"Chain Scenario" for Josephson Tunneling with π Shift in $YBa_2Cu_3O_7$

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We point out that all current Josephson-junction experiments probing directly the symmetry of the superconducting state in $YBa_2Cu_3O_7$ can be interpreted in terms of the bilayer antiferromagnetic spin fluctuation model, which renders the superconducting state with the order parameters of extended s symmetry, but with the opposite signs in the bonding and antibonding Cu-O plane bands. The essential part of our interpretation includes the Cu-O chain band which would have the order parameter of the same sign as antibonding plane band. We show that in this case net Josephson currents along and perpendicular to the chains have a phase shift equal to π.

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In the last year, starting with the pioneering work of Wollman *et al.* [1], substantial progress has been made [2–7] in probing the symmetry of the superconducting state in $YBa_2Cu_3O_7$ (YBCO) by means of Josephson tunneling. In all these experiments except those of [4] the relative phase of the tunneling currents in YBCO contacts parallel to a and to b crystallographic axes were measured. In most cases it was found that the phases are opposite, as expected, for instance, for $d_{x^2-y^2}$. To the contrary, in Ref. [4] tunneling current parallel to c was measured, which for pure $d_{x^2-y^2}$ is expected to vanish [8], and a nonzero, although small, value was found.

Interpretation of the experiments [1–7] is additionally obscured by the fact that the only object studied so far has been orthorhombic YBCO, where a $d + s$ state is formally allowed and one can speak only about the weight of d or s components. Some authors [9] suggested that a strong anisotropy of the Fermi surface can explain the edge-contact experiments even without a large d component. However, the underlying assumption is that the plane electrons themselves are subject to strong orthorhombic effects, while both in calculations [10] and in the experiment [11] the main manifestation of orthorhombicity is the presence of the chains, while the planes themselves remain fairly tetragonal. This fact cannot be neglected when judging about pairing symmetry (see, e.g., Ref. [12]).

In a previous work [13], we noticed that if the order parameters (OP) in chain and plane bands had opposite signs and if the tunneling current along the chains was dominated by the chain band, this could explain the Josephson experiments in YBCO (this suggestion has been recently elaborated on by others [14]). While in Ref. [13] a number of reasons have been proposed for the sign reversal of the OP, neither Ref. [13] nor Ref. [14] suggested any microscopical reason for the tunneling current being dominated by chains.

In this Letter we propose another quantitative "chain scenario" for the above-mentioned Josephson tunneling experiments. This scenario is based on a recently proposed bilayer antiferromagnetic spin fluctuation model for superconductivity in YBCO [15] where the symmetry of the pairing state for the plane electrons is such that the bonding and antibonding plane bands have OP of opposite signs while angular symmetry is extended s. The physical reason for such sign reversal is that the unit cell of YBCO includes two CuO_2 planes (a "bilayer"), and the spin fluctuations are known to be perfectly correlated antiferromagnetically between the two planes in a bilayer. The third Cu-O layer is formed by CuO chains, running along the crystallographic b direction (Cartesian axis y), lowering the crystal symmetry to the orthorhombic one. We will argue that if this chain's layer is properly taken into account, the extended s spin fluctuation model of Ref. [15] leads to a situation when the net tunneling currents along a and along b have opposite signs.

The Fermi surface of YBCO is believed to consist of four sheets: two plane bands, which are bonding (B) and antibonding (A) combinations of the individual planes' states, the chain (C) band, and a small pocket which is not relevant for the current discussion. Since the bands A and B have different parity with respect to $z \to -z$ reflection, the above- mentioned spin fluctuations can work as pairing agents only for interband, $A \leftrightarrow B$, scattering. This leads [15] to the above-discussed sign reversal of the order parameter between the two bands. The Fermi surface of YBCO, as calculated by Andersen *et al.* [10], is shown in Fig. 1. According to calculations [16], the chain band is very light, so that its contribution to the total density of states is small (~15%), while its contribution in the plasma frequency $\omega_{py}^2 \propto N(0)v_{Fy}^2$ is considerable (~50%). This was confirmed by the experiment: The maximal Fermi velocity was calculated [17] to be $\sim 6 \times 10^7$ cm/s and corresponds to the point where the chain Fermi surface crosses the Γ-Y line. This value agrees with Raman experiments [18]. The calculated plasma frequency anisotropy $\omega_{py}^2/\omega_{px}^2 \simeq 1.75$, as discussed in Ref. [19], is in agreement with the optical and transport measurements.

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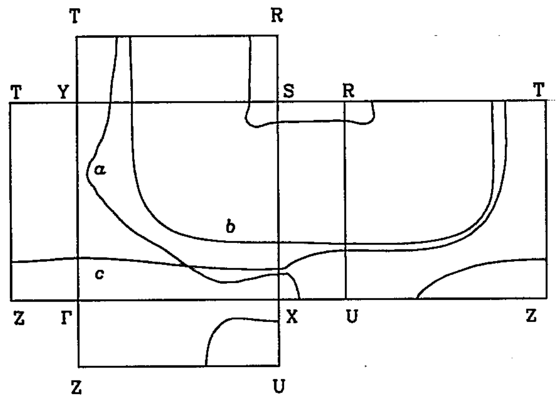

FIG. 1. Fermi surface of $YBa_2Cu_3O_7$ (from Ref. [10]).

Band A is, in calculations, rather heavy, which also agrees with the experiment [11,20]. Band B is light again. Both A and B bands are nearly tetragonal. Their relative contribution to the normal-state transport is defined by the partial plasma frequencies (Table I). Importantly, bands A and C at $q_z = 0$ can cross by symmetry; they are degenerate with $\epsilon = E_F$ at $\mathbf{q} = (\approx 0.8\pi/a, \approx 0.2\pi/B, 0)$. For all $q_z \neq 0$ these bands hybridize. This is the reason for YBCO being the most three dimensional of all high-T_c cuprates. An extremal orbit in the $q_z = \pi/c$ plane, which appears because of the A-C hybridization, has been seen in de Haas–van Alphen experiments [21].

Now we make a link to the above-mentioned model for the superconducting state, as suggested in Ref. [15]. The key feature of the model is that the bands of the different parity, A and B, have OP of the opposite signs [22]. The sign of the OP in band C was not discussed in Ref. [15]. Apparently because this band hybridizes with band A, but not band B, one can assume that C and A have OP of the same sign, while B has OP of the opposite sign. How can this fact manifest itself in Josephson tunneling?

To answer this question, let us consider the tunneling currents between two superconductors, L and R, each having several conducting bands, labeled by subscripts i, j. The total Josephson current through the system is given by a sum of the currents between each pair of bands (Li, Rj): $J_{\rm tot} = \sum_{(i,j)} J_{ij}$. For simplicity let us assume that the OP Δ_i in individual bands are isotropic. Then, using a standard technique [23], one easily finds the Josephson current between the bands i and j:

TABLE I. Partial contributions of the chain, plane-bonding, and plane-antibonding bands to the density of states and plasma frequencies of YBCO (from Ref. [17]).

n	$\frac{N(n)}{N}$	$\left(\frac{\omega_{\rm pl}(n)}{\omega_{\rm pl}}\right)_x$	$\left(\frac{\omega_{\rm pl}(n)}{\omega_{\rm pl}}\right)_y$	$\left(\frac{v(n)^2}{v^2}\right)_x$	$\left(\frac{v(n)^2}{v^2}\right)_y$
Bonding	23%	60%	37%	77%	40%
Antibonding	55%	37%	15%	19%	7%
Chain	22%	3%	47%	4%	54%

$$J_{ij} = \frac{\pi T}{eR_{ij}} \sum_{\omega_m} \frac{\mathrm{Im}(\Delta_{Li}^* \Delta_{Rj})}{\sqrt{|\Delta_{Li}|^2 + \omega_m^2}\sqrt{|\Delta_{Rj}|^2 + \omega_m^2}}. \quad (1)$$

Here R_{ij} is the normal-state resistance of a tunnel junction for the bands (i, j), $R_{ij} = \max\{R_{Lij}, R_{Rij}\}$,

$$R_{L(R)ij}^{-1} = 2e^2 \int_{v_x>0} D_{ij} v_{n,Li(Rj)} \frac{d^2 S_{Li(Rj)}}{(2\pi)^3 v_{F,Li(Rj)}}, \quad (2)$$

v_n is the projection of the Fermi velocity v_F on the direction normal to the junction plane, and dS is an element of the Fermi surface for the corresponding band. Equation (1) is a straightforward generalization of the well-known result [24] to the case of several conducting bands.

Further simplification of Eq. (1) takes place at low temperatures $T \ll T_c$:

$$J_{ij} = \frac{2\,\mathrm{Im}(\Delta_i^* \Delta_j)}{eR_{ij}(|\Delta_i| + |\Delta_j|)} K\left(\frac{|\Delta_i| - |\Delta_j|}{|\Delta_i| + |\Delta_j|}\right)$$
$$\approx \begin{cases} \mathrm{Im}(\Delta_i^* \Delta_j)\log 4|\Delta_j/\Delta_i|/eR_{ij}|\Delta_j|, & (\Delta_i \ll \Delta_j), \\ \pi\,\mathrm{Im}(\Delta_i^* \Delta_j)/eR_{ij}(|\Delta_i| + |\Delta_j|), & (\Delta_i \approx \Delta_j), \end{cases} \quad (3)$$

where $K(t)$ is the complete elliptic integral and indices L, R are omitted for simplicity.

The effective transparency D_{ij} in Eq. (2) can be evaluated for some models of the potential barrier $U(x)$ between L and R. For instance, for a specular barrier $U(x) = U_0 \delta(x - x_0)$, the probability for a quasiparticle to tunnel from the band i in L into the band j in R can be found by matching the solutions of the Schrödinger equation on both sides using the boundary conditions [25]

$$\Psi_L(x_0) = \Psi_R(x_0),$$
$$U_0 \Psi_L(x_0) = \frac{1}{2m_{Li}} \frac{\partial \Psi_L(x_0)}{\partial x} - \frac{1}{2m_{Lj}} \frac{\partial \Psi_R(x_0)}{\partial x}. \quad (4)$$

The second condition is conservation of the probability current $J(x) = -i\,\mathrm{Im}(\Psi^* \partial \Psi/\partial x)/2m(x)$. It is important to note that, as was shown in Ref. [25], $m_{i,j}$ are the effective band masses of quasiparticles in L and R, which differ from both the bare electron mass and the masses renormalized by the many-body correlation effects (i.e., essentially the local density approximation band masses). As a result, the effective transparency D_{ij} in Eq. (2) is determined by the band velocities:

$$D_{ij} = \frac{v_{n,Li} v_{n,Rj}}{(v_{n,Li} + v_{n,Rj})^2/4 + U_0^2}. \quad (5)$$

In the low transparency limit $U_0 \gg v$, we have $D_{ij} = D_0 v_{Li,n} v_{Rj,n}$, where D_0 is a constant.

Let us now apply these results to the junction between YBCO, L, and a conventional superconductor R ($\Delta_R \ll \Delta_{A,B,C}$). We choose $\Delta_R = |\Delta_R| \exp i\varphi$ and put the OP phase in the A band of YBCO equal to zero: $\Delta_A = |\Delta_A|$. Then $\Delta_B = -|\Delta_B|$ and $\Delta_C = |\Delta_C|$. Making use of Eqs. (1)–(3) and (5) we obtain the Josephson currents in the x and y directions $J_{x,y} = J_{x,y}^{\rm crit} \sin\varphi$, where

$$\begin{aligned} J_x^{\rm crit} &= J_A + J_B = |J_A| - |J_B|, \\ J_y^{\rm crit} &= J_A + J_B + J_C = |J_A| - |J_B| + |J_C|, \end{aligned} \quad (6)$$

and in the limit $\Delta_R \ll \Delta_{A,B,C}$

$$\begin{aligned} &|J_A| : |J_B| : |J_C| \\ &\approx R_A^{-1} \log\left|\frac{4\Delta_A}{\Delta_R}\right| : R_B^{-1} \log\left|\frac{4\Delta_B}{\Delta_R}\right| : R_C^{-1} \log\left|\frac{4\Delta_C}{\Delta_R}\right| \\ &\approx v_A : v_B : v_C \,. \end{aligned} \quad (7)$$

According to Eq. (2) there is no contribution of the band C to the current in the x direction (i.e., perpendicular to the chains). Substituting the values for v from Table I into Eq. (7) and neglecting the small x/y anisotropy of v_A/v_B, we get

$$J_A : J_B : J_C \approx 1 : 2 : 2 \,. \quad (8)$$

Now we observe that $|J_A| < |J_B|$, while $|J_C + J_A| > |J_B|$, *unless* $|\Delta_A|$, $|\Delta_B|$, and $|\Delta_C|$ differ drastically [so that the logarithmic terms in Eq. (7) become important]. To check this possibility, let us come back to the bilayer antiferromagnetic spin fluctuation model of Ref. [15]. The essence of the model is that the coupling interaction is the interband A-B interaction. A nonessential feature of the model was that the densities of states in both bands were assumed equal. To estimate the effect of N_A being about twice larger than N_B, let us consider the weak coupling limit for a BCS superconductor near T_c with interband interaction only. Then close to T_c we have

$$\Delta_A = \text{const} \times V_{AB} N_B \Delta_B, \quad \Delta_B = \text{const} \times V_{AB} N_A \Delta_A \,, \quad (9)$$

where V is the pairing interaction, and we obtain for the ratio of the gaps $|\Delta_A/\Delta_B| = \sqrt{N_B/N_A}$, i.e., counterintuitively, the band with the *smaller* density of states, in our case, bonding band, develops a *larger* gap. Including Δ_C in Eq. (9) assuming $N_C \ll N_A$, $V_{BC} \approx V_{CC} \approx 0$, we obtain $|\Delta_C/\Delta_B| = V_{AC}/V_{AB}$.

Thus, we can safely exclude the possibility of $|\Delta_B|$ being too small, but there are no arguments within the chosen model that Δ_C cannot be arbitrarily small. One can find in the literature many indirect estimates of the chain gap (see, e.g., [12] and references therein); however, the only experiment we are aware of that *directly* addresses this issue is that of Bauer, Genzel, and Habermeier [26], who compared normal/superconducting optical conductivity ratios for pure YBCO and YBCO doped with Fe (which substitute Cu in the chains). They found that the main effect of doping was that a gaplike structure at $\omega \sim 150$ cm^{-1} shifts down to $\sim$50 cm^{-1}, while the maximal gap at $\omega \sim 300$ cm^{-1} does not change. The lower energy can be naturally interpreted as the chain gap and the higher one as the plane gap. Thus one can be confident that the relations between J_A, J_B, and J_C indeed hold.

Now, since the currents $J_x^{\rm crit} = J_A + J_B > 0$ and $J_y^{\rm crit} = J_A + J_B + J_C < 0$ are of different signs, the same arguments that are usually applied to $d_{x^2-y^2}$ pairing (see, e.g., Ref. [27]) are valid, and lead to the conclusion that the free energy minima of two junctions along the x and y directions will correspond to the phase differences $\phi = 0$ and $\phi = \pi$, respectively. Thus the intrinsic phase shift π between the x and y directions takes place. Such a state is indistinguishable from a $d_{x^2-y^2}$ state for those experiments which probe the phase difference for two edge contacts; however, for the tunnel current perpendicular to the planes the model correctly gives a nonzero value.

The discussion above is relevant for the experiments such as Refs. [2,3,7], which deal with YBCO-conventional superconductor contacts. Let us now discuss the case of YBCO-YBCO contacts [5,6] (grain-boundary junctions). The condition for a π contact is now $|J_{AC}| - |J_{BC}| + |J_{AA}| + |J_{BB}| - 2|J_{AB}| < 0$, analogous to Eq. (6). A standard analysis [6] says that if a ring of N grain-boundary junctions consists of an *odd number of* π junctions, a spontaneous half-integer magnetic flux of $(n + 1/2)\Phi_0$ will be trapped in a ring, whereas for an *even number* of π junctions an integer flux of $n\Phi_0$ will be trapped. The findings of Ref. [6] suggest the grain-boundary junctions are π contacts.

To derive the criterion for a π contact from our model, we start from the expression for the currents $J_{ij} \propto v_i v_j \,{\rm Im}(\Delta_{Li}^* \Delta_{Rj})/(|\Delta_{Li}| + |\Delta_{Rj}|)$, which follows from Eqs. (3) and (5). Using the relation $\Delta_A/\Delta_B = \sqrt{N_B/N_A}$, and introducing $|\Delta_C/\Delta_B| = V_{AC}/V_{AB} = \alpha$, we find that the condition

$$\frac{\alpha v_A v_C \sqrt{N_B}}{\sqrt{N_B} + \alpha\sqrt{N_A}} - \frac{\alpha v_B v_C}{1 + \alpha} + \frac{v_B^2}{2} + \frac{v_A^2 \sqrt{N_B}}{2\sqrt{N_A}} - \frac{2 v_A v_B \sqrt{N_B}}{\sqrt{N_A} + \sqrt{N_B}}$$

is negative. Substituting data from Table I, $v_A : v_B : v_C \sim 1 : 2 : 2$, $N_A : N_B : N_C \sim 2 : 1 : 1$ one finds that the above condition holds when $\alpha \gtrsim 0.45$, that is, when the chain gap is at least half the maximal gap. As discussed above, a reasonable estimate of the ratio α is close to one-half, and so it looks like the condition for existence of the π shifts in grain-boundary junctions is barely satisfied. However, in this kind of experiment the effect must be very sensitive to the value of the chain gap. We will return to this issue later.

Our final point concerns the experiments on twinned samples. Naively, one can assume that the OP in the chain bands have the same sign in all domains, and thus the tunneling currents from different domains cancel. It is easy to see, however, that this is not the case. The superconducting state in each domain is degenerate with respect to changing signs of the OP in all bands simultaneously. Thus the relative phase of the OP in neighboring domains will be set by proximity effects.

Arguments similar to those used above for tunneling currents lead to the conclusion that OP in two adjacent domains with opposite orientations will have opposite signs of the OP in the same bands, thus maintaining the proper a/b asymmetry for the whole crystal.

To summarize, we suggest that recent Josephson-junction experiments that discovered the π phase shift between the tunneling currents in the a and b directions in YBCO can be fully understood in terms of the $s^{\pm}$ pairing symmetry, when order parameters in bonding and antibonding plane bands have opposite signs, provided that the chain band is properly taken into account. This model is able to explain nonzero tunneling current perpendicular to the planes, as well as independence of the experimental results on twinning.

A "smoking gun" for this model would be an experiment on YBCO with the superconductivity in the chains intentionally destroyed by doping at the Cu sites (Fe, Ga), which should be compatible with the conventional s pairing. An interesting property of our chain scenario is that the experiments with the YBCO-conventional superconductor junctions [1–3,7] should be much less sensitive to such doping than the experiments with the grain boundary junctions [5,6], since in the latter case the condition on the chain gap is much more severe (and is only barely satisfied, according to the estimation given above). To the contrary, in the former case we are in the regime where the correspondent condition is definitely fulfilled. Interestingly, the only tunneling experiment on YBCO which indeed showed no π shifts was that of Ref. [5], which was using grain boundary junctions. This fact is a strong argument in favor of the suggested model.

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