Cases of resonant tunneling important for high-T_c cuprates

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Some basic assumptions made by the present author in his work about c-axis transport in layered cuprates are examined on simple models. First, a one-dimensional model is considered with a localized center slightly displaced from the middle of the barrier in order to find out whether this displacement prevents resonant tunneling. Second, a three-dimensional model is analyzed with two resonant centers in the median plane; the goal is to establish whether tunneling through such centers can be coherent. The results provide support for the basic assumptions. [S0163-1829(97)13517-2]

I. INTRODUCTION

In Refs. 1–3 an idea was proposed that the mechanism of c-axis transport in underdoped $YBa_2Cu_3O_x$ is resonant tunneling through localized centers in the barrier between two CuO_2 bilayers formed in place of broken CuO chains. It was supposed that the tunneling through centers having the same binding energy happens coherently and therefore the amplitudes are added, whereas the tunneling through centers with different energies is incoherent, and therefore the probabilities are summed up. The coherence leads to an important consequence, namely that the electron momentum in the (ab) plane is conserved during tunneling. Whether this is true has to be checked.

Another important problem is that in other layered high-T_c cuprates, such as $Bi_2Sr_2CaCu_2O_{8+\delta}$,[4,5] and $Tl_2Ba_2CuO_{6+\delta}$,[6,7] the resistivity ratio ρ_c/ρ_{ab} varies with temperature as $\exp(E/T)$, and this is very much reminiscent of resonant tunneling behavior. However, there are no chains between the CuO_2 layers, and, actually, the median plane is empty. It is widely believed that the doping of the CuO_2 layers with holes in $Bi_2Sr_2CaCu_2O_{8+\delta}$ originates from the BiO layers. They are located around the median plane at distances approximately equal to 1 Å. If the localized centers in the barrier are associated with these layers, the question is whether this small displacement from the middle can reduce substantially the resonant tunneling probability.

Although the answer, at least for the second problem, can be obtained from some previous articles, e.g., Refs. 8 and 9, their authors were concerned with rather general cases, and this made the results somewhat hard to comprehend. Therefore we find it useful to consider the simplest models in a straightforward way in order to leave no doubts and to present the results in a most transparent form.

II. ONE-DIMENSIONAL CASE, ONE CENTER

We will start with the second problem, since it can be solved in the framework of a one-dimensional mode. Let us consider a rectangular barrier with a potential U at $0<z<d$ with a center located at z_0 $(0<z_0<d)$ described by a potential energy $-(\beta/2m)\delta(z-z_0)$. The Schrödinger equation can be presented in the form

$$\frac{d^2\Psi}{dz^2}-\alpha^2\Psi=-\beta\delta(z-z_0)\Psi(z_0), \tag{1}$$

where

$$\alpha=[2m(U-E)]^{1/2}. \tag{2}$$

Its general solution is

$$\Psi(z)=[A-(\beta/2\alpha)\Psi(z_0)\theta(z-z_0)e^{-\alpha z_0}]e^{\alpha z}+[B+(\beta/2\alpha)\Psi(z_0)\theta(z-z_0)e^{\alpha z_0}]e^{-\alpha z}. \tag{3}$$

The solutions beyond the barrier are

$$\Psi(z)=e^{i\kappa z}+re^{-i\kappa z}, \quad z<0$$
$$\Psi(z)=pe^{i\kappa(z-d)}, \quad z>d, \tag{4}$$

where $\kappa=(2mE)^{1/2}$, r is the amplitude of the reflected wave, and p is of the penetrated wave.

The boundary conditions are the continuity of Ψ and $d\Psi/dz$ at the interfaces. From these four conditions we define the constants A, B, r, and p. They are

$$A=\frac{1}{2}\left(1+\frac{i\kappa}{\alpha}\right)+\frac{r}{2}\left(1-\frac{i\kappa}{\alpha}\right),$$
$$B=\frac{1}{2}\left(1-\frac{i\kappa}{\alpha}\right)+\frac{r}{2}\left(1+\frac{i\kappa}{\alpha}\right), \tag{5}$$

$$r=\frac{(\beta/\alpha)\Psi(z_0)[(1-i\kappa/\alpha)e^{\alpha(d-z_0)}+(1+i\kappa/\alpha)e^{-\alpha(d-z_0)}-2(1+\kappa^2/\alpha^2)\sinh(\alpha d)}{(1-i\kappa/\alpha)^2e^{\alpha d}-(1+i\kappa/\alpha)^2e^{-\alpha d}}\approx\frac{(\beta/\alpha)\Psi(z_0)e^{-\alpha z_0}-(1+i\kappa/\alpha)}{1-i\kappa/\alpha}, \tag{6}$$

$$p=\frac{(\beta/\alpha)\Psi(z_0)[(1-i\kappa/\alpha)e^{\alpha z_0}+(1+i\kappa/\alpha)e^{-\alpha z_0}]-4i\kappa/\alpha}{(1-i\kappa/\alpha)^2e^{\alpha d}-(1+i\kappa/\alpha)^2e^{-\alpha d}}\approx\frac{(\beta/\alpha)\Psi(z_0)e^{\alpha(z_0-d)}}{1-i\kappa/\alpha}-\frac{(4i\kappa/\alpha)e^{-\alpha d}}{(1-i\kappa/\alpha)^2}. \tag{7}$$

0163-1829/97/55(17)/11735(3)/$10.00

We assumed here that $z_0,\ d-z_0 \gg 1/\alpha$.

From Eqs. (3), (5), and (6) (here we have to use the full expression) we obtain $\Psi(z_0)$:

$$\Psi(z_0) \approx -\left(\frac{2i\kappa}{\alpha}\right) e^{\alpha(d-z_0)}\{(1-\beta/2\alpha)(1-i\kappa/\alpha)e^{\alpha d}-(\beta/\alpha) \times(1+i\kappa/\alpha)\cosh[\alpha(d-2z_0)]\}^{-1} \tag{8}$$

and

$$p \approx (\beta/\alpha)e^{\alpha(z_0-d)}(1-i\kappa/\alpha)^{-1}\Psi(z_0) \approx -\left(\frac{2i\beta\kappa}{\kappa^2+\alpha^2}\right)\left\{\left(1-\frac{\beta}{2\alpha}\right)e^{\alpha d+2i\varphi} - \frac{\beta}{\alpha}\cosh[\alpha(d-2z_0)]\right\}^{-1}, \tag{9}$$

where $\varphi = \arctan(\alpha/\kappa)$.

The transparency coefficient is equal to the absolute square of this expression. It is exponentially small except in a small ''coherence interval'' of energies around $2\alpha=\beta$, or

$$U-E_0=\beta^2/(8m), \tag{10}$$

provided that the resonant center is located close to the middle of the barrier: $z_0 \approx d/2$. Our main goal is to find out to what extent this condition is stringent. One sees readily that the requirement is

$$|d-2z_0| \leqslant 1/\alpha = [2m(U-E)]^{-1/2}. \tag{11}$$

As it was said already, in $Bi_2Sr_2CaCu_2O_{8+\delta}$ the displacement of the BiO layers from the center is approximately 1 Å. Even in this case, if $U-E_0=1$ eV, $1/\alpha=2$ Å, and the actual resonant levels might be more shallow. One sees that practically all localized centers formed from broken chains in $YBa_2Cu_3O_x$ and from BiO layers in $Bi_2Sr_2CaCu_2O_{8+\delta}$ can serve for resonant tunneling at proper energies. The only remaining question is their coherence, which may be violated either by the environment, or by their distance from each other. The latter problem we are going to analyze in the next section.

III. THREE-DIMENSIONAL CASE, TWO CENTERS

This time we suppose that there are two centers located in the median plane: the first at $(0,d/2)$, and the second at $(\rho_0,d/2)$. This time we have to solve the three-dimensional Schrödinger equation. Performing a Fourier transformation with respect to ρ, we obtain

$$\frac{d^2\Psi_k}{dz^2}-\alpha_k^2\Psi_k=-\beta\Psi^{(k)}(d/2)\,\delta[z-(d/2)], \tag{12}$$

where

$$\Psi(\rho,z)=\int \Psi_k(z)e^{i\mathbf{k}\rho}d^2\mathbf{k}/(2\pi)^2, \tag{13}$$

$$\alpha_k=[2m(U-E)+k^2]^{1/2}, \tag{14}$$

$$\Psi^{(k)}(d/2)=\Psi(0,d/2)+\Psi(\rho_0,d/2)e^{-i\mathbf{k}\rho_0}. \tag{15}$$

The boundary conditions for a normal incidence are

$$\Psi_k(0)=(2\pi)^2\delta(\mathbf{k})+r_k, \quad \Psi_k(d)=p_k. \tag{16}$$

From Eqs. (12), (16) we obtain formulas similar to Eqs. (5)–(7), where $\alpha_k=(\alpha^2+k^2)^{1/2}$ enters instead of α, $q=(\kappa^2-k^2)^{1/2}$ instead of κ, $\Psi^{(k)}(d/2)$ instead of $\Psi(z_0)$, and the terms without Ψ in the numerators of Eqs. (6) and (7) acquire a factor $(2\pi)^2\delta(\mathbf{k})$.

The self-consistency relations are

$$\Psi(0,d/2)=\int \frac{d^2\mathbf{k}}{(2\pi)^2}\,(A_k e^{\alpha_k d/2}+B_k e^{-\alpha_k d/2}),$$

$$\Psi(\rho_0,d/2)=\int \frac{d^2\mathbf{k}}{(2\pi)^2}\,(A_k e^{\alpha_k d/2}+B_k e^{-\alpha_k d/2})e^{i\mathbf{k}\rho_0}.$$

Substituting A_k and B_k we get equations defining Ψ at both centers:

$$\Psi(0,d/2)-\int \frac{d^2\mathbf{k}}{(2\pi)^2}\frac{\beta}{\alpha_k}\left(\frac{1}{2}+\frac{1+iq/\alpha_k}{1-iq/\alpha_k}e^{-\alpha_k d}\right)[\Psi(0,d/2)+\Psi(\rho_0,d/2)e^{-i\mathbf{k}\rho_0}]=-\frac{2i\kappa e^{-\alpha d/2}}{\alpha(1-i\kappa/\alpha)},$$

$$\Psi(\rho_0,d/2)-\int \frac{d^2\mathbf{k}}{(2\pi)^2}\frac{\beta}{\alpha_k}\left(\frac{1}{2}+\frac{1+iq/\alpha_k}{1-iq/\alpha_k}e^{-\alpha_k d}\right)[\Psi(0,d/2)e^{i\mathbf{k}\rho_0}+\Psi(\rho_0,d/2)]=-\frac{2i\kappa e^{-\alpha d/2}}{\alpha(1-i\kappa/\alpha)}, \tag{17}$$

where α and κ are the same, as in the previous section. The symmetry of the integrals with respect to $\mathbf{k}\rightarrow-\mathbf{k}$ leads to the conclusion

$$\Psi(\rho_0,d/2)=\Psi(0,d/2), \tag{18}$$

and hence

$$\Psi(0,d/2)=-\frac{2i\kappa e^{-\alpha d/2}}{\alpha(1-i\kappa/\alpha)}\left[1-\int \frac{d^2\mathbf{k}}{(2\pi)^2}\frac{\beta}{2\alpha_k}\left(1+2\frac{1+iq/\alpha_k}{1-iq/\alpha_k}e^{-\alpha_k d}\right)(1+e^{-i\mathbf{k}\rho_0})\right]^{-1}. \tag{19}$$

Since the minimal value of α_k, is α, the second term of the integrand vanishes at $d\rightarrow\infty$. The remaining integral is divergent. This is due to the fact that in the three-dimensional case the δ-function potential has no finite eigenvalues. Therefore we must consider some potential with a finite range. Since the precise eigenvalue is of no importance, we simply cut off the integral at some $k=K$. Assuming ρ_0 to be larger than $1/\alpha$ and the range of the potential, $1/K$, we can calculate the square bracket in the denominator of Eq. (19) close to the resonance and obtain

$$\Psi(0,d/2)\approx\frac{2\kappa e^{-\alpha d/2}}{\kappa+i\alpha}\left[\frac{\varepsilon-\varepsilon_0}{2[\varepsilon_0(\varepsilon_0+K^2/2m)]^{1/2}}-\frac{\beta}{2\pi d}\frac{\kappa-i\alpha}{\kappa+i\alpha}(1+e^{-\alpha\rho_0^2/(2d)})e^{-\alpha d}\right]^{-1}, \tag{20}$$

where $\varepsilon_0=(1/2m)(\beta/8\pi)^2[K^2-(4\pi/\beta)^2]^2$ is the resonant value of $\epsilon=U-E$.

From the formula, similar to Eq. (7) we can obtain the Fourier component of the penetrated wave

$$p_k\approx i\beta\Psi(0,d/2)(1+e^{i\mathbf{k}\rho_0})e^{-\alpha_k d/2}(q+i\alpha_k)^{-1}, \tag{21}$$

and, transforming to real space, we get for two centers

$$P^{(2)}=\int p_k d^2k/(2\pi)^2=\frac{2i\beta\alpha\kappa}{\pi d(\kappa+i\alpha)^2}(1+e^{-\alpha\rho_0^2/d})\left[\frac{(\varepsilon-\varepsilon_0)e^{\alpha d}}{2[\varepsilon_0(\varepsilon_0+K^2/2m)]^{1/2}}-\frac{\beta}{2\pi d}\frac{\kappa-i\alpha}{\kappa+i\alpha}(1+e^{-\alpha\rho_0^2/(2d)})\right]^{-1}. \tag{22}$$

The dependence on ρ_0 in the square bracket can be neglected, as we will see in a moment. Then, in this case, if $\rho_0\ll\sqrt{d/\alpha}$, the amplitude is doubled compared to the case of one center, and that means coherence of tunneling through the two centers. In the general case of many centers, if the average distance between them is less than $\sqrt{d/\alpha}$, i.e., their density is larger than α/d, we can introduce the average amplitude, substituting the bracket $(1+e^{-\alpha\rho_0^2/d})$ in Eq. (21) by the density of the centers. This, however, does not take into account that the energies of the centers can be slightly different. If this scatter of eigenvalues, although small, is still sufficiently large, so that the absolute limiting values of the first term in the square bracket of Eq. (22) are larger than the second term, then this bracket can be replaced by

$$-i\delta\left(\frac{(\varepsilon-\varepsilon_0)e^{\alpha d}}{2[\varepsilon_0(\varepsilon_0+K^2/2m)]^{1/2}}\right)=-2i\pi[\varepsilon_0(\varepsilon_0+K^2/2m)]^{1/2}\times e^{-\alpha_0 d}\delta(\varepsilon-\varepsilon_0);$$

this expression does not depend on ρ_0. The principal part of Eq. (22) does not contribute to the result.

Summation over centers, i.e., integration over their energies ε_{0j}, gives

$$\overline{P}=\frac{4\beta\alpha_0\kappa_0}{d(\kappa_0+i\alpha_0)^2}[\varepsilon_0(\varepsilon_0+K^2/2m)]^{1/2}e^{-\alpha_0 d}\left(\frac{dn_j}{d\varepsilon}\right)_0, \tag{23}$$

where $dn_j/d\varepsilon$ is the density of localized states. This penetration amplitude exceeds the amplitude of direct tunneling, if $dn_j/d\varepsilon$ is sufficiently large, i.e., if all the localized states have approximately the same energy or are concentrated around few discrete values (the experimental curves for high-frequency c conductivity[10] can be considered as evidence of the latter situation). The factor $[\varepsilon_0(\varepsilon_0+K^2/2m)]^{1/2}e^{-\alpha_0 d}(dn_j/d\varepsilon)_0$ plays the role of n_j, which was introduced in Refs. 1 and 2. The coefficient t, appearing there in the tunneling Hamiltonian, is the product of $4\beta\alpha/(\kappa d)$ and some ''interaction energy'' having the order of the barrier U.

The main result, which we obtained here, is that coherent tunneling through different centers is possible, if their energies do not differ too much and if their density is higher than one center per area d/α. For $Bi_2Sr_2CaCu_2O_{8+\delta}$ the distance between the closest double layers is $d=15$ Å. If we assume $|\varepsilon_0|=1$ eV, we obtain $1/\alpha=2$ Å, but it is likely that the localized levels are more shallow, and so we take $1/\alpha=4$ Å. From this we get the characteristic area of the order of 60 Å^2; more than one center per such an area looks quite realistic. One has to consider also our basic assumption $e^{-\alpha d}\ll 1$; in this case $e^{-\alpha d}\approx 0.024$.

The above estimates are rather transparent and, despite the simplicity of the models, provide support to the assumptions made by the present author in Refs. 1–3 and hence, to the resonant tunneling mechanism of the c-axis transport in layered cuprates.

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