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Resonant tunneling in high- T_c superconductors

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<u>Abstract.</u> A review is presented of the author's work on resonance tunneling as an electron transport mechanism along the c axis in high-temperature layered cuprates. A formulation of the problem is given, qualitative aspects of the mechanism are described, and physical properties calculated. Comparisons are made with experimental data for the temperature dependence of normal conductivity, the frequency dependence of optical conductivity, and the stationary supercurrent along the c axis. For the latter, the resonance tunneling coherence of different centers is shown to be of crucial importance. Weakened interplane coupling and vortex fluctuations are invoked to explain the sharp drop in T_c and the rise in the $2\Delta(0)/T_c$ ratio with decreasing oxygen content. Simple example models are given to demonstrate major aspects of resonance tunneling.

1. Introduction

The mechanism of conductivity, and hence, superconductivity, along the *c* axis in high- T_c layered cuprates has always been somewhat mysterious. The long period in this direction means a long distance between CuO₂ complexes of single, double or triple layers, and in the absence of the CuO chains, which exist only in the optimally doped YBa₂Cu₃O₇ and in YBa₂Cu₄O₈ (YBCO124), the hopping between distant CuO₂ layers should be negligible. Systematic experimental studies of the normal conductivity of single crystals of YBa₂Cu₃O_x with x < 7, i.e., with broken chains [1], showed that whereas the in-plane resistivity ρ_{ab} behaved 'metallically', i.e., decreased with temperature, the *c*-axis resistivity ρ_c showed 'insulating' behavior (see Fig. 1).

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At first this was explained as a consequence of the 'Anderson localization' in the c direction. However, this explanation was rejected, first, on the basis of the scaling theory, and then by direct estimates [2], which showed that localization in the c direction requires a larger impurity concentration than localization on the plane. Attempts to explain the conductivity along the c axis in the absence of chains led to many controversial assumptions. One was the universal existence of 'normal metal layers' (see, e.g., Refs [3-5]); this hypothesis was not confirmed by angle-resolved photoemission spectroscopy (ARPES) in $Bi_2Sr_2CaCu_2O_{8+\delta}$ (BSCCO), which showed that there are no other Fermi surfaces, except those of the CuO₂ planes (see Ref. [6]). The other was the RVB mechanism, associated with the existence of 'spinons' and 'holons' [7, 8] (or, for superconductivity, 'pair tunneling' [9]); however, in the presence of chains the ARPES experiments demonstrated a definite hybridization in the one-electron spectra of chains and planes [10], and this completely ruled out such a mechanism. There exist several



Figure 1.Temperature dependences of ρ_{ab} and ρ_c for YBa₂Cu₃O_{6.66} [1].

attempts to connect the *c*-axis conductivity with 'off-diagonal disorder', i.e., some sort of scattering by impurities lying between the CuO_2 planes, which enhances the hopping between planes (see Ref. [11] and references therein). It is difficult, however, to understand the mechanism of such an enhancement unless some further assumptions are made, and this can substantially alter the picture.

At the same time the solution of this mystery is almost obvious. The metallic conductivity of layered cuprates is due to doping of the CuO₂ planes by holes. In YBCO the origin is the oxygen atoms in the CuO chains, which have a tendency to attract electrons from the planes. In the case of optimally doped YBa₂Cu₃O_x with x = 7 the chains are metallic (Fig. 2a), and the energy bands of the planes and chains intersect (Fig. 3a). However, in the 'underdoped' samples with x < 7 the chains are broken (Fig. 2b). Nevertheless, the remaining oxygen atoms can form localized states for electrons and can attract them from the planes (Fig. 3b). It is easy to see that this mechanism can lead not only to doping but also to transport of holes between the planes (Fig. 4). In order for this mechanism to be effective, it must correspond to the so-called 'resonant tunneling'.

The idea of this phenomenon was first proposed by D Bohm [12] in 1951 and is now extensively used in the physics of semiconductors. If the electrons tunnel through a potential barrier, the probability is exponentially small. However, if in the bulk of the barrier there exists a potential well, the probability can become almost 1. For this, two conditions must be fulfilled: (1) the well must be exactly in the



Figure 2. Scheme of CuO_2 planes and CuO chains in (a) optimally doped and (b) underdoped YBCO (real space).



Figure 3. (a) Energy bands of planes and chains in optimally doped YBCO; and (b) energy bands of planes and localized states of broken chains in underdoped YBCO (energy space).



Figure 4. Scheme of doping and *c*-axis transport in underdoped YBCO (real space).

middle of the barrier, and (2) the energy of the electron must be equal to that of the bound state in the well. For the centers formed by broken CuO chains in YBCO, the first requirement is satisfied automatically. As for the second requirement, the energy of the localized states is in general quite different from the Fermi energy (see Fig. 3b). At finite temperatures the Fermi distribution has an exponential tail, and the holes in it may have the necessary energy. This leads to an exponential temperature dependence of ρ_c .

This explanation is very likely for underdoped YBCO, but the question is whether it can be used for superconductors based on Bi, Tl, or Hg which have no chains. The temperature dependence of the in-plane resistivity ρ_{ab} of such layered cuprates is always 'metallic' but ρ_c exhibits various kinds of behavior, from 'metallic' to 'insulating', in different samples. However, as can be seen from the theory described below, the behavior of the resistivity components can be confusing, and much clearer conclusions can be drawn from the temperature dependence of the ratio ρ_c/ρ_{ab} . In BSCCO and the talliumbased superconductors this ratio grows approximately exponentially with decreasing temperature [13–16], which can be considered as evidence of the same resonant tunneling mechanism.

It is generally accepted that the doping of the CuO_2 planes in these substances is accomplished by oxygen atoms in the BiO layers in BSCCO, or similar layers in other substances, in the same way as by the CuO chains of YBCO. The BiO layers are, however, slightly displaced from the middle of the barrier. Therefore, a question appears as to what are the permissible limits of such a displacement. This is a rather simple quantum-mechanical problem, and its solution is given in Appendix I [17]. The result is that the actual displacement is so small that it does not qualitatively influence the tunneling probability, and hence, we can conclude that the resonant tunneling mechanism of interplane transport is very general.

The contents of this review are ordered in the following way. In Section 2, the temperature dependence of the static normal c conductivity is calculated [18, 19]. In Section 3, theoretical predictions are compared with the experimental data of Ref. [1]. Section 4 is devoted to normal optical conductivity along the c axis, including a comparison with experiment [20]. In Section 5, superconductivity along the c axis is considered [19]; special attention is drawn to the case when the resonant tunneling through different centers is incoherent or partially coherent [21]. In Section 6, an analysis is given of how the critical temperature is suppressed by decreasing the concentration of resonant centers [21, 22]. Appendix I deals with the question about the role of displacement of the resonant center with respect to the barrier center [17]. The coherence of resonant tunneling through two centers is considered in Appendix II [17].

2. Normal static conductivity

We will assume that the resonant 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 CuO_2 planes 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 more numerous than the resonant centers. The Hamiltonian of the model ist

$$H = \sum_{n} \left\{ \int \psi_{n}^{+}(\rho) \xi \psi_{n}(\rho) d^{2}\rho + U_{n} + t \sum_{j} \left[\tilde{\psi}_{n+1}^{+}(\rho_{j}) \tilde{\psi}_{n}(\rho_{j}) \exp\left(\mathrm{i}\frac{e}{c}A_{z}d\right) + \tilde{\psi}_{n}^{+}(\rho_{j}) \tilde{\psi}_{n+1}(\rho_{j}) \exp\left(-\mathrm{i}\frac{e}{c}A_{z}d\right) \right] \right\},$$
(1)

where the first term is the kinetic energy, the second corresponds to scattering within the plane leading to a finite life time, and the third is associated with the resonant tunneling between CuO₂ planes. Here ψ_n refers to plane $n, \tilde{\psi}$ means the part of the ψ operator that corresponds to the energy of the resonant impurity E_j , and ρ_j are 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 (the distance between the planes), and A_z is assumed to vary substantially at distances much larger than d.

In order to calculate the current, we first define the contribution to the thermodynamic potential Ω of second order in A_z and lowest order in t. Since we have to take averages over electronic states, the correction in the first approximation after summation over spins is given by (see Ref. [19])

$$\Delta \Omega = -T \left(\frac{etd}{c}\right)^2 \int_0^\beta d\tau \int_0^\beta d\tau'$$

$$\times \sum_n \sum_{jj'} \widetilde{G}_n(\rho_j - \rho_{j'}, \tau - \tau') \widetilde{G}_{n+1}(\rho_{j'} - \rho_j, \tau' - \tau)$$

$$\times \left[A_z(\tau) - A_z(\tau')\right]^2. \tag{2}$$

First, we perform summation over j, j'. Here, we must distinguish two limiting cases. Resonant tunneling through different centers can be coherent or incoherent. If the energies of the centers are very different, they are definitely incoherent. The permitted 'coherence' interval, which we denote as η , is by order of magnitude the average binding energy $U - E_0$ times the direct tunneling amplitude $exp(-\alpha d)$, where $\alpha = \hbar^{-1} \sqrt{2m(U-E_0)}$ (see Appendix I). The difference in energies can be due to different surroundings. This is, however, not the only origin of incoherence. If the centers are too far apart, i.e., their concentration is very low, they will also act incoherently. An example of two centers is considered in Appendix II. The characteristic distance proves to be of the order of $\sqrt{d/\alpha}$. If the distance between the CuO₂ layers is large, and the binding energy is small, there will be many centers within such distances, and all centers with the same energy will be coherent. This is the actual case except for very strongly underdoped samples; the latter will be considered later.

As shown in Appendix II, resonant tunneling enhances the probability only in the case when the energies of the localized states are clustered around some discrete values with a high density (there is some indication of this in the infrared data, see Section3). Then the tunneling processes through centers belonging to the same cluster will be coherent, and the summation over impurities can be replaced by a summation over such clusters, namely,

$$\sum_{j}^{(i)} \to v_{i} \eta \int d^{2} \rho_{j}, \qquad (3)$$

where *i* denotes a certain cluster, and v_i is the corresponding density of states. With this substitution, the contribution of every cluster to free energy (2) has to be calculated, and then the summation over clusters performed. For simplicity we will consider a model with only one such cluster, i.e., where the energies of all localized states are close to each other. This introduces two adjustable parameters: the constant prefactor depending on *t*, η and *v*; and the energy of the localized state. From Eqn (2) we obtain the 'thermodynamic' current

$$j_{z}(\tau) = -c \frac{\delta \Delta \Omega}{\delta A_{z}(\tau)} = \frac{4}{c} d(etv\eta)^{2} \int_{0}^{\beta} d\tau' \int d^{2}\rho \widetilde{G}_{n}(\rho, \tau - \tau')$$
$$\times \widetilde{G}_{n+1}(-\rho, \tau' - \tau) \left[A_{z}(\tau') - A_{z}(\tau) \right].$$
(4)

Here, the \widetilde{G} functions include the in-plane scattering. According to our assumption, this scattering is uncorrelated at different planes and, so, independently averaged functions must be used. Therefore, both functions are equal and depend only on the coordinate differences. Passing to the Fourier representation in τ and ρ , we obtain

$$j_{z}(i\omega_{0}) = \frac{4}{c}d(etv\eta)^{2}T\sum_{m}\int d^{2}k(2\pi)^{-2}$$

$$\times \left[\widetilde{G}(k,i\omega_{m}+i\omega_{0})\widetilde{G}(k,i\omega_{m})\right]$$

$$-\widetilde{G}(k,i\omega_{m})\widetilde{G}(k,i\omega_{m})]A_{z}(i\omega_{0}).$$
(5)

It is important to mention that, due to the coherence of tunneling through centers belonging to the same cluster and to the randomness of their locations, the electron conserves its momentum in the plane after hopping.

Now, we perform two operations. First, we find the analytical continuation to real frequencies. The k integration refers to a tiny energy interval of width η around the energy of the cluster E. Hence,

$$\int \mathrm{d}^2 k (2\pi)^{-2} f(k) \to \frac{\mathrm{d} v_{\mathrm{e}} \eta}{2} \int f(E) \frac{\mathrm{d} \phi}{2\pi} \,, \tag{6}$$

where v_e is the three-dimensional electron density of states (i.e., the 2D-density with spins times 1/d; note that it is not the same as v in (4) — the 2D density of resonant states), and the integration is over the Fermi contour in the plane. For simplicity we assume isotropy in the plane. Then $v_e = m/(\pi d)$ and can be considered as independent of energy. We obtain

$$j_{z}(\omega_{0}) = \frac{2}{c} (etv\eta d)^{2} v_{e} \eta \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega$$

$$\times \left[\tanh\left(\frac{\omega}{2T}\right) \operatorname{Im} G_{R}(\omega, E) G_{R}(\omega + \omega_{0}, E) \right.$$

$$+ \tanh\left(\frac{\omega + \omega_{0}}{2T}\right) G_{A}(\omega, E) \operatorname{Im} G_{R}(\omega + \omega_{0}, E)$$

$$- \tanh\left(\frac{\omega}{2T}\right) \operatorname{Im} G_{R}^{2}(\omega, E) \right] A_{z}(\omega_{0}) .$$

$$(7)$$

[†] Everywhere, except specially mentioned cases, we use units with $\hbar = 1$.

The coefficient connecting $j_z(\omega_0)$ and $A_z(\omega_0)$ (denoted by -Q) vanishes at $\omega_0 = 0$.

The static conductivity is defined by the relation

$$\sigma_{\rm c} = {\rm i}c \left(\frac{\partial Q(\omega_0)}{\partial \omega_0}\right)_{\omega_0 = 0}.$$
(8)

From this we obtain

$$\sigma_{\rm c} = (etv\eta d)^2 v_{\rm e} \eta \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \frac{1}{T} \cosh^{-2} \left(\frac{\omega}{2T}\right) \left[\operatorname{Im} G_{\rm R}(\omega, E) \right]^2$$
$$= (etv\eta d)^2 v_{\rm e} \eta \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \frac{1}{T} \cosh^{-2} \left(\frac{\omega}{2T}\right)$$
$$\times \left[\frac{1/2\tau}{(\omega - E)^2 + (1/2\tau)^2} \right]^2, \tag{9}$$

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

The integrand in Eqn (9) is a product of two δ -functionlike factors. Since we assume $1/2\tau$ to be much less than *T*, the second factor can be replaced by $\pi\tau\delta(\omega - E)$, and after that we obtain

$$\sigma_{\rm c} = \frac{1}{2} \left(e t v \eta d \right)^2 v_{\rm e} \eta \tau \left(T \cosh^2 \frac{E}{2T} \right)^{-1}. \tag{10}$$

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

$$\frac{\rho_c}{\rho_{ab}} = \frac{1}{\eta} \left(\frac{v}{tv\eta d}\right)^2 T \cosh^2 \frac{E}{2T} \,. \tag{11}$$

For generality, let us consider the case of incoherent tunneling [21]. This means that not the amplitudes but the probabilities should be added, and in formula (2) the summation over impurities should be performed with j = j'. We obtain

$$j_{z}(\tau) = \frac{4}{c} d(et)^{2} v \eta \int_{0}^{\beta} \mathrm{d}\tau' \int \widetilde{G}_{n}(0, \tau - \tau') \widetilde{G}_{n+1}(0, \tau' - \tau) \\ \times \left[A_{z}(\tau') - A_{z}(\tau) \right].$$
(12)

Passing to Fourier components, we get

$$j_{z}(i\omega_{0}) = \frac{4}{c} d(et)^{2} v \eta T \sum_{m} \int d^{2}k \, d^{2}k' (2\pi)^{-4}$$
$$\times \left[\widetilde{G}_{n}(k, i\omega_{m} + i\omega_{0}) \widetilde{G}_{n+1}(k', i\omega_{m}) - \widetilde{G}_{n}(k, i\omega_{m}) \widetilde{G}_{n+1}(k', i\omega_{m}) \right] A_{z}(i\omega_{0}) .$$
(13)

One can see that in the incoherent case the quasimomentum in the plane is not conserved after hopping from one plane to another. The two independent k integrations are substituted according to formula (6). Then we perform the analytical continuation to real frequencies. The result will be the same as before, except for the substitution of one of the v's in (11) by $v_e d/2$. Since v is supposed to be large (see Appendix II), incoherence is likely to reduce the conductivity. Actually, it is difficult to get an independent estimate of the constant prefactor, and since otherwise there is no change, we can consider the question of coherence not very important for normal conductivity. We will see the same to be true for high-frequency conductivity. The situation, however, will be drastically different for superconductivity (see Section 5).

3. Comparison with experiment

A comparison with experimental data [1] was performed on the basis of Eqn (11) written in the form

$$\frac{\rho_c}{\rho_{ab}} = AT \cosh^2 \frac{T_0}{T} \tag{14}$$

by choosing optimal values for the constants A and T_0 (Fig. 5a-e). One sees that the fit is good for moderate oxygen concentrations, and worse in both limits, i.e., for metallic and completely broken chains; hence, in these limits our theory does not reflect all the details of the plane-chain relations (see also the end of this section). The constant T_0 in the middle region (Fig. 5b-d) remains essentially independent of the oxygen concentration: $\overline{T}_0 \approx 548$ K, or $E \approx 47$ meV (it has to be remembered that the energy *E* is actually the difference $E - \mu$) and is somewhat smaller at the edges.

Our theory fails close to x = 7, where the chains are metallic and their energy levels tend to form a band. Since the *c*-axis conductivity is essentially exponential, the smallest activation energy shows up; therefore, it is likely to be smaller than in the intermediate region. In the vicinity of the metal– insulator transition, there is a competing mechanism of doping: direct thermal excitation from the valence band to the conduction band. Due to the low concentration of resonant centers, direct tunneling becomes the main mechanism of transport. The probability does not depend on temperature, and therefore, the main temperature dependence of the resistivity comes from the thermal excitation exponent with a smaller activation energy. Despite this, such processes are negligible far from the transition, since the direct, unassisted tunneling probability is very small.

Contrary to T_0 , the constant

$$A = \frac{1}{\eta} \left(\frac{v}{tv\eta d}\right)^2 \tag{15}$$

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

$$4 = a(x-b)^{-m},$$
 (16)

where x is the number of oxygen atoms per unit cell, we obtain the following optimal values for the constants:

$$a = 0.073, \quad b = 6.34, \quad m = 1.62.$$
 (17)

The fit is presented in Fig. 6. It is remarkably good, and the values (17) are very reasonable.

The concentration x = 6.34 corresponds to the metal– insulator transition, and this shows that the resonant centers and doping centers are essentially the same, as we argued in Section 1. It is most likely that the density of localized states *v* is proportional to the concentration of oxygen atoms in



Figure 5. Best fit of Eqn (14) to the experimental data [1] for YBCO with different oxygen contents.



Figure 6. Dependence of the constant A from formula (14) on oxygen content; fitting of Eqn (16).

broken chains. The value m = 1.62 < 2 means that the Fermi velocity entering into Eqn (15) decreases with increasing difference x - 6.34; this could be expected.

4. Pseudogap in the optical conductivity

The energy difference between the resonant centers and the Fermi level can be surpassed not only by a finite temperature but also by absorption of a photon. Therefore, in underdoped YBCO and in other substances with the resonant tunneling mechanism of *c*-axis transport one can expect the appearance of a gap in the absorption of polarized infrared radiation at low temperatures. The corresponding threshold should not depend on temperature. Such a phenomenon was observed in [24, 25] (Fig. 7) and was originally associated with the 'spin gap' observed in the temperature dependence of the Knight shift above T_c and the 'pseudogap' found by angle-resolved photoemission spectroscopy (ARPES) in normal BSCOO. The latter can be measured rather precisely, and it never exceeds the true gap in the superconducting state, whereas the gap observed in the *c*-axis infrared conductivity is definitely larger.



Figure 7. Experimental data on optical conductivity along the c axis obtained in Refs [24, 25].

According to our concept, such a gap should be absent in $YBa_2Cu_3O_{6.95}$ and in $YBa_2Cu_4O_8$ (the small depression of the conductivity at temperatures slightly above T_c can be explained by fluctuations [26]).

We will start with Eqn (7) derived in the previous section. 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

$$\operatorname{Re} \sigma(\omega_{0}) = -c \, \frac{\operatorname{Im} Q(\omega_{0})}{\omega_{0}} = \frac{2}{\omega_{0}} (etv\eta d)^{2} v_{e} \eta$$
$$\times \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \left(\tanh \frac{\omega + \omega_{0}}{2T} - \tanh \frac{\omega}{2T} \right)$$
$$\times \operatorname{Im} G_{\mathrm{R}}(\omega, E) \operatorname{Im} G_{\mathrm{R}}(\omega + \omega_{0}, E) , \qquad (18)$$

where the notation is the same as before, and in particular,

$$-\text{Im}\,G_{\rm R}(\omega, E) = \frac{1/2\tau}{(\omega - E)^2 + (1/2\tau)^2}$$
(19)

(τ is the scattering time in the plane). This function is close to $\pi\delta(\omega - E)$, and if we assume that its width is $1/2\tau \ll \omega_0$, then both delta functions in Eqn (18) will be well separated (this limit is opposite to that assumed for static conductivity). Performing the integration over ω , we obtain

$$\operatorname{Re}\sigma(\omega_{0}) = \frac{\left(etv\eta d\right)^{2} v_{e}\eta}{\tau \omega_{0}^{3}} \left[n_{\mathrm{F}}(E - \omega_{0}, T) - n_{\mathrm{F}}(E + \omega_{0}, T) \right]$$
(20)

In order to avoid guesses about the frequency dependence of τ , it is necessary to simultaneously measure the optical conductivity in the *ab* plane and to take the ratio σ_c/σ_{ab} , as we did previously for the static conductivity (the static σ_{ab} will be divided by $\omega_0^2 \tau^2$, and so τ will be absent in the ratio). Unfortunately, these data were not obtained, and we have to use what is available.

Now, we will compare our predictions with the experimental data obtained for YBa₂Cu₃O_{6,7} ($T_c = 63$ K) in Refs [24, 25] (Fig. 7). In order to apply formula (20), we have to know the in-plane scattering probability $1/\tau$ as a function of temperature and frequency, and this has not yet been definitely established. At the lowest temperatures above $T_{\rm c}$ (T = 70 K, 110 K), we use the assumption $1/\tau = \text{const} \times \omega_0$ (const \ll 1). Apart from the constant prefactor, there is only one fitting parameter in Eqn (20), namely, E (we cannot mechanically take the value obtained from the static conductivity, since it may be sample-dependent). The result (for $\omega_0 > 3T$) is presented in Fig. 8 for $E = 47 \text{ meV} (379 \text{ cm}^{-1})$, which is virtually the same as that defined from the temperature dependence of the static conductivity. The error bars in this plot represent the 'wiggling' of the experimental curves (see Fig. 7); those taken at lower temperatures may reflect the uneven distribution of resonance levels. The fitting is worse for data taken at lower frequencies.

This may be due to the failure of our assumption that $1/\tau = \text{const} \times \omega_0$.

So we see that the resonant tunneling concept explains the data on the infrared conductivity along the c axis reasonably well. There exist, however, other explanations assuming the



Figure 8. Best fit of Eqn (20) with $1/\tau = \text{const} \times \omega_0$ to experimental data [20, 21] at low temperatures YBa₂Cu₃O_{6.7}; $T_c = 63$ K, $2\Delta \sim 5T_c = 27$ meV.

formation of some sort of a bound state. One is based on the idea of spin-charge separation (RVB) and the formation of spinon pairs, i.e., of a gap in the spinon density of states [27, 28]. Since the current in the c direction requires recombination of spinons and holons [7, 29], the c-axis conductivity would show activation behavior. This idea can also explain the 'spin gap' [30], i.e., the decrease in the electron spin susceptibility in the underdoped YBCO with decreasing temperature, starting far above $T_{\rm c}$. The general problem with the spin-charge separation 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, as in layered cuprates with overdoping. Another objection could be the fact that since the spin susceptibility is due only to unpaired spinons, and these are the only ones responsible for the *c*-axis conductivity, both should have the same temperature dependence, and this is not observed experimentally.

Another explanation of the spin gap is based on the idea of 'preformed pairs' of holes in the case of strong attraction (see, e.g., Ref. [31]). This idea could also give an explanation of the pseudogap in the ARPES experiments [32, 33]. In this framework the pseudogap in the optical conductivity could be attributed to the fact that the tunneling of pairs between the CuO₂ planes is prohibited due to their double charge. It seems, however, that this is not the proper explanation for the same reason as the previous one, namely, the different temperature dependence of the spin susceptibility and the c conductivity. Besides, as we mentioned at the beginning of this section, the value obtained for the gap in the c conductivity is too large for this explanation to be correct.

5. Interlayer superconductivity

Below T_c we have to take into account the Gorkov anomalous Green's functions F (see Ref. [23]). This time, we will not expand in A_z and keep the exponential factors entering into the Hamiltonian (1). On the other hand, we will only consider the external field constant in time, and this permits the cancellation of the terms with the G functions from the very beginning. For coherent resonant tunneling, we obtain

$$j_{z} = 4e(tv\eta)^{2}T\sum_{m} \int d^{2}k(2\pi)^{-2}\widetilde{F}_{n}(k,\omega_{m})\widetilde{F}_{n+1}(k,\omega_{m})$$
$$\times \sin\left(\varphi_{n}-\varphi_{n+1}+2eA_{z}\frac{d}{c}\right)$$
$$\equiv J_{c}\sin\left(\varphi_{n}-\varphi_{n+1}+2eA_{z}\frac{d}{c}\right), \qquad (21a)$$

and for the incoherent resonant tunneling, the result is

$$j_{z} = 4et^{2}\nu\eta T \sum_{m} \int d^{2}k(2\pi)^{-2}\widetilde{F}_{n}(k,\omega_{m}) \int d^{2}k'(2\pi)^{-2}$$
$$\times \widetilde{F}_{n+1}(k',\omega_{m}) \sin\left[2eA_{z}\frac{d}{c}+\varphi_{n}-\varphi_{n+1}\right]$$
$$\equiv J_{c}^{(\text{inc})} \sin\left[2eA_{z}\frac{d}{c}+\varphi_{n}-\varphi_{n+1}\right].$$
(21b)

We see that the current has a Josephson nature. Passing, as previously, to the energy integration, we obtain from (21a)

$$J_{\rm c} = 2e(tv\eta)^2 dv_{\rm e}\eta T \sum_m \int \frac{\mathrm{d}\phi}{2\pi} \frac{\Delta^2(\omega_m,\phi)}{\left[\omega_m^2 + E^2 + \Delta^2(\omega_m,\phi)\right]^2},$$
(22a)

and from (21b)

$$J_{c}^{(inc)} = e(tdv_{e}\eta)^{2}v\eta T \sum_{m} \int \frac{\mathrm{d}\phi_{1}}{2\pi} \frac{\varDelta(\omega_{m},\phi_{1})}{\omega_{m}^{2} + E^{2} + \varDelta^{2}(\omega_{m},\phi_{1})}$$
$$\times \int \frac{\mathrm{d}\phi_{2}}{2\pi} \frac{\varDelta(\omega_{m},\phi_{2})}{\omega_{m}^{2} + E^{2} + \varDelta^{2}(\omega_{m},\phi_{2})} . \tag{22b}$$

It is well known that in layered cuprates the order parameter $\Delta(\phi_1)$ is rather anisotropic, and additionally, under a $\pi/2$ rotation in the plane it can be either even (s symmetry) or odd (d symmetry). It is easy to see that formula (22a) gives a finite result in both cases, since the integrand depends only on $\Delta^2(\phi)$. However, the incoherent formula gives a finite result only for the s case and zero for the d case. This leads to very important consequences.

For the moment, let us consider the case of a not too underdoped sample described by the coherent formula. Since in the sum over frequencies the most important are $\omega_m \sim \Omega \gg T$, where Ω is the characteristic phonon frequency (see below), the sum can be approximated by the integral

$$T\sum_{m} \rightarrow \frac{1}{2\pi} \int_{-\infty}^{\infty} \mathrm{d}\omega$$

The BCS equation for $\Delta(\omega)$ in the temperature technique and with explicit phonons, according to G Eliashberg (see [23]), contains the phonon propagator $\Omega^2/[\Omega^2 + (\omega_m - \omega_{m_1})^2]$. Since in the integral $\omega_{m_1} \sim \Delta$, for $\omega_m \gg \Delta$ we can substitute

$$\Delta(\omega_m) \approx \Delta \frac{\Omega^2}{\omega_m^2 + \Omega^2} \ll (\Omega, E) \,. \tag{23}$$

For simplicity, we assume $E \ge \Omega$. Then, after substitution of Eqn (23) into (22a) and integration over ω_m , we get

$$J_{\rm c} = \frac{1}{2} e d (t v \eta)^2 v_{\rm e} \eta \frac{\Delta^2 \Omega}{E^4}$$
(24)

if $\varepsilon \ll E$. Here Δ^2 means $\overline{\Delta^2}$. The only temperature dependence of J_c is that of $\Delta^2(T)$. One must, however, have in mind that we imposed strong inequalities: $\Delta \ll \Omega \ll E$, which might not be true. Therefore, the details of the temperature dependence may be more complex.

In order to estimate the value of J_c , we substitute $(tv\eta)^2$ from Eqn (15):

$$J_{\rm c} \approx \frac{ev^2 v_{\rm e} \hbar}{2Ad} \, \frac{\Delta^2 \Omega}{E^4} \,, \tag{25}$$

where we have inserted \hbar in order to use ordinary units. The estimate depends on the particular choice of unknown quantities entering into this equation, but in all cases it is likely to be confined to the range

$$J_{\rm c} \sim 10^5 - 10^7 \,\,{\rm A}\,\,{\rm cm}^{-2}\,.$$
 (26)

The surprisingly large value is due to the fact that Δ decreases rather slowly when the energy deviates from the Fermi level [see (26)] contrary to the normal-state distribution function. The experimental value obtained in [34] for YBa₂Cu₃O_x with x = 6.7 at T = 4.2 K is $J_c = 1.5 \times 10^6$ A/cm², which falls within the estimated limits.

Expressions (22a, b) represent the limiting cases, and it is interesting how the crossover occurs, i.e., how the current changes with a gradual decrease in the concentration of resonant centers. In Appendix II, a formula is derived for the total tunneling probability through two centers per unit surface of the barrier; it corresponds to the one-center expression multiplied by

$$2 + 2\exp\frac{-\alpha\rho_0^2}{2d},\qquad(27)$$

where ρ_0 is the distance between the two centers, *d* is the thickness of the barrier, $\alpha = \sqrt{2m(U - \varepsilon_0)}$, and $U - \varepsilon_0$ is the binding energy at 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

$$4\exp\frac{-\alpha\rho_0^2}{2d} + 2\left(1 - \exp\frac{-\alpha\rho_0^2}{2d}\right),\tag{28}$$

and the first term may be interpreted as the coherent part, and the second as the incoherent part.

This formula can be used for an interpolation between two limiting cases. On average, $\rho_0^{-2} \sim nc$ is the concentration of resonant centers in the plane (*c* is the atomic concentration). Therefore, we can construct an interpolation

$$J_{\rm c} = \exp\left(-\frac{c^{(0)}}{c}\right) J_{\rm c}^{\rm coh} + J_{\rm c}^{\rm inc} , \qquad (29)$$

where $c^{(0)} \sim \alpha/(dn)$. In the case of d-type pairing, the incoherent part vanishes, and hence, J_c decreases exponentially with the atomic concentration of the resonant centers when the latter becomes less than $c^{(0)} \sim \alpha/(dn)$ (for BSCCO $c^{(0)} \sim 3\%$). It would be interesting to check this expression experimentally.

6. Critical temperature of underdoped samples

One of the unusual features of high- T_c cuprates is the relatively high BCS ratio, $2\Delta(0)/T_c$ (see, e.g., Ref. [35]). Contrary to its conventional value 3.52, it is close to 5 in optimally doped YBCO and around 7 in BSCCO. Usually, this is explained by the strong interaction between electrons. On the basis of the Eliashberg theory, within the formal limits of its applicability (the 'Migdal theorem'), the ratio can reach even higher values. On the other hand, in the limit of very strong interaction, 'preformed pairs', or 'bipolarons' are formed; then the binding energy of pairs and $T_{\rm c}$ are more or less disconnected, $T_{\rm c}$ being the Bose condensation temperature of these preformed pairs. In the bipolaron version, the increase in the electron-phonon interaction enhances the binding energy and at the same time raises the effective mass of bipolarons, decreasing their Bose-condensation temperature.

In these approaches the essential quantity is the ratio of electron interaction to their Fermi energy: the increase of this ratio moves the electron system in the direction of 'preformed pairs' and increases the BCS ratio. This all seemed, until recently, very clear but some results of the recent photoemission experiments with underdoped BSCCO [32, 33, 36], where the so-called 'pseudogap' was discovered, cannot be explained in that way. Of course, the pseudogap, i.e., the presence of a gap in the quasiparticle spectrum above T_c and its amazing thermal stability in strongly underdoped samples, was the most spectacular among the new phenomena. There

was, however, another surprise (see Ref. [36]): in the same experiments it was found that the BCS ratio could reach values over 20, and at the same time the Fermi surface was virtually unchanged compared to the optimally doped substance. This made it likely that the Fermi energy also remained the same, and since there was no reason to suspect a strong increase in the interaction of electrons, the conventional explanation of the large BCS ratio did not work. What then can be the action of underdoping? We propose an explanation based on the destruction of superconductivity by phase fluctuations in low-dimensional systems.

According to modern ideas, the antiferromagnetic insulator phase is formed as a result of a Mott transition at halffilling of the band (one can have in mind, as a simple example, the spin–Peierls transition in a 1D metal). A small doping destroys the antiferromagnetic phase; a metallic phase appears instead with an almost half-filled band and a large Fermi surface. Differences in the doping concentration influence its volume very little, since the original half-filling is always present. However, the concentration of oxygen atoms in the CuO chains, or BiO layers, which can serve as resonant tunneling centers, varies considerably. If it becomes very small, the connection between the CuO₂ bilayers is disrupted, and fluctuations of the phase suppress the critical temperature without any essential change in the electron concentration or their interaction.

Our estimate will be based on the method developed by K Efetov and A Larkin [37]. If there is no magnetic field and only phase fluctuations are important, we can write the following expression for the free energy:

$$F = \sum_{n} \int dx \, dy \left\{ \frac{n_{\rm s}^{(0)}}{8m} \left[\left(\frac{\partial \varphi_n}{\partial x} \right)^2 + \left(\frac{\partial \varphi_n}{\partial y} \right)^2 \right] + 4\beta \delta n_{\rm s} \left[1 - \cos(\varphi_n - \varphi_{n+1}) \right] \right\}, \quad (30)$$

where $n_s^{(0)}$ is the superconducting electron density in one layer, φ_n is the phase of the order parameter in the *n*th layer, $\beta \sim T_c^{(0)^2}/\varepsilon_F$ is some scaling energy, and δ is a dimensionless constant defining the connection between the layers. If the atomic concentration of the resonant centers *c* exceeds $c^{(0)}$, the tunneling is coherent, and formula (24) applies. It may be written as $\delta = \delta_0 c^2$, since we can assume that *v* is proportional to *c* (here $\delta_0 \ll 1$). If, on the other hand, $c < c^{(0)}$, then $\delta = \delta_0 c^2 \exp(-c^{(0)}/c)$, according to (29). Strictly speaking, *F* is the Ginzburg–Landau free energy, which is valid only in the vicinity of T_c , but expression (30) is very general, and it is very likely to be applicable beyond this vicinity, at least for purpose of estimates. As in Ref. [37], we will assume that a long-range order along the *c* axis described by an order parameter $\langle \exp(i\varphi) \rangle$ exists. Using the mean-field approximation, we obtain from the last term in (30)

$$-2\beta\delta n_{\rm s}^{(0)}\langle \exp({\rm i}\varphi)\rangle\exp(-{\rm i}\varphi_n)$$
.

The critical temperature can be defined by the self-consistency condition at infinitesimal $\langle \exp(i\varphi) \rangle$ (see Ref. [37]):

$$1 = \left(\frac{2\beta\delta n_{\rm s}^{(0)}}{T}\right) \int {\rm d}^2\rho \langle \exp\left[{\rm i}\varphi(0) - {\rm i}\varphi(\rho)\right] \rangle \,. \tag{31}$$

The average is taken over one two-dimensional layer and is defined by fluctuations; $n_{\rm s}^{(0)}$ means that the superconducting electron density is defined by the 2D mean-field BCS-type theory with critical temperature $T_{\rm c}^{(0)}$.

The strongest fluctuations in a two-dimensional superconductor are those associated with spontaneous formation of 'pancake' vortices. The appearance of such vortices leads to the so-called Berezinskiĭ–Kosterlitz–Thouless (BKT) transition [38, 39]. Indeed, the velocity of the superfluid in a quantum vortex is (in ordinary units) $v_s = \hbar/2m\rho$, where ρ is the distance from the axis (see, e.g., [35], Section 18). The corresponding kinetic energy is

$$E_{\rm v} = \frac{n_{\rm s}m}{2} \int_{\xi_0}^R v_{\rm s}^2 \, 2\pi\rho \, {\rm d}\rho = \frac{n_{\rm s}\hbar^2}{4m} \ln \frac{R}{\xi_0} \, .$$

Here *R* is the radius of the sample and ξ_0 is the radius of the core, or the coherence length; we assume that the penetration depth, if exists, is much larger than *R*. Since the vortex can appear anywhere, its entropy is equal to the logarithm of the cross sections

$$S_{\mathrm{v}} = \ln\left(rac{\pi R^2}{\pi \xi_0^2}
ight) = 2\lnrac{R}{\xi_0} \,.$$

The vortex can appear if its free energy $F_v = E_v - TS_v$ is negative, i.e., at temperatures higher than

$$T_{\rm BKT} = \frac{\pi n_{\rm s}}{8m} \,. \tag{32}$$

There is a delicate point at this moment [40]. In order for the vortex to appear, there must be a medium, which is the superfluid. Similar transitions can happen in a crystal, where the role of vortices is played by dislocations, or in a system of spins lying in the plane (XY-model). In these cases there is no doubt of the existence of the medium. For a superfluid, however, the question is not so clear. On the one hand, it can be assumed that there exists a 2D superfluid with a very distant T_c ; then n_s is some constant defining T_{BKT} , and the latter is a given parameter of the theory (this is done in Refs [37, 38, 40] and all subsequent literature on the BKT transition). On the other hand, we can assume that there exists only one possibility of a finite n_s , namely, real 3D superconductivity. In this case, n_s is a function of temperature, and formula (32) must be considered as an equation defining T_{BKT} . We will take this approach, since it seems more natural. Unlike the case of liquid ⁴He, if we at low temperatures substitute *n* for n_s , we obtain a Fermi energy that is even much higher than $T_c^{(0)}$. This time, n_s is the true superconducting density in two dimensions. In the vicinity of $T_{\rm c}$ it can be estimated as $n_{\rm s} = (n_{\rm s}/n) \times n$, where $n_{\rm s}/n \sim (T_{\rm c} - T)/T_{\rm c}$, and *n* is the effective 2D electron density. Then

$$\varepsilon_0 \sim \frac{n}{m} \gg T_{\rm c}^{(0)} > T_{\rm BKT} \,. \tag{33}$$

This would mean

$$\frac{n_{\rm s}}{n} \sim \frac{T_{\rm c} - T_{\rm BKT}}{T_{\rm c}} \sim \frac{T_{\rm BKT}}{\varepsilon_0} \ll 1.$$
(34)

Therefore T_{BKT} must be very close to the real T_c .

According to Refs [41, 42, 43], the correlator entering into Eqn (31) is equal to

$$\langle \exp\left[\mathrm{i}\varphi(0) - \mathrm{i}\varphi(\rho)\right] \rangle = A \exp\left(-\frac{\rho}{\xi}\right),$$
 (35)

where $A \sim 1$, and the correlation radius ξ is given by

$$\xi = \xi_0 \exp\left\{ b \left(\frac{T_{\rm BKT}}{T - T_{\rm BKT}} \right)^{1/2} \right\}.$$
(36)

Here ξ_0 is the usual superconducting coherence length and *b* is some constant; for qualitative estimates we can assume that it is of the order of unity, as in Ref. [41]. Substituting Eqn (35) into condition (31) that defines the critical temperature, we obtain

$$\frac{\beta \delta n_{\rm s}^{(0)} \xi^2}{T} \sim 1. \tag{37}$$

Here we substitute Eqn (36) and $\beta \sim T_c^{(0)^2}/\varepsilon_0$, $\xi_0^2 \sim v^2/T_c^{(0)^2} \sim \varepsilon_0/(mT_c^{(0)^2})$, $n_s^{(0)} \sim n \sim \varepsilon_0 m$ (we assume here that $T_c \approx T_{BKT} \ll T_c^{(0)}$), and obtain an equation for $x = (T_c - T_{BKT})/T_c$:

$$\frac{x}{\delta} = \exp\left(\frac{2b}{\sqrt{x}}\right). \tag{38}$$

For very small δ we get from (38) $x \approx [\ln(1/\delta)]^{-2}$ or, since according to (34), $x \sim T_c/\varepsilon_0 \approx T_{BKT}/\varepsilon_0$,

$$T_{\rm c} \sim \frac{\varepsilon_0}{\left[\ln(1/\delta)\right]^2} \,. \tag{39}$$

Substituting

$$\delta = \begin{cases} \delta_0 c^2, & c > c^{(0)}, \\ \delta_0 c^2 \exp\left(-\frac{c^{(0)}}{c}\right), & c < c^{(0)}, \end{cases}$$
(40)

we obtain

$$T_{\rm c} \sim \begin{cases} \frac{\varepsilon_0}{\left[B + 2\ln(1/c)\right]^2}, & c > c^{(0)}, \\ \frac{\varepsilon_0}{\left[B + 2\ln(1/c) + c^{(0)}/c\right]^2}, & c < c^{(0)}, \end{cases}$$
(41)

where $B \sim 1$ and $\varepsilon_0 \sim 10^3$ K. The second formula can also serve as an interpolation between different extremal regions. This relation gives the connection between the real T_c and the concentration of resonant centers when $T_c \ll T_c^{(0)}$. At larger values of δ , when Eqn (41) formally predicts $T_c \gtrsim T_c^{(0)}$, the true T_c remains equal to $T_c^{(0)}$.

Since it is difficult to measure the concentration c directly, the theory can be verified by finding a relation between J_c and T_c ; formulas (29) and (41) can be considered as a parametric representation of this dependence.

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 that predicted in [44, 45] for impurity suppression of the d-type order parameter. Since there is little hope that systematic measurements of T_c and J_c on the same samples will be performed in the 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.

The $\Delta(0)$ entering into the BCS ratio is obtained experimentally either as a singularity in the density of states from the tunneling conductance or as the energy gap from ARPES. In principle, one can use the following reasoning. The disruption of the connection between the planes makes the system more two-dimensional, and this reduces the phase transition temperature. However, it is much easier to form a bound state of two particles in a space with reduced dimensionality. Hence, there will be a tendency toward 'performed pairs,' the same as with increasing interaction. This idea is supported by the existence of the 'pseudogap' in the ARPES experiments: Δ remains finite far above T_c , particularly in strongly underdoped samples. Hence, Δ , as a feature of a one-particle excitation spectrum, can persist even without long-range order, being some sort of local characteristic. We have no theory at present explaining the pseudogap and its stability with temperature. Our only goal was to draw attention to the fact that the existence of a pseudogap does not necessarily mean the presence of long-range order, the same as the presence of long-range order does not necessarily lead to a gap in the spectrum of one-particle excitations (see Ref. [46]); this can result in huge values of the BCS ratio.

Appendix I

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

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

where

α

$$= \left[2m(U-E)\right]^{1/2}.$$
 (I.2)

Its general solution is

$$\Psi(z) = \left[A - \frac{\beta}{2\alpha} \Psi(z_0) \theta(z - z_0) \exp(-\alpha z_0) \right] \exp \alpha z + \left[B + \frac{\beta}{2\alpha} \Psi(z_0) \theta(z - z_0) \exp \alpha z_0 \right] \exp(-\alpha z) . \quad (I.3)$$

The solutions beyond the barrier are

$$\Psi(z) = \exp(i\varkappa z) + r \exp(-i\varkappa z), \quad z < 0,$$

$$\Psi(z) = p \exp\left[i\varkappa(z-d)\right], \quad z > d,$$
 (I.4)

where $\varkappa = (2mE)^{1/2}$, r and p are the amplitudes of the reflected and penetrated waves, respectively.

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

$$A = \frac{1}{2} \left(1 + \frac{i\varkappa}{\alpha} \right) + \frac{r}{2} \left(1 - \frac{i\varkappa}{\alpha} \right),$$

$$B = \frac{1}{2} \left(1 - \frac{i\varkappa}{\alpha} \right) + \frac{r}{2} \left(1 + \frac{i\varkappa}{\alpha} \right),$$

(I.5)
(B/a) $\Psi(z_{\perp})$

$$r = \frac{(\rho/\alpha) \Psi(z_0)}{(1 - i\varkappa/\alpha)^2 \exp \alpha d - (1 + i\varkappa/\alpha)^2 \exp(-\alpha d)}$$

$$\times \left\{ \left(1 - \frac{i\varkappa}{\alpha} \right) \exp\left[\alpha (d - z_0) \right] + \left(1 + \frac{i\varkappa}{\alpha} \right) \exp\left[- \alpha (d - z_0) \right] \right\}$$

$$- \frac{2(1 + \varkappa^2/\alpha^2) \sinh \alpha d}{(1 - i\varkappa/\alpha)^2 \exp \alpha d - (1 + i\varkappa/\alpha)^2 \exp(-\alpha d)}$$

$$\approx \frac{(\beta/\alpha) \Psi(z_0) \exp(-\alpha z_0) - (1 + i\varkappa/\alpha)}{1 - i\varkappa/\alpha}, \qquad (I.6)$$

$$p = \frac{(\beta/\alpha)\Psi(z_0)\left[(1 - i\varkappa/\alpha)\exp(\alpha z_0) + (1 + i\varkappa/\alpha)\exp(-\alpha z_0)\right]}{(1 - i\varkappa/\alpha)^2\exp\alpha d - (1 + i\varkappa/\alpha)^2\exp(-\alpha d)} - \frac{4i\varkappa/\alpha}{(1 - i\varkappa/\alpha)^2\exp\alpha d - (1 + i\varkappa/\alpha)^2\exp(-\alpha d)} \approx \frac{(\beta/\alpha)\Psi(z_0)\exp\left[\alpha(z_0 - d)\right]}{1 - i\varkappa/\alpha} - \frac{(4i\varkappa/\alpha)\exp(-\alpha d)}{(1 - i\varkappa/\alpha)^2}.$$
 (I.7)

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

From Eqns (I.3), (I.5) and (I.6) (here we have to use the full expression), we obtain

$$\Psi(z_0) \approx -\left(\frac{2i\varkappa}{\alpha}\right) \exp\left[\alpha(d-z_0)\right] \left\{ \left(1-\frac{\beta}{2\alpha}\right) \left(1-\frac{i\varkappa}{\alpha}\right) \times \exp\alpha d - \frac{\beta}{\alpha} \left(1+\frac{i\varkappa}{\alpha}\right) \cosh\left[\alpha(d-2z_0)\right] \right\}^{-1} (I.8)$$

and

$$p \approx \frac{\beta}{\alpha} \exp\left[\alpha(z_0 - d)\right] \left(1 - \frac{i\varkappa}{\alpha}\right)^{-1} \Psi(z_0)$$
$$\approx -\left(\frac{2i\beta\varkappa}{\varkappa^2 + \alpha^2}\right) \left\{ \left(1 - \frac{\beta}{2\alpha}\right) \exp(\alpha d + 2i\varphi) - \frac{\beta}{\alpha} \cosh\left[\alpha(d - 2z_0)\right] \right\}^{-1}, \quad (I.9)$$

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

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

$$U - E_0 = \frac{\beta^2}{8m} \,, \tag{I.10}$$

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

$$|d - 2z_0| \leq \frac{1}{\alpha} = \left[2m(U - E)\right]^{-1/2}.$$
 (I.11)

As has been said already, in $Bi_2Sr_2CaCu_2O_{8+\delta}$ the displacement of the BiO layers from the center is approximately 1 A. Even if $U - E_0 = 1 \text{ eV}$, $1/\alpha = 2 \text{ A}$, and the actual resonant levels might be more shallow. One sees that practically all localized centers formed from broken chains in underdoped YBCO and from BiO layers in BSCCO can support resonant tunneling at proper energies.

Appendix II

This time we suppose that there are two centers located in the median plane: the first at (0, d/2), and the second at $(\rho_0, d/2)$ (see Fig. 9). Here we have to solve the 3D Schrödinger equation. Performing a Fourier transformation with respect to ρ , we obtain

$$\frac{\mathrm{d}^2 \Psi_k}{\mathrm{d}z^2} - \alpha_k^2 \Psi_k = -\beta \Psi^{(k)} \left(\frac{d}{2}\right) \delta\left(z - \frac{d}{2}\right), \qquad (\mathrm{II.1})$$



Figure 9. Resonant tunneling through two centers in the median plane.

where

$$\Psi(\rho, z) = \int \frac{\mathrm{d}^2 k}{(2\pi)^2} \Psi_k(z) \exp(\mathrm{i}k\rho) \,, \tag{II.2}$$

$$\alpha_k = \left[2m(U-E) + k^2\right]^{1/2},\tag{11.3}$$

$$\Psi^{(k)}\left(\frac{d}{2}\right) = \Psi\left(0, \frac{d}{2}\right) + \Psi\left(\rho_0, \frac{d}{2}\right) \exp(-ik\rho_0). \quad (II.4)$$

The boundary conditions for a normal incidence are

$$\Psi_k(0) = (2\pi)^2 \delta(k) + r_k, \quad \Psi_k(d) = p_k.$$
 (II.5)

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

The self-consistency relations are

$$\Psi\left(0,\frac{d}{2}\right) = \int \frac{d^2k}{(2\pi)^2} \left[A_k \exp\left(\frac{\alpha_k d}{2}\right) + B_k \exp\left(-\frac{\alpha_k d}{2}\right)\right],$$
$$\Psi\left(\rho_0,\frac{d}{2}\right) = \int \frac{d^2k}{(2\pi)^2} \left[A_k \exp\left(\frac{\alpha_k d}{2}\right) + B_k \exp\left(-\frac{\alpha_k d}{2}\right)\right] \exp ik\rho_0$$

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

$$\begin{split} \Psi\left(0,\frac{d}{2}\right) &- \int \frac{\mathrm{d}^{2}k}{(2\pi)^{2}} \frac{\beta}{\alpha_{k}} \left[\frac{1}{2} + \frac{1 + \mathrm{i}q/\alpha_{k}}{1 - \mathrm{i}q/\alpha_{k}} \exp(-\alpha_{k}d)\right] \\ &\times \left[\Psi\left(0,\frac{d}{2}\right) + \Psi\left(\rho_{0},\frac{d}{2}\right) \exp(-\mathrm{i}k\rho_{0})\right] \\ &= -\frac{2\mathrm{i}\varkappa\exp(-\alpha d/2)}{\alpha(1 - \mathrm{i}\varkappa/\alpha)} , \\ \Psi\left(\rho_{0},\frac{d}{2}\right) - \int \frac{\mathrm{d}^{2}k}{(2\pi)^{2}} \frac{\beta}{\alpha_{k}} \left[\frac{1}{2} + \frac{1 + \mathrm{i}q/\alpha_{k}}{1 - \mathrm{i}q/\alpha_{k}} \exp(-\alpha_{k}d)\right] \\ &\times \left[\Psi\left(0,\frac{d}{2}\right) \exp\mathrm{i}k\rho_{0} + \Psi\left(\rho_{0},\frac{d}{2}\right)\right] \\ &= -\frac{2\mathrm{i}\varkappa\exp(-\alpha d/2)}{(1 - \mathrm{i}\varkappa/\alpha)} , \end{split}$$
(II.6)

 $-\frac{\alpha(1-i\varkappa/\alpha)}{\alpha}$

where α and \varkappa are the same as in Appendix I. The symmetry of the integrals with respect to $k \rightarrow -k$ leads to the conclusion

$$\Psi\left(\rho_0, \frac{d}{2}\right) = \Psi\left(0, \frac{d}{2}\right),\tag{II.7}$$

and hence,

$$\Psi\left(0,\frac{d}{2}\right) = -\frac{2i\varkappa\exp(-\alpha d/2)}{\alpha(1-i\varkappa/\alpha)} \left\{1 - \int \frac{d^2k}{(2\pi)^2} \frac{\beta}{2\alpha_k} \times \left[1 + 2\frac{1+iq/\alpha_k}{1-iq/\alpha_k}\exp(-\alpha_k d)\right] \left[1 + \exp(-ik\rho_0)\right]\right\}^{-1}.$$
(II.8)

Since the minimum value of α_k is α , the second term of the integrand vanishes at $d \to \infty$. 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 to be 1/K, we can calculate the square bracket in the denominator of Eqn (II.8) close to the resonance and obtain

$$\Psi\left(0,\frac{d}{2}\right) \approx \frac{2\varkappa \exp(-\alpha d/2)}{\varkappa + i\alpha} \left\{ \frac{\varepsilon - \varepsilon_0}{2\left[\varepsilon_0(\varepsilon_0 + K^2/2m)\right]^{1/2}} - \frac{\beta}{2\pi d} \frac{\varkappa - i\alpha}{\varkappa + i\alpha} \left[1 + \exp\left(-\frac{\alpha \rho_0^2}{2d}\right) \right] \exp(-\alpha d) \right\}^{-1},$$
(II.9)

where

$$\varepsilon_0 = \frac{1}{2m} \left(\frac{\beta}{8\pi}\right)^2 \left[K^2 - \left(\frac{4\pi}{\beta}\right)^2\right]^2$$

is the resonant value of $\varepsilon = U - E$.

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

$$p_k \approx i\beta \Psi\left(0, \frac{d}{2}\right) \left[1 + \exp(ik\rho_0)\right] \exp\left(-\frac{\alpha_k d}{2}\right) (q + i\alpha_k)^{-1}.$$
(II.10)

and, transforming to real space, we obtain the value of the amplitude at $\rho = 0$ for two centers

$$P^{(2)} = \int \frac{\mathrm{d}^2 k}{(2\pi)^2} p_k = \frac{2\mathrm{i}\beta\alpha\varkappa}{\pi d(\varkappa + \mathrm{i}\alpha)^2} \left[1 + \exp\left(-\frac{\alpha\rho_0^2}{d}\right) \right] \\ \times \left\{ \frac{(\varepsilon - \varepsilon_0)\exp\alpha d}{2\left[\varepsilon_0(\varepsilon_0 + K^2/2m)\right]^{1/2}} - \frac{\beta}{2\pi d}\frac{\varkappa - \mathrm{i}\alpha}{\varkappa + \mathrm{i}\alpha} \right. \\ \left. \times \left[1 + \exp\left(-\frac{\alpha\rho_0^2}{2d}\right) \right] \right\}^{-1}.$$
(II.11)

The dependence on ρ_0 in the square bracket can be neglected, as we will see in a moment. Then, if $\rho_0 \ll \sqrt{d/\alpha}$, the amplitude is doubled compared to the case of one center, and this means coherence of tunneling through two centers.

The condition $\rho_0 \ll \sqrt{d/\alpha}$ can easily be understood. Despite the fact that the tunneling occurs with the use of a resonant center, all the same the probability depends exponentially on the length of the trajectory. If the latter is tilted at an angle θ to the normal, its length becomes $d/\cos\theta \approx d(1+\theta^2/2)$, and hence the amplitude acquires a factor $\exp(-\alpha d\theta^2/2)$. Therefore, the typical values of θ will be $(\alpha d)^{-1/2}$. The transverse momentum component will be $k_{\perp} \sim \alpha \sin \theta \sim \alpha \theta \sim (\alpha/d)^{1/2}$. The corresponding wavelength $\lambda \sim k_{\perp}^{-1} \sim \sqrt{d/\alpha}$ is the distance of coherence.

In the general case of many centers, with an average distance between them less than $\sqrt{d/\alpha}$, i.e., if their planar density is larger than α/d , we can introduce an average amplitude, substituting the bracket $[1 + \exp(-\alpha\rho_0^2/d)]$ in (II.11) by the density of the centers. This, however, does not take into account that the energies of the centers may 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 (II.11) are larger than the second term, then this bracket can be replaced by

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

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

this expression does not depend on ρ_0 . The principal part of (II.11) does not contribute to the result.

Summation over centers gives

$$\bar{P} = \frac{4\beta\alpha_0\varkappa_0}{d(\varkappa_0 + i\alpha_0)^2} \left[\varepsilon_0\left(\varepsilon_0 + \frac{K^2}{2m}\right)\right]^{1/2} \exp(-\alpha_0 d)\nu, \quad (\text{II.12})$$

where v is the density of localized states. This penetration amplitude exceeds the amplitude of direct tunneling if v is sufficiently large, i.e., if all the localized states have approximately the same energy or are clustered around a few discrete values (the experimental curves for high-frequency c conductivity at low temperatures can be considered as evidence of the latter situation, see Fig. 7). The factor $[\varepsilon_0(\varepsilon_0 + K^2/2m)]^{1/2} \exp(-\alpha_0 d)$ plays the role of η that was introduced in Section 2. The coefficient t, appearing in the tunneling Hamiltonian, is the product of $4\beta\alpha/(\varkappa d)$ and some 'interaction energy,' which is of the order of the barrier U in magnitude.

Qualitatively the same but a physically more interesting result can be obtained if we consider the tunneling probability per unit area. The corresponding expression is

$$W = \left\langle \int \frac{d^2 k_1}{(2\pi)^2} p_{k_1} \exp(ik_1\rho) \int \frac{d^2 k_2}{(2\pi)^2} p_{k_2}^* \exp(-ik_2\rho) \right\rangle$$
$$= \int \frac{d^2 k}{(2\pi)^2} |p_k|^2,$$

where $\langle ... \rangle$ is the average over the area. Substituting p_k , we obtain the connection between tunneling probabilities with two centers and with one center

$$W^{(2)} = W^{(1)} \left[2 + 2 \exp\left(-\frac{\alpha \rho_0^2}{2d}\right) \right].$$
 (II.13)

The main result obtained here is that coherent tunneling through different centers is possible if their energies do not differ too much and if their planar density is higher than one center per area $2d/\alpha$. For BSCCO the distance between the closest double layers is d = 15 A. If we assume $|\varepsilon_0| = 1$ eV, we obtain $1/\alpha = 2$ A, but it is likely that the localized levels are shallower, and so we take $1/\alpha = 4$ A. From this we obtain a characteristic area of the order of 120 A²; more than one center per such an area looks quite realistic. One has also to take into account our basic assumption: $exp(-\alpha d) \ll 1$; in this case $\exp(-\alpha d) \approx 0.024$.

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