin, Phys. Rev. B **42**, 10 230 (1990).

[2] M. Tachiki *et al.*, Z. Phys. B Condens. Matter **80**, 161 (1990).

[3] A. A. Abrikosov, Physica C **182**, 191 (1992).

[4] H. Ding *et al.*, Phys. Rev. Lett. **74**, 2784 (1995).

[5] P. W. Anderson and Z. Zhou, Phys. Rev. Lett. **60**, 132 (1988); **60**, 2557 (1988).

[6] P. B. Littlewood and C. M. Varma, Phys. Rev. B **45**, 12 636 (1992).

[7] S. Chakravarty *et al.*, Science **261**, 337 (1993).

[8] A. J. Rojo and K. Levin, Phys. Rev. B **48**, 16 861 (1993).

[9] B. Veal *et al.* (unpublished).

[10] I. M. Lifshitz and V. Ya. Kirpichenkov, Zh. Eskp. Teor. Fiz. **77**, 989 (1979) [Sov. Phys. JETP **50**, 499 (1979)].

[11] A. A. Abrikosov, L. P. Gor'kov, and I. E. Dzyaloshinsky, *Quantum Field Theory Methods in Statistical Physics* (Pergamon, New York, 1965).