Coherent versus incoherent resonant tunneling in high-T_c cuprates

A. A. Abrikosov
Materials Science Division, Argonne National Laboratory, 9700 South Cass Avenue, Argonne, Illinois 60439
(Received 21 April 1997)

An analysis is performed of the resonant tunneling transport along the c axis in the case where the concentration of localized resonant centers is low and the tunneling via different centers becomes incoherent. In this case the planar component of the quasimomentum is not conserved in the process of interlayer hopping. For the normal conductivity, as function of temperature and frequency, this leads only to a change of a prefactor. However, the supercurrent along the c axis vanishes if the order parameter is of d type and the tunneling is incoherent. An interpolation is proposed, describing a partially coherent case, when the interference terms are suppressed, but still present. A rapid decrease of the critical temperature with concentration of resonant centers and the possibility of a $d\rightarrow s$ phase transition are predicted. [S0163-1829(98)01213-2]

I. INTRODUCTION

The problem of the c-axis conductivity in high-T_c layered cuprates was always considered as one of the mysteries of these substances. The low-temperature semiconductorlike behavior in underdoped $YBa_2Cu_3O_{7-\delta}$ (YBCO) contradicted the metallic behavior of the in-plane conductivity; the c-axis frequency-dependent conductivity in the same substances revealed a definite ''pseudogap'' which was absent in the optimally doped samples. At the same time a significant supercurrent observed along the c axis in underdoped YBCO (Ref. 1) contradicted the idea of absence of coherence between different CuO_2 layers. A detailed description of the experimental situation and theoretical ideas can be found in review articles.[2,3]

In order to resolve these contradictions the present author proposed in his previous papers[4–6] the concept of resonant tunneling for the c-axis transport in underdoped YBCO. The idea was that if the doping of the CuO_2 planes by holes resulted from binding of electrons by oxygen atoms in the intermediate CuO chains (complete, or broken), these atoms could as well transmit the holes from one plane to another one. In order for this mechanism to be effective, it should correspond to ''resonance tunneling'' discovered by Bohm in 1951.[7] This phenomenon happens under two conditions: (a) the energy of the particle has to be equal to the energy of the bound state, and (b) the binding center has to be in the middle of the potential barrier. This is good for YBCO but does not fit, strictly speaking, to other layered cuprates, since there the doping agents are layers slightly displaced from the center (e.g., the BiO layers in $Bi_2Sr_2CaCu_2O_{8+\delta}$). Therefore, in the paper,[8] it was demonstrated that a small displacement of resonance centers from the median plane between two CuO_2 (single, double, or triple) layers does not reduce their effectiveness in transferring electrons; this explained the similarity of the temperature dependence of ρ_c/ρ_{ab} in Bi- and Tl-based cuprates to underdoped YBCO. In the same paper one of the major assumptions of the proposed mechanism was analyzed—the coherence of resonant tunneling via different centers; it was established that this idea is correct, provided that the resonant centers are not too rare. There appears, however, an important question: what happens with the normal and superconducting current along the c axis when the density of resonant centers decreases? Definitely, the coherence will be reduced, and it eventually disappears. The answer to this question is of principal importance, since, as it was shown in the paper,[9] the connection between different CuO_2 layers is crucial for superconductivity in strongly underdoped layered cuprates.

In this paper we will first analyze the c-axis normal conductivity in the case of incoherent resonance tunneling. We will see that it is, most likely, reduced compared to the coherent case but the temperature and frequency dependence do not differ from the coherent case. Contrary to that, the supercurrent exists only in the case of an s-type order parameter but is absent for a d-wave type. Then we will extend the calculation of the dependence of T_c on the concentration of resonant centers, performed in Ref. 9, to the region, where the coherence is gradually reduced. We will give arguments in favor of a possible $d\rightarrow s$ phase transition.

II. NORMAL STATE, INCOHERENT RESONANT TUNNELING

We will first go through the arguments of Ref. 5 (denoted as I) and consider formula $(2_{(\mathrm{I})})$ for the addition to the free energy due to the electromagnetic field. There is a summation over the resonant centers: $\Sigma_{jj'}$. In the case where the resonant tunneling through different centers is coherent, both summations are independent, i.e., the amplitudes are summed up. The sums are then substituted according to formula $(3_{(\mathrm{I})})$, and the resulting current is given by formula $(4_{(\mathrm{I})})$.

Here we would like to make some clarification. According to Ref. 8, the coherent resonant tunneling amplitude is proportional to the density of states at the localized centers (dn_j/dE_j) times the coherence energy interval η (in I it was denoted, as δ), which is of the order of the bandwidth times $\exp(-\alpha d)$—the direct tunneling amplitude. If all the centers would be exactly equivalent and have the binding energy E_0, (dn_j/dE_j) would be equal to $nc_j\delta(E_j-E_0)$, where n is the planar density of atoms in the median plane, c_j is the atomic concentration of resonant centers (oxygens). This is, however, not the real case, since different centers have a different environment, and this smears out slightly their binding energies. Nevertheless, in order for the resonant tunneling to exceed direct tunneling, (dn_j/dE_j) must be sufficiently large, i.e., the levels must be clustered within a narrow interval, not larger than η. In the general case there can be a finite number of such ''clusters'' centered at some discreet energies; this is likely the real case, as can be seen from the frequency-dependent c-axis conductivity at sufficiently low temperatures.[10,11] The quantity $(dn_j/dE_j)\eta$ was denoted in I, as n_j; it is proportional but not exactly equal to nc_j, the concentration of resonant centers in the median plane.

After the Fourier transformation we obtain Eq. $(5_{(\mathrm{I})})$. It should be stressed that the planar momenta entering the Green functions of the neighboring layers are equal; this follows directly from the coherence of tunneling through different centers. Actually the $\mathbf{k}$ integration is limited to an energy interval of the order of η around the resonance, and so the integral in Eq. $(5_{(\mathrm{I})})$ should include $\eta\delta[\varepsilon(\mathbf{k})-E_j]$, or, in the case of several ''clusters,'' the sum over all of them. This means, strictly speaking, that instead of $\int_{E-\varepsilon}^{E+\varepsilon} dE_j$ we will have $\eta\Sigma_{E_j}$. If there are many ''clusters'' this can be modeled by $q\int_{E-\varepsilon}^{E+\varepsilon} dE_j$, with $q\ll 1$.

In the case of incoherent tunneling $\rho_j=\rho_{j'}$ in Eq. $(2_{(\mathrm{I})})$. We obtain, therefore, the result

$$\begin{aligned} j_z(\tau) &= -c\,\frac{\delta\Delta\Omega}{\delta A_z(\tau)} \\ &= \frac{4}{c}\,d(et)^2 n_j \int_0^\beta d\tau' \widetilde{G}_n(0,\tau-\tau') \\ &\quad \times \widetilde{G}_{n+1}(0,\tau'-\tau)[A_z(\tau')-A_z(\tau)], \end{aligned} \tag{1}$$

instead of Eq. $(4_{(\mathrm{I})})$. Passing to the Fourier representation, we obtain

$$\begin{aligned} j_z(i\omega_0) &= \frac{4}{c}\,d(et)^2 n_j T\eta^2 \sum_m \int d^2k\,d^2k' \\ &\quad \times \delta[\varepsilon(\mathbf{k})-E_j]\delta[\varepsilon(\mathbf{k}')-E_j](2\pi)^{-4} \\ &\quad \times [\widetilde{G}_n(\mathbf{k},i\omega_m+i\omega_0)\widetilde{G}_{n+1}(\mathbf{k}',i\omega_m) \\ &\quad - \widetilde{G}_n(\mathbf{k},i\omega_m)\widetilde{G}_{n+1}(\mathbf{k}',i\omega_m)]A_z(i\omega_0). \end{aligned} \tag{2}$$

What concerns the imaginary time dependences, and, after the Fourier transformation, the frequency dependences, is that there are no changes.

Since, in the normal state the energy spectrum in the plane is almost isotropic, the change, compared to the coherent case, consists in substitution of one of n_j by $d(\nu_e/2)\eta$, where $d(\nu_e/2)$ is the electronic density of states per one plane per one spin projection. Since, as we argued before, n_j is actually $(dn_j/dE_j)\eta$, the planar density of electronic states at the resonant energy is substituted instead of (dn_j/dE_j). The latter is of the order of $nc_j/\Delta E_j$-the total amount of resonant centers divided by the width of the cluster. Hence, the reduction due to the absence of coherence is of the order of $(\Delta E_j/E_j)/c_j$. As it was said before, the resonant tunneling concept is true only, if the ratio $(\Delta E_j/E_j)$ is very small. Therefore, most likely, the coherence enhances the transport, even in the normal case.

Apart from a different coefficient, the formulas describing the temperature and frequency dependence of the c-axis conductivity remain the same, as in I and in Ref. 6. From the fitting of the coefficient A in I to experimental data we can also conclude that its dependence on oxygen concentration is in favor of coherent tunneling.

III. SUPERCONDUCTING STATE, INCOHERENT AND PARTIALLY COHERENT TUNNELING

The difference between coherent and incoherent tunneling becomes much more pronounced in the superconducting state. We can repeat all the derivation performed in Ref. 5 up to formula (17) for the current. Here for the incoherent case we obtain

$$\begin{aligned} j_z &= 4et^2 n_j \eta^2 T \sum_m \int d^2k \widetilde{F}_n(\mathbf{k},\omega_m)\delta[\varepsilon(\mathbf{k})-E_j] \\ &\quad \times \int d^2k' \widetilde{F}_{n+1}(\mathbf{k}',\omega_m)\delta[\varepsilon(\mathbf{k}')-E_j] \\ &\quad \times \sin[2eA_z(d/c)+\varphi_n-\varphi_{n+1}] \\ &\equiv J_c \sin[2eA_z(d/c)+\varphi_n-\varphi_{n+1}]). \end{aligned} \tag{3}$$

Performing the same transformations, as in the previous section we obtain

$$J_c = \frac{1}{2}\,ed(t\nu_e\eta)^2\left[\int \Delta(\theta)d\theta/(2\pi)\right]^2 \Omega \sum_j \left(\frac{n_j}{E_j^4}\right), \tag{4}$$

where the integration $d\theta$ is performed over the Fermi surface and Ω is the characteristic phonon frequency. In the case of d-type symmetry the integral $\int\Delta(\theta)d\theta/(2\pi)=0$, and hence $J_c=0$. This does not happen in the case of an s-type symmetry.

For the coherent case we obtain, instead of Eq. (4),

$$J_c = \frac{1}{2}\,edt^2\nu_e\eta\left[\int \Delta^2(\theta)d\theta/(2\pi)\right]\Omega \sum_j \left(\frac{n_j^2}{E_j^4}\right). \tag{5}$$

This current does not vanish even in the case of d-type symmetry.

Expressions (4) and (5) represent the limiting cases, and it is interesting, how the crossover happens, i.e., how the current changes with a gradual decrease of the concentration of resonant centers. In Ref. 8 a formula was derived for the Fourier component of the amplitude of the penetrated wave via two centers [see formula (21) in Ref. 8]. In order to illustrate the coherence we defined there the amplitude in real space at $\rho=0$ [formula (22) in Ref. 8]. Actually we need the total probability integrated over the surface of the barrier, and for two centers it is easy to see from Eq. (21) in Ref. 8 that the one-center expression is multiplied by

$$2+2e^{-\alpha\rho_0^2/(2d)}, \tag{6}$$

where ρ_0 is the distance between the two centers, d is the thickness of the barrier and $\alpha=\sqrt{(2m|U|)}$, $|U|$ being the binding energy of the center. The first term in this expression is the sum of probabilities, and the second term comes from interference. The whole expression can be presented in a form

$$4e^{-\alpha\rho_0^2/(2d)}+2(1-e^{-\alpha\rho_0^2/(2d)}), \tag{7}$$

and the first term can be interpreted as the coherent part, whereas the second represents the incoherent part. On the average $\rho_0^{-2}\sim nc_j$, the concentration of resonant centers in the plane. Therefore we can write an interpolation

$$J_c=e^{-s\alpha/(dnc_j)}J_c^{\rm coh}+J_c^{\rm in}, \tag{8}$$

where $s\sim 1$. In the case of d-type paring the incoherent part vanishes, and hence, J_c decreases exponentially with the atomic concentration of the resonant centers, when the latter becomes less than $c_j^{(0)}\sim\alpha/(dn)$.

In this connection the results of the work[9] on the dependence of T_c on the concentration of resonant centers have to be somewhat revised. In the final formula (9) in Ref. 9 the quantity δ is proportional to c_j^2 only until the atomic concentration of resonant centers is large enough: $c_j\gg c_j^{(0)}$ (for the Bi-based superconductor $c_j^{(0)}\sim 3\%$). If $c_j\ll c_j^{(0)}$, an exponential factor appears in δ, according to Eq. (8), and it contains the major dependence of T_c on the concentration. Hence, we get

$$T_c\sim\varepsilon_0/[B+2\ln(1/c_j)+sc_j^{(0)}/c_j]^2, \tag{9}$$

where $B\sim 1$ and $\varepsilon_0\sim 10^3$ K. This formula can serve also as an interpolation between different extremal regions.

The following possibility appears. If superconductivity with a d-type order parameter is sufficiently suppressed, another type of superconductivity can appear with a ''subdominant'' order parameter. In order to survive, this order parameter must be of the s type, and hence a $d\rightarrow s$ (or $d\rightarrow d+is$) transition can be expected in sufficiently underdoped samples, similar to the one predicted[12,13] for impurity suppression of the d-type order parameter. In principle, this can lead to a flattening of the angle-resolved photoemission spectroscopy curves for the momentum-dependent gap in drastically underdoped samples, which was observed experimentally.[14] Since there is little hope that systematic measurements of T_c and J_c on the same samples will be performed in near future, they can be replaced by a much simpler measurement of the T_c dependence on heating time in vacuum in order to trace the $d\rightarrow s$ transition, as a kink in this dependence.

ACKNOWLEDGMENTS

I would like to express my deep gratitude to Professor Ted Geballe, whose question: ''What happens in the incoherent case?'' originated this work. I would like also to thank Dr. David Hinks and Dr. Hong Ding for useful discussions. This work was supported by the Department of Energy under Contract No. W-31-109-ENG-38.

[1] M. Rapp *et al.*, Phys. Rev. Lett. **77**, 928 (1996).
[2] S. L. Cooper and K. E. Gray, in *Physical Properties of High Temperature Superconductors IV*, edited by D. M. Ginsberg (World Scientific, Singapore, 1994).
[3] A. V. Puchkov, D. N. Basov, and T. Timusk, J. Phys.: Condens. Matter **8**, 10 049 (1996).
[4] A. A. Abrikosov, Phys. Rev. B **52**, R7026 (1995).
[5] A. A. Abrikosov, Physica C **258**, 53 (1996).
[6] A. A. Abrikosov, Phys. Rev. B **54**, 12 003 (1996).
[7] D. Bohm, *Quantum Theory* (Prentice Hall, New York, 1951).
[8] A. A. Abrikosov, Phys. Rev. B **55**, 11 735 (1997).
[9] A. A. Abrikosov, Phys. Rev. B **55**, R6149 (1997).
[10] C. C. Homes *et al.*, Phys. Rev. Lett. **71**, 1645 (1993).
[11] C. C. Homes *et al.*, Physica C **254**, 265 (1995).
[12] A. A. Abrikosov, Phys. Rev. B **53**, R8910 (1996).
[13] G. Preosti and M. Palumbo, Phys. Rev. B **55**, 8430 (1997).
[14] H. Ding *et al.*, Nature (London) **382**, 51 (1996).