“Chain scenario” for Josephson tunneling with $\pi$-shift in YBa$_2$Cu$_3$O$_7$

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We point out that all current Josephson-junction experiments probing directly the symmetry of the superconducting state in YBa$_2$Cu$_3$O$_7$, 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 the phase shift equal to $\pi$.

In the last year, starting with the pioneering work of Wollman et al.\cite{1}, substantial progress has been made\cite{2,3,4,5,6,7} in probing the symmetry of superconducting state in YBa$_2$Cu$_3$O$_7$ by mean of Josephson tunneling. In all these experiments except of\cite{4} the relative phase of the tunneling currents in YBCO contacts parallel to $a$ and to $b$ crystallographic axes was 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.\cite{4} tunneling current parallel to $c$ was measured, which for pure $d_{x^2-y^2}$ is expected to vanish\cite{4}, and non-zero, although small, value was found. Interpretation of the experiments\cite{2,3,4,5,6,7} is additionally obscured by the fact that the only object studied so far has been orthorhombic YBa$_2$Cu$_3$O$_7$, where a $d+s$ state is formally allowed and one can speak only about the weight of $d$– or $s$–components. Some authors\cite{4} suggested that a strong anisotropy of the Fermi surface can explain the edge-contact experiments even without large $d$–component. However, the underlying assumption is that the plane electrons themselves are subject to strong orthorhombic effects, while both in calculations\cite{10} and in the experiment\cite{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.\cite{12}).

In a previous work\cite{13}, we noticed that if the order parameters (OP) in chain and plane bands had opposite sign and if the tunneling current along the chains were dominated by the chain band, this could explain the Josephson experiments in YBCO (this suggestion has been recently elaborated on by others\cite{14}). While in Ref.\cite{14} a number of reasons have been proposed for the sign reversal of the OP, none of Refs.\cite{13,14} 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\cite{15} where the symmetry of the pairing state for the plane electrons is such that the bonding and antibonding plane bands have OP of the opposite signs while angular symmetry is extended $s$.

We will argue that within this model, if the detailed Fermi surface properties of YBa$_2$Cu$_3$O$_7$, as calculated in LDA and measured experimentally, are taken into account, it follows that the net tunneling currents along $a$ and along $b$ must have opposite signs.

The Fermi surface of YBa$_2$Cu$_3$O$_7$ is believed to consist of four sheets: Two plane bands, which are bonding ($b$) and antibonding ($a$) combinations of the individual planes’ states (in the calculations they are well splitted by the energy which ranges from 0.05 to 0.5 eV, depending on the wave vector), the chain ($c$) band, and a small pocket formed mainly by apical oxygen states (which is not discussed here). The Fermi surface of YBa$_2$Cu$_3$O$_7$, as calculated by Andersen et al.\cite{10} is shown in Fig. 1. The $c$ band has been detected by positron annihilation technique and the corresponding sheet of the Fermi surface is in perfect agreement with LDA calculations. According to calculations\cite{10}, this band is very light, so that its contribution to the total density of states is small ($\sim 15\%$), while its contribution in the plasma frequency $\omega_{py}^2 \propto N(0)v_{Fy}^2$ is considerable ($\sim 50\%$). These
finding are confirmed by the experiment: Maximal Fermi velocity was calculated \cite{7} to be \(\sim 6 \times 10^7\) cm/s and corresponds to the point where the chain Fermi surface crosses the \(\Gamma-Y\) line. This value agrees well with the Raman experiments \cite{8}. Calculated plasma frequency anisotropy \(\omega_{ph}^2/\omega_{ph}^2 \approx 1.75\), as discussed in Ref. \cite{9}, is in agreement with the optical and transport measurements.

Band \(a\) is, according to calculations, rather heavy. In particular, it has extended van Hove singularities which have also been discovered experimentally \cite{10,11}. 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, for instance they are degenerate with \(\epsilon = E_F\) at \(q = (\approx 0.8\pi/a, \approx 0.2\pi/b, 0)\). 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 \(q_z = 0\) plane, which appears because of the \(a-c\) hybridization, has been seen in de Haas-van Alphen experiments \cite{12}. These facts provide indirect support for the calculations as regards \(a-b\) splitting and \(a-c\) hybridization.

Now we make link to the above mentioned model for the superconducting state, suggested in Ref. \cite{13}. The key feature of the model is that the bands of the different parity, \(a\) and \(b\), have OP of the opposite signs. The sign of the OP in band \(c\) was not discussed in Ref. \cite{13}. 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 \(i, j\). For simplicity let us assume that the OP \(\Delta_i\) in individual bands is isotropic. In order to evaluate the Josephson current between each of these bands we make use of a standard formalism of the integrated over energy quasiclassical Green functions \cite{24}, which should be completed by the boundary conditions \cite{25} on both sides of the barrier. Assuming that the tunnel junction transparency is small \(D(p) \ll 1\) one can proceed perturbatively and expand the boundary conditions \cite{26} in powers of \(D\). Keeping only the linear terms one gets

\[ g_{Li}(p) - g_{Li}(-p) = \frac{1}{2} D_{ij}(p) f_{Lj}(p) f_{Li}(-p) - f_{Li}(p) f_{Rj}(-p), \]

where the functions \(g\) and \(f\) are respectively the normal and anomalous quasiclassical Green functions on the left- or on the righthand side of the barrier. As we are interested only in the linear in \(D(p)\) contribution to the Josephson current it is sufficient to substitute for the anomalous Green functions the unperturbed values, \(f_{Li}(p) = \Delta_{Li}(p) / \sqrt{\Delta_{Li}(p)^2 + \omega_{m}^2}\). Then, using

\[ J = - (2\pi)^{-2} e^{-T} \int_{m} \int \left( d^{2}S / v_{F} \right) v_{F}(p) g(p, \omega_m), \]

we arrive at the general expression for the Josephson current between the bands \(i\) and \(j\) \((J_{ij} = \sum_{ij} J_{ij})\):

\[ J_{ij} = \frac{\pi T}{e R_{ij}} \sum_{\omega_m} \frac{\Delta_{Li} \Delta_{Rj}}{\sqrt{\Delta_{Li}^2 + \omega_m^2} \sqrt{\Delta_{Rj}^2 + \omega_m^2}}. \] (1)

Here \(R_{ij}\) is the normal state resistances of a tunnel junction for the bands \((i, j)\), and is the maximal of the two resistances, \(R_L\) and \(R_R\):

\[ R_{ij}^{-1} = 2 \pi e \int_{v_x > 0} D_{ij} v_n L_i(R_i) \frac{d^{2}S_{Li}(R_j)}{(2\pi)^{2} v_{F,Li}(R_i)}, \] (2)

\(v_n\) is the projection of the Fermi velocity \(v_F\) on the direction normal to the junction plane, \(dS\) is an element of the Fermi surface for the corresponding band. Eq. 1 is a straightforward generalization of the well known Ambegaoko-Baratoff result \cite{26} to the case of several conducting bands.

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

\[ J_{ij} = \frac{2 \Delta_i \Delta_j}{e R_{ij} (|\Delta_i| + |\Delta_j|)} K \left( \frac{|\Delta_i| - |\Delta_j|}{|\Delta_i| + |\Delta_j|} \right) \] (3)

\[ \approx \Delta_i \log |\Delta_i|/|\Delta_j|, \quad \Delta_i \ll \Delta_j \]

\[ \approx \Delta_i \log (|\Delta_i| + |\Delta_j|)/|\Delta_j|, \quad \Delta_i \approx \Delta_j \]

where \(K(t)\) is the complete elliptic integral. The first case corresponds to a contact \(YBa_2Cu_3O_7-\delta\) conventional superconductor, and the second to a grain boundary contact.

Estimate of the effective barrier transparencies \(D_{ij}\) in Eq. 2 can be obtained for certain models of the potential barrier \(U(x)\) between \(L\) and \(R\). Let us consider the case of a specular reflecting barrier \(U(x) = U_0 \delta(x - x_0)\). Transmission probability for a quasiparticle from the band \(i\) in \(L\) to tunnel into the band \(j\) in \(R\) is found by matching solutions of Schrödinger equations on both sides of the barrier using boundary conditions at the barrier \cite{27}.

\[ \Psi_L(x_0) = \Psi_R(x_0) \]

\[ U_0 \Psi_L(x_0) = \frac{1}{2 m_{ij}} \frac{\partial \Psi_L(x_0)}{\partial x} - \frac{1}{2 m_{ij}} \frac{\partial \Psi_R(x_0)}{\partial x} \] (4)

The second condition is conservation of the probability current \(J(x) = -i m \left( \Psi^* \partial \Psi / \partial x \right) / 2 m(x)\). It is important to note that, as was shown in Refs. \cite{26} \(m_{ij}\) are effective band masses of quasiparticles in \(L\) and \(R\), and are neither the bare electron mass \(m_0\), nor the masses renormalized by many-body correlation effects, i.e., essentially the LDA band masses. As a result, effective barrier transparency coefficient \(D_{ij}\) in Eq. 2 is determined by the band velocities:
In the low transparency limit, \( U_0 \gg v \), we have \( D_{ij} = D_0(v_{Li,n}v_{Ri,n}) \), where \( D_0 \) is a constant. Thus, for a conventional superconductor on the righthand side, we have \( \Delta_R \ll \Delta_{a,b,c} \), and:

\[
J_a : J_b : J_c 
\approx R_a^{-1} \log \left( \frac{\Delta_a}{\Delta} \right) : R_b^{-1} \log \left( \frac{\Delta_b}{\Delta} \right) : R_c^{-1} \log \left( \frac{\Delta_c}{\Delta} \right)
\]

\[
\approx v_a : v_b : v_c.
\]

From Eq.2 we observe that band \( c \) does not contribute into the tunneling current in the \( x \) direction (i.e., perpendicular to the chains), which is quite natural. Correspondingly, the total current along \( x \) is

\[
J_x = J_a + J_b = |J_a| - |J_b|
\]

\[
J_y = J_a + J_b + J_c = |J_a| - |J_b| + |J_c|
\]

Substituting the values for \( v \) from Table 1 in Eq.3 we get

\[
J_a : J_b : J_c \approx 1 : 2 : 2
\]

Now we observe that \( |J_a| < |J_b| \), while \( |J_a + J_b| > |J_b| \), unless \( |\Delta_a|, |\Delta_b|, \) and \( |\Delta_c| \) differ drastically (so that the log terms in Eq.3 become important). To check this possibility, let us come back to the bilayer antiferromagnetic spin fluctuation model of Ref. 13. The essence of the model is that the coupling interaction is interband \( a-b \) interaction. A non-essential 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 that \( N_b \), let us consider the weak coupling limit for a BCS superconductor near \( T_c \) with interband interaction only. In this limit,

\[
\Delta_a = \text{const} \cdot V_{ab} N_b \Delta_a \quad \Delta_b = \text{const} \cdot V_{ab} N_a \Delta_a,
\]

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 \( \Delta_c \) in Eqs.2 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 \( \Delta_c \) cannot be arbitrary small. However, there are various experimental indications that this is not the case, for instance optical experiments of Bauer et al [22], 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 structures at \( \omega \approx 150 \text{ cm}^{-1} \) shifts down to \( \approx 50 \text{ cm}^{-1} \), while the maximal gap at \( \omega \approx 300 \text{ cm}^{-1} \) 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 relations between \( J_a, J_b, \) and \( J_c \) indeed hold.

Now, since \( J_c \) and \( J_a \) are in-phase, and \( J_b \) is out-of-phase with both of them, it becomes obvious that the net current along \( x \) and along \( y \) should have a phase shift \( \pi \). Such a state is indistinguishable from \( d_x^2 - y^2 \) state for those experiments which probe phase difference for two edge contacts; however, for the tunnel current perpendicular to the planes the model correctly gives a non-zero value.

The discussion above is relevant for the experiments like Refs. 3, 4, which deal with YBCO-conventional superconductor contacts. Let us now discuss the case of YBCO-YBCO contacts (5), (6), (7), (8), (9), (10), (11). The condition for a \( \pi \)-contact is now \( |J_{ac} - J_{bc}| + |J_{aa} + J_{bb} - 2|J_{ab}| < 0 \), analogous to Eq.5. According to Eqs.3, 4, the corresponding currents are \( J_{ij} \propto v_i v_j \Delta_i \Delta_j / (|\Delta_i| + |\Delta_j|) \). To estimate currents, let us use the relations between the order parameters: \( \Delta_a/\Delta_b = \sqrt{N_b/N_a} \) and introduce \( |\Delta_c/\Delta_b| = V_{ac}/V_{ab} = \alpha \). Then the condition is

\[
\frac{\alpha v_a v_c \sqrt{N_a}}{\sqrt{N_b + \alpha \sqrt{N_a}}} - \frac{\alpha v_b v_c}{1 + \alpha} + \frac{v_d^2}{2} + \frac{\alpha v_b \sqrt{N_b}}{\sqrt{N_a + \sqrt{N_b}}} < 0.
\]

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 \( \alpha \approx 0.45 \), in other words, when chain gap is at least half the maximal gap. As discussed above, a reasonable estimate of the ratio \( \alpha \) is close to one half, so it looks like the condition for existing of the \( \pi \)-shifts in grain-boundary junctions is barely satisfied. However, in this kind of experiments 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 easy to see, however, that it is not the case. 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 the proximity effects. Arguments similar to those used above for the 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 \( a/b \) symmetry for the whole crystal.

To summarize, we suggest that recent Josephson junctions experiments that discovered \( \pi \) phase shift between the tunneling currents in \( a \) 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 sign, provided that the chain band is properly taken into account. This model is able to explain non-zero 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. A particularly interesting property of our “chain scenario” is that the experiments with the YBCO-conventional superconductor junctions should be substantially less sensitive to such doping than the experiments with the grain boundary junctions, since in the latter case the condition on the chain gap is much more severe. Interestingly, the only tunneling experiment on YBCO which indeed showed no $\pi$-shifts was that of [5], which was using grain boundary junctions. This fact is a strong argument in favor of suggested model.

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TABLE I. Partial contributions of the chain, plane- bonding and plane-antibonding bands to the density of states and plasma frequencies of YBa$_2$Cu$_3$O$_7$- (from Ref. [16]).

| \(n\) | \(N(n)/N\) | \(\omega_{pl}(n)/\omega_{pl}\) | \(\omega_{pl}(n)/\omega_{pl}\) | \(\omega_{pl}(n)/\omega_{pl}\) | \(\omega_{pl}(n)/\omega_{pl}\) |
|------|-------------|----------------|----------------|----------------|----------------|
| bonding | 23% | 60% | 37% | 77% | 40% |
| antibonding | 55% | 37% | 15% | 19% | 7% |
| chain | 22% | 3% | 47% | 4% | 54% |

Fermi surface of YBa$_2$Cu$_3$O$_7$, from Ref. [10].