Critical Josephson Current in a Model Pb/YBCO Junction

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Abstract

In this article we consider a simple model for a $c$–axis Pb/YBa$_2$Cu$_3$O$_{7-\delta}$ Josephson junction. The observation of a nonzero current in such a junction by Sun et al. [A. G. Sun, D. A. Gajewski, M. B. Maple, R. C. Dynes, Phys. Rev. Lett. 72, 2267 (1994)] has been taken as evidence against $d$–wave superconductivity in YBa$_2$Cu$_3$O$_{7-\delta}$. We suggest, however, that the pairing interaction in the CuO$_2$ planes may well be $d$–wave but that the CuO chains destroy the tetragonal symmetry of the system. We examine two ways in which this happens. In a simple model of an incoherent junction, the chains distort the superconducting condensate away from $d_{x^2-y^2}$ symmetry. In a specular junction the chains destroy the tetragonal symmetry of the tunneling matrix element. In either case, the loss of tetragonal symmetry results in a finite Josephson current. Our calculated values of the critical current for specular junctions are in good agreement with the results of Sun and co-workers.

74.50.+r, 74.20.Fg
I. INTRODUCTION

The debate over the symmetry of the order parameter in the high $T_c$ copper–oxide superconductors has intensified over the last few years because of a number of suggestive experimental findings. The discovery of linear low temperature behaviour in the penetration depths of single crystals of YBa$_2$Cu$_3$O$_{7-\delta}$ (YBCO) and Tl$_2$CaBa$_2$Cu$_2$O$_{8-\delta}$ has been taken as support for $d$–wave superconductivity, although such experiments have been unable to exclude anisotropic $s$–wave models. NMR relaxation rates have been interpreted in terms of a $d$–wave order parameter. More recently, angle resolved photoemission experiments (ARPES) have been able to map out the Fermi surface in the normal and superconducting states for Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ and have found an anisotropic gap with nodes located approximately along the diagonals of the Brillouin zone. This is strongly suggestive of a $d$–wave gap although the experiments have been criticized because they sample only the surface states of the crystals.

A recent generation of experiments has attempted to resolve the issue of order parameter symmetry by measuring its relative phase between different regions of the Brillouin zone. These experiments are all based on the fact that the current through a Josephson junction depends on the phase difference between the condensates on either side. Some of the experiments which have been performed have attempted to measure the phase difference between electrons tunneling through different faces of a single crystal of YBCO. In a $d$–wave material, these electrons will have a phase of $\pi$ relative to each other. Two of the experiments suggest that YBCO has a $d$–wave order parameter while the third suggests an $s$–wave order parameter. More recently, there have been experiments which attempt to detect phase shifts of $\pi$ across YBCO/YBCO junctions in which the crystals are misaligned. These phase shifts, which are a signature of $d$–wave symmetry, have been found in both of the cited experiments.

The experiment in which we are interested in this article is that of Sun et al. It is
slightly different than the others: it relies on the fact that in a $c$–axis Pb/YBCO junction (in which the junction face is perpendicular to the YBCO $c$–axis) the Josephson current will vanish if YBCO has a $d$–wave gap. Since the experiment finds a small, but finite Josephson current ($J_c R_n = 0.3 - 0.9$ mV, where $R_n$ is the normal state resistance of the junction and $J_c$ is the critical Josephson current) the authors conclude that the order parameter cannot be purely $d$–wave. On the other hand, their results are also inconsistent with simple $s$–wave theory since the measured critical voltages $J_c R_n$ are an order of magnitude lower than expected. Following Ambegoakar and Baratoff\textsuperscript{22}, and assuming that the gaps in the YBCO and Pb are $\Delta_Y \sim 14\text{meV}$ and $\Delta_P \sim 1.4\text{meV}$ respectively, they find

$$J_c R_n = \frac{2}{e} \frac{\Delta_Y \Delta_P}{\Delta_Y + \Delta_P} K \left( \frac{|\Delta_Y - \Delta_P|}{\Delta_Y + \Delta_P} \right) \sim 8 \text{ mV}$$

where $K$ is the complete elliptic integral of the first kind.

In fact, the experiment of Sun et al\textsuperscript{21} does not immediately rule out YBCO having a $d_{x^2-y^2}$ order parameter. Tanaka\textsuperscript{23} has shown, that while the usual treatment of the barrier as a second order perturbation does lead to a vanishing Josephson current, higher order terms in the perturbation series will not vanish. Unfortunately, attempts by one of the current authors\textsuperscript{24} to fit the experimental results with a fourth order calculation have been unsuccessful. On the other hand, it may be reasonable to expect that YBCO does not have a gap structure with a full $d_{x^2-y^2}$ symmetry since (optimally doped) YBCO is not tetragonal. Band structure calculations\textsuperscript{25,26} show that the CuO chains both contribute a piece of Fermi surface with orthorhombic symmetry and distort the band structure in the CuO$_2$ planes. O’Donovan et al.\textsuperscript{27} have a simple model of this: they consider a single CuO$_2$ plane in which the Fermi surface is distorted slightly away from tetragonal symmetry. They find that the reduced symmetry is strongly reflected in the gap, which picks up a small extended $s$–wave component while retaining its nodal structure. Another point of view is that of Xu et al.\textsuperscript{28}, who treat YBCO as having tetragonal symmetry but take the gap to be $s + id$. Despite the very different starting points, both of these articles reach the conclusion that a gap which
is roughly ten percent $s$–wave will explain the results of Sun et al.

In this article, we suggest that the nonzero critical current seen in Pb/YBCO $c$–axis Josephson junctions may be due to the CuO chains. We consider a phenomenological model for YBCO in which the unit cell contains a CuO$_2$ plane and a CuO chain and calculate the tunneling current for a Pb/YBCO junction as a function of the chain–plane coupling strength. In Sec. II, we introduce our model for YBCO. In section III we derive an expression for the critical Josephson current. In Sec. V we discuss the results of numerical calculations. We finish with a brief conclusion in Sec. V.

II. MODEL

We wish to consider a simple model for a Pb/YBCO Josephson junction. For the sake of clarity, we will take the Pb (YBCO) to be on the left (right) side of the junction. We treat the Pb as an ordinary free electron metal with an isotropic BCS gap. The YBCO is treated with a simplified model in which there are alternating layers of chains and planes. The planes and chains are weakly coupled by coherent electron hopping and the planes contain a BCS–like pairing interaction with a $d_{x^2−y^2}$ symmetry. The chains are driven superconducting by a proximity effect. This model is related to models studied elsewhere in which both layers are treated as planes and (with the exception of Ref. [35] where it is $d$–wave) the order parameter is $s$–wave. It should be emphasized that this model is only suitable for weak chain–plane coupling. As the coupling is increased, the pairing potential begins to affect electrons in the chains directly. The problem becomes more complicated in this case and has only been examined in various special limits.

The experiment we wish to describe is one in which the $c$–axis of the YBCO is normal to the junction. Furthermore, we assume that the tunneling junction is adjacent to a CuO$_2$ plane. Then our Hamiltonian can be written:

$$H = H_0^l + H_0^r + T$$

(1)

where $H_0^l$ and $H_0^r$ describe the uncoupled Pb and YBCO subsystems and $T$ describes the
coupling through the junction. We define \( c_{k\sigma}, a_{1k\sigma} \) and \( a_{2k\sigma} \), to be the electron annihilation operators with wavevector \( k \) and spin \( \sigma \), in the Pb, YBCO planes and YBCO chains respectively. We can write

\[
\begin{align*}
H^l_0 - N^l\mu &= \sum_{k,\sigma} \epsilon(k) c_{k\sigma}^\dagger c_{k\sigma} \\
&\quad - \sum_k \left[ \Delta^l c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger + \Delta^l c_{-k\downarrow} c_{k\uparrow} \right] 
\end{align*}
\] (2a)

\[
\begin{align*}
H^r_0 - N^r\mu &= \sum_{k,\sigma} \left[ a_{1k\sigma}^\dagger a_{1k\sigma} \xi_1(k) + a_{2k\sigma}^\dagger a_{2k\sigma} \xi_2(k) \right] \\
&\quad + \sum_{k,\sigma} \left[ t(k) a_{1k\sigma}^\dagger a_{2k\sigma} + t^*(k) a_{2k\sigma}^\dagger a_{1k\sigma} \right] \\
&\quad - \sum_k \left[ \Delta^r a_{1\downarrow}^\dagger a_{1\downarrow} + \Delta^r a_{1\downarrow} a_{1\uparrow} \right] 
\end{align*}
\] (2b)

\[
T = \sum_{k,q} T_{kq} c_{k\sigma}^\dagger a_{1q\sigma} + T^{*}_{kq} a_{1q\sigma}^\dagger c_{k\sigma}
\] (2c)

The normal state dispersion in the Pb is \( \epsilon = \hbar^2 k^2/2m^* - \mu \), and the mean field order parameter, \( \Delta^l \), is isotropic. The dispersions \( \xi_1 \) and \( \xi_2 \) are the normal state dispersions of the YBCO planes and chains in the limit of no chain–plane coupling:

\[
\begin{align*}
\xi_1 &= -2\sigma_1 [\cos(k_x) + \cos(k_y)] - \mu_1 \\
\xi_2 &= -2\sigma_2 \cos(k_y) - \mu_2
\end{align*}
\] (3a)

\[
\begin{align*}
\xi_1 &= -2\sigma_1 [\cos(k_x) + \cos(k_y)] - \mu_1 \\
\xi_2 &= -2\sigma_2 \cos(k_y) - \mu_2
\end{align*}
\] (3b)

with \(-\pi < k_x, k_y < \pi\) and where \( \mu_1 \) and \( \mu_2 \) include information about both the chemical potential and the offset of the bands from one another. The strength of the plane–chain coupling is given by \( t(k) \) which, in the tight binding limit, depends only on \( k_z \). To simplify matters further, we take the chain–plane distances to be the same on either side of a chain, so that

\[
t(k_z) = t_0 \cos(k_z/2),
\] (4)

with \(-\pi < k_z < \pi\). The mean field order parameter in the YBCO, \( \Delta^r_k \), is a thermal average of electron pairs in the CuO\(_2\) planes only. This is because we make the ansatz that the pairing is localised to the planes:
\[ \Delta^r_k = \sum_{k} V_{kk'} \langle a_{1-k'} a_{1k'} \rangle, \quad (5) \]

where \( V_{kk'} \) is the BCS–like pairing interaction in the planes. If, for simplicity, we assume that the pairing interaction is separable, so that \( V_{kk'} = V \eta_k \eta_{k'} \), with \( \eta_k = \cos(k_x) - \cos(k_y) \) for a d–wave interaction, then we may write \( \Delta^r_k = \Delta^r_0 \eta_k \).

We will find it convenient to work within the Nambu formalism, in which we define

\[
C(k) = \begin{bmatrix} c_{k\uparrow} \\ c_{-k\downarrow} \end{bmatrix} \quad (6a)
\]

and

\[
A(k) = \begin{bmatrix} a_{1k\uparrow} \\ a_{1-k\downarrow} \\ a_{2k\uparrow} \\ a_{2-k\downarrow} \end{bmatrix} \quad (6b)
\]

so that the uncoupled Hamiltonians may be written,

\[
H^0 = \sum_{k} C^\dagger(k) \mathcal{H}^l_0(k) C(k) + \sum_{k} A^\dagger(k) \mathcal{H}^r_0(k) A(k). \quad (7a)
\]

with

\[
\mathcal{H}^l_0(k) = \begin{bmatrix} \epsilon(k) & -\Delta^l \\ -\Delta^{l*} & \epsilon(-k) \end{bmatrix} \quad (7b)
\]

and

\[
\mathcal{H}^r_0 = \begin{bmatrix} \xi_1(k) & -\Delta^r_k & t(k) & 0 \\ -\Delta^{r*}_{-k} & -\xi_1(-k) & 0 & -t^*(-k) \\ t^*(k) & 0 & \xi_2(k) & 0 \\ 0 & -t(-k) & 0 & -\xi_2(-k) \end{bmatrix}. \quad (7c)
\]

The eigenvalues of the Hamiltonian matrices are \( E^l/r_i(k) \) with \( E^l_i = (E^l, -E^l) \),

\[
E^l = \sqrt{\epsilon^2 + \Delta^{l2}}, \quad (8a)
\]
and $E_i^r = (E_i^+, E_i^-, -E_i^-, -E_i^+)$,

$$E_{\pm}^r = \frac{\xi_1^2 + \xi_2^2 + \Delta_k^2}{2} + t^2 \pm \sqrt{\left[\frac{\xi_1^2 - \xi_2^2 + \Delta_k^2}{2}\right]^2 + t^2[(\xi_1 + \xi_2)^2 + \Delta_k^2]}.$$  

(8b)

and the unitary transformations which diagonalise the Hamiltonian are

$$U^l(k) = \frac{1}{\sqrt{2E}} \begin{bmatrix} \Delta^l & \Delta^l \\ \frac{\xi_1}{\sqrt{E^l - \epsilon}} & \frac{\xi_2}{\sqrt{E^l + \epsilon}} \\ \frac{\xi_2}{\sqrt{E^l - \epsilon}} & \frac{\xi_1}{\sqrt{E^l + \epsilon}} \end{bmatrix}$$

(9a)

and $U_{ij}^r = U_i^r(E_j)$,

$$U_i^r(E_j) = \frac{1}{\sqrt{\mathcal{C}}} \begin{bmatrix} (E_j^r - \xi_2)A \\ -(E_j^r + \xi_2)B \\ tA \\ tB \end{bmatrix}$$

(9b)

$$A = t^2 - (\Delta_k^+ + E_j^r + \xi_1)(E_j^r + \xi_2)$$

$$B = t^2 - (\Delta_k^- + E_j^r - \xi_1)(E_j^r - \xi_2)$$

$$C = A^2[t^2 + (E_j^r - \xi_2)^2] + B^2[t^2 + (E_j^r + \xi_2)^2].$$

(9c)

The Hamiltonian may, therefore, be written

$$H_0 - N\mu = \sum_k \sum_{i=1}^2 \hat{C}_i^\dagger(k) \hat{C}_i(k) E_i^l(k)$$

$$+ \sum_k \sum_{i=1}^4 \hat{A}_i^\dagger(k) \hat{A}_i(k) E_i^r(k)$$

(10)

where, for example, $\hat{C}_i(k) = \sum_j U_{ij}^l(k) C_j(k)$.

In the normal state, the YBCO band energies are
\[ \varepsilon_{\pm} = \frac{\xi_1 + \xi_2}{2} \pm \sqrt{\frac{(\xi_1 - \xi_2)^2}{4} + t^2}. \] 

(11)

and their Fermi surfaces are given by \( t^2 = \xi_1 \xi_2 \). In Fig. 1(a) we plot the Fermi surfaces in the \( k_x k_y \) plane for a range of \( t \). When \( t = 0 \), the two pieces of Fermi surface are just the Fermi surfaces of the isolated planes and chains, given by \( \xi_1 = 0 \) and \( \xi_2 = 0 \) respectively. There is a Fermi surface crossing at \( \xi_1 = \xi_2 = 0 \). As \( t \) is increased, the Fermi surfaces are pushed apart, and the crossing becomes an avoided crossing. Far away from the avoided crossing, the each piece of Fermi surface is predominantly chain or plane in character. However, near the avoided crossing, the two bands are hybridizations of the chain and plane states. In the superconducting state this has the important effect of distorting the gap away from the \( d_{x^2-y^2} \) symmetry of the pairing interaction. In Figs. 1(b) and (c), we show the quasiparticle band structure [given by Eq. (8b)] in the superconducting state along the two paths \( k_y = 0 \) and \( k_y = 8k_x/3 \) (with \( k_z = 0 \) in both cases). For comparison purposes, we show the same spectra in the \( t = 0 \) limit. Along \( k_y = 0 \), the two pieces of Fermi surface are far enough apart that one piece is predominantly chain–like while the second is predominantly plane–like. If we take the term “gap” to mean a local minimum in \( E_{\pm} \) along paths of the type \( k_y = \alpha k_x \) then we can see that there is a double gap structure along the \( k_y = 0 \) direction. The larger of the two gaps can be identified with the CuO\(_2\) plane and is perturbed from \( |\Delta_k| \) by a term of order \( |\Delta_k| t^2/(\xi_1^2 - \xi_2^2) \). The second gap is the induced gap in the chains, and it is of order \( |\Delta_k| t^2/(\xi_1^2 - \xi_2^2) \). The second path, \( k_y = 8k_x/3 \), passes through the avoided crossing. In Fig. 1(c), the band structure near the Fermi surface has little in common with the band structure in the \( t = 0 \) limit, and the two gaps are nearly equal to each other, but very different from \( \Delta_k \). It is the effect of the chain–plane coupling in this region of the Brillouin zone which produces the finite \( c \)–axis Josephson current.

The shape of the Fermi surfaces in Fig. 1(a) was chosen to qualitatively resemble the results of first principles band structure calculations. Such calculations find a Fermi surface that has four pieces, two of which are similar to the ones shown in Fig. 1(a). The remaining two pieces of Fermi surface have a (nearly) tetragonal symmetry. These have not
been accounted for here since the goal is to describe the effects of orthorhombic distortion with a simple model.

III. JOSEPHSON CURRENT

The current generated by $T$ is $e\dot{N}^l$, where $N^l = \sum_{k,\sigma} c^\dagger_{k\sigma} c_{k\sigma}$ is the number of electrons in the Pb and $\dot{N}^l = -i/\hbar [N^l, T]$ so that

$$\langle \dot{N}^l \rangle = 2\text{Im} \sum_{k,q,\sigma} T_{kq} \langle c^\dagger_{k\sigma} a_{1q\sigma} \rangle. \quad (12)$$

Taking $T$ as a perturbation we find that, to lowest order, the Josephson current is

$$I = -\frac{2e}{\hbar^2} \text{Re} \sum_{k,q,\sigma} T_{kq} \int_{-\infty}^{t} dt' e^{\eta t'} \langle [c^\dagger_{k\sigma}(t) a_{1q\sigma}(t), T(t')] \rangle, \quad (13)$$

where $\eta$ is positive and vanishingly small, and the expectation value is now taken with respect to the uncoupled system. Equation (13) has both a supercurrent contribution, which depends on the expectation values $\langle c^\dagger_{k\sigma}(t) c_{k\sigma}(t') \rangle$ and $\langle a_{1k\sigma}(t) a_{1k\sigma}(t') \rangle$, and a quasiparticle contribution, which depends on $\langle c^\dagger_{k\sigma}(t) c_{k\sigma}(t') \rangle$ and $\langle a^\dagger_{1k\sigma}(t) a_{1k\sigma}(t') \rangle$. In our case, the voltage across the junction is zero and the quasiparticle part vanishes. The supercurrent can be evaluated by rewriting the electron creation and annihilation operators in terms of the superconducting quasiparticle operators and noting that, for example,

$$\hat{C}_m(k, t) = e^{-iE_m(k)t/\hbar} \hat{C}_m(k, 0). \quad (14)$$

It follows directly that

$$J = \frac{4e}{\hbar} \text{Im} \sum_{i,j,k,q} T_{kq} T_{-k-q} U^*_{i1j}(k) U^*_{j1i}(k) U^*_{i1j}(q) U^*_{j1i}(q) \frac{f(E^l_i(k)) - f(E^r_j(q))}{E^l_i(k) - E^r_j(q)}. \quad (15)$$

This is the basic equation for the Josephson current in the absence of an external voltage.

For our particular model, this expression becomes

$$J(\phi) = \frac{4e}{\hbar} \sum_{k,q} |T_{kq}|^2 \frac{\text{Im}[\Delta^l \Delta^r]}{2E^l[E^r E^l - E^r]^2} \left\{ \frac{E^r - \xi_2^2}{E^l + E^r} + 2 \frac{E^r f(E^l) - E^l f(E^r)}{E^l - E^r} \right\}. \quad (16)$$

where $\Delta = \Delta^l \Delta^r$ is the order parameter.
In this equation $k$ is the variable of integration for all terms associated with the Pb (i.e. all variables with superscript $l$) and $q$ is the variable of integration for all terms associated with the YBCO. We have also used $T_{kq} = T_{k+q}^*$, which follows from time reversal symmetry. The phase $\phi$ is the complex phase of $\Delta^l \Delta^r_q$. Equation (13) can be written $J(\phi) = J_c \sin(\phi)$, which defines the critical current $J_c$.

Although Eq. (16) is complicated in appearance, its behaviour can actually be understood fairly easily. First of all, since $E_+ > |\xi_2|$ everywhere (see, eg., Fig. [1]) the sign of the coefficient of the first term is the same as the sign of $\Delta_q$. Furthermore, the term inside the square brackets can easily be seen to be positive and decreasing with increasing $T$. A similar argument holds for the second term in Eq. (16), except that $E_2^2 - \xi_2^2$ changes sign between different regions of the Brillouin zone. In Fig. [1] however, we can see that $E_2^2 - \xi_2^2 < 0$ near the Fermi surface, so that at low enough temperatures (recall that $T$ is less than one tenth of the $T_c$ of YBCO here) the sign of the temperature dependent part of the second term is also determined by $\Delta_q$. Whether $J_c$ is an increasing or decreasing function of $T$, then, depends on the strength with which the integrand contributes to the integral in different regions of the Brillouin zone.

It is simple to show that, in the limit $t_0 \to 0$, Eq. (16) becomes the well known equation of Ambegoakar and Baratoff:

$$J = \frac{2e}{\hbar} \sum_{k,q} |T_{k,q}|^2 \frac{\text{Im}[\Delta^l \Delta^r_q]}{E^l E^r} \times \left\{ \frac{f(E^l) - f(E^r)}{E^l - E^r} - \frac{f(E^l) - f(-E^r)}{E^l + E^r} \right\},$$

with $E^r = [\xi_2^2 + \Delta^r_q]^2]^{1/2}$. Provided that $|T_{kq}|$ is invariant under $\pi/2$ rotations in the $q_x q_y$ plane, the Josephson current will vanish for a $d$-wave order parameter.

In order to proceed with Eq. (16) it is necessary to choose a form for the tunneling matrix element. The two common choices are

$$|T_{k,q}|^2 = |T|^2, \quad (18a)$$

(which describes an incoherent tunneling process) and
which describes a specular tunneling process\(^3\)). In Eq. (18b), \(P\) is the probability of transmission through the barrier for a single electron, \(L^l\) and \(L^r\) are the thicknesses of the Pb and YBCO perpendicular to the junction and \(v^l\) and \(v^r\) are the semiclassical electron velocities in the \(z\)-direction: \(v^l_z = \partial \epsilon / \partial k_z\) and

\[
|v^r_z| = \left| \frac{\partial \epsilon_{\pm}}{\partial q_z} \right|
\]

\[
= |t_0 \sin(q_z/2)| \frac{|t(q_z)|}{\sqrt{\xi_1^2 - \xi_2^2 + 4t^2(q_z)}}. \tag{19}
\]

The \(\delta\)-function in Eq. (18b) conserves the momentum parallel to the junction face.

In the case of specular tunneling, the choice of \(v^r_z\) plays an important role in determining the magnitude of the Josephson current. For a single band material, in which there are only CuO\(_2\) planes, \(v_z = t_0 \sin(q_z)\) so that the entire Fermi surface contributes to the tunneling process, and the Josephson current vanishes because of the antisymmetry of the \(d\)-wave order parameter. In Eq. (13), however, there is a weighting factor which is only appreciable in regions where \(|\xi_1 - \xi_2| < 2|t|\). Physically, this means that currents can only flow along the \(z\)-axis in regions of the Brillouin zone near to where the Fermi surfaces cross: electrons travelling in the \(z\)-direction must hop between the chains and planes and, since the chain–plane coupling is coherent (conserves \(q\)), hopping can only take place in regions where the chain and plane Fermi surfaces are close together. In the \(q\)-space integral in Eq. (16), \(v^r_z\) has the effect of restricting the integral to one small region of the Brillouin zone over which the order parameter is roughly constant. Because of this Eq. (16) is not able to distinguish whether YBCO is \(s\)-wave or \(d\)-wave for small \(t_0\).

Another useful way of looking at \(v^r_z\) is that it destroys the antisymmetry of the integrand under rotations of \(\pi/2\). For small \(t_0\), the Josephson current is approximately given by Eq. (17). The integral is non–vanishing, however, because of \(|T_{kq}|'s lack of symmetry.

We will finish this section with a brief derivation of the normal state junction resistance \(R_n\), which is necessary to determine the critical voltage, \(J_cR_n\). The calculation is similar to
the one performed above for the supercurrent and, as before, we begin with Eq. (13). In this case, however, we are finding the quasiparticle current, \( J_n \), driven through the junction in the normal state by a voltage \( V \), and the supercurrent contribution to the integral vanishes. The voltage is taken into account by shifting the operators \( c_{k\sigma} \) by a phase \( \exp(\frac{i e V t}{\hbar}) \).

Performing the integration over \( t' \) in Eq. (13), we find that, for small \( V \) and \( T = 0 \), we regain Ohm’s law: \( J_n = R_n^{-1} V \). For incoherent tunneling

\[
R_n^{-1} = \frac{8\pi e^2 |T|^2 N_l(0)}{\hbar} \sum_q \sum_{\sigma=\pm} \frac{t^2}{t^2 + \xi^2} \delta(\varepsilon_{\pm}),
\]

while for specular tunneling,

\[
R_n^{-1} = \frac{8e^2 P}{\hbar L r} \sum_q |v_r(q)| \sum_{\sigma=\pm} \frac{t^2}{t^2 + \xi^2} \delta(\varepsilon_{\pm}).
\]

The advantage of reporting \( J_c R_n \) instead of \( J_c \) is that \( J_c R_n \) is independent of the strength of the tunneling matrix element.

IV. RESULTS AND DISCUSSION

In this section we present the results of numerical calculations of the Josephson current through a \( c \)-axis junction. In Fig. 2 the dependence of the critical voltage at \( T = 0 \) on the chain–plane coupling is shown for an incoherent junction [Eq. (18a)]. The voltage scale of \( J_c R_n \) is tens of \( \mu V \), which is two orders of magnitude lower than the value found from the Ambegaokar–Baratoff formula (assuming both materials to be \( s \)-wave), and a full order of magnitude lower than found in the experiments of Sun et al. For small \( t_0 \) we have a quadratic increase in \( J_c R_n \) with \( t_0 \) which is due to the distortion of the gap away from \( d_{x^2-y^2} \) symmetry by the chain–plane coupling. Increasing the coupling further, however, does not increase \( J_c R_n \) indefinitely. The maximum in the critical voltage is due to the fact that chain plane coupling, as well as breaking the symmetry, reduces the gap in the CuO\(_2\) planes. This is a feature which is particular to proximity effect models. In the inset figure we plot the temperature dependence of \( J_c R_n \) for a relatively weak \( t_0 = 10 \) meV chain–plane
coupling. The shape of the curve differs slightly from single band models by the fact that the maximum value of $J_c R_n (J_c R_n \sim 0.026 \text{ mV})$ does not occur at $T = 0$, but at $T \sim 0.4 \text{ meV}$. This happens at temperatures which are low enough that $f(E') \sim 0$. As we have mentioned in the discussion following Eq. (16), whether $J_c$ is an increasing or decreasing function of $T$ depends on the sign of the order parameter in the regions of the Brillouin zone which contribute most to the integral. Since the induced gap in the chain is smaller than the gap in the Pb in the region of the Brillouin zone where the chain and plane Fermi surfaces are far apart, the temperature dependence of $J_c R_n$ at low $T$ is determined by the induced gap. In Fig. 1 we can see that $\Delta_q < 0$ in the region where the induced gap is small so that $J_c R_n$ is an increasing function of $T$. At larger values of $T$, thermal excitation of quasiparticles in the Pb determines the temperature dependence of the critical voltage. It is clear from this discussion that $J_c R_n(T)$ will not have this kind of non-monotonic behaviour for an $s$-wave gap.

In our discussion of the current through an incoherent junction, we have used the word “gap” in a loose sense to describe the state of the condensate. The fact that the structure of the gap can be distorted by the chains highlights the fundamental difference between the gap and the order parameter, which is defined in Eq. (5). From the definition, it is clear that the order parameter has the $d_{x^2-y^2}$ symmetry of the pairing interaction regardless of the strength of the chain–plane coupling. In fact, our intuitive definition of the “gap” is more closely related to the anomalous Green’s function, $F$, which describes both the density and phase of the superconducting condensate. We can rewrite Eq. (15) for the Josephson current in terms of $F$:

$$J = \frac{4e}{\beta} \operatorname{Im} \sum_{\mathbf{k} \mathbf{q}} T_{\mathbf{k} \mathbf{q}} T_{-\mathbf{k} - \mathbf{q}} F^\dagger(l; i\zeta_l) F^r_{11}(\mathbf{q}; i\zeta_l),$$

(21)

where $F^l$ is the anomalous Green’s function in the Pb, $F^r_{11} \equiv -\langle T a_{1-k1}(-i\tau) a_{1k1}(0) \rangle$ is the anomalous Green’s function in the CuO$_2$ plane, $\beta$ is the inverse temperature, $\zeta_l = (2l+1)\pi/\beta$ are the fermion Matsubara frequencies and $\beta$ is the inverse temperature. Equation (21) makes it clear that Josephson junctions are sensitive to the structure of the condensate and
not the pairing interaction. In a single band material

$$F(k; \omega) = -\frac{\Delta_k}{\omega^2 - E^2},$$  \hspace{1cm} (22)

where $E$ is the quasiparticle energy. In our multiband model,

$$F_{11}(k; \omega) = -\frac{\Delta_k(\omega^2 - \xi^2_z)}{(\omega^2 - E^2_+)(\omega^2 - E^2_-)}.$$ \hspace{1cm} (23)

By comparing Eqs. (23) and (22) we can see how the chains affect the symmetry of the condensate, and that $F_{11}$ does not share the symmetry of $\Delta_k$. The point we would like to emphasize with this discussion, then, is that a finite current through an incoherent $c$–axis junction does seem to suggest that the condensate is not $d$–wave, but does not not rule out the possibility that the pairing interaction is $d$–wave.

In Figs. 3(a) and (b) we plot $J_cR_n$ for a specular junction, in which the tunneling matrix element is given by Eq. (18b). For an isotropic Fermi surface and gap, the specular and incoherent cases yield identical results. As we can see in Fig. 3(a), however, the critical voltage is a full order of magnitude larger for a specular junction than for an incoherent junction. Furthermore, $J_cR_n$ is a monotonically decreasing function of $T$. In Fig. 3(b), the dependence of both $J_c$ and $J_cR_n$ on $t_0$ is shown. As expected, $J_c$ vanishes as $t_0 \to 0$, although here the reason is that the Fermi velocity of electrons in the $z$–direction, $v^r_z$, vanishes. From Eq. (20b), it is clear that $R_n^{-1}$ also vanishes as $v^r_z \to 0$, so that the product $J_cR_n$ is nonvanishing. This is very different from the case of incoherent tunneling where $R_n$ is largely independent of $t_0$. It seems, then, that our model for specular tunneling is in good agreement with the observations of Sun et al.\textsuperscript{21} From Fig. 3(c) we can see that for $t_0 = 40$ meV, the critical voltage is around 1 mV, while Sun and his co–workers find critical voltages of 0.3–0.9 mV. This value of $t_0$ is also consistent with the observed anisotropy of the penetration depth, $\lambda_c/\lambda_{ab}$, as we have shown using a closely related model.\textsuperscript{8}

The large difference between the results of the specular and incoherent tunneling is a reflection of the important difference between the roles of the chains in the two types of tunneling. As we discussed earlier, an incoherent junction is sensitive to the symmetry of
the condensate over the entire Brillouin zone. For a specular junction, on the other hand, the most important effect of the chains is to change the component of the Fermi velocity perpendicular to the junction. In Sec. III we showed that the tunneling is strongly weighted in favour of electrons with a large perpendicular component so that only one small region of the Brillouin zone, near where the chain and plane Fermi surfaces cross, contributes to the total tunneling current. The symmetry of the order parameter is largely irrelevant in this case. In the case of specular tunneling, then, the $c$–axis tunneling current is less a probe of the symmetry of the condensate than it is of the normal state band structure.

We would like to finish this section with a brief discussion of an unresolved issue which is relevant to this work. Experiments on $c$–axis Josephson junctions have been performed with both twinned and untwinned crystals, and find similar values for the critical currents. Dynes has suggested that the total critical current through a junction, in which one of the materials is heavily twinned and has a gap which changes sign under rotations of $\pi/2$, should vanish. This is because the phase locking of the condensate at twin boundaries causes overall phase shifts of $\pi$ between adjacent regions. Adjacent regions should therefore have Josephson currents in opposite directions, and the total current should vanish. This argument is problematic for the work presented in this article. The argument is uncertain, however, because the behaviour of the order parameter at twin boundaries is not well understood.

V. CONCLUSION

In this article we have calculated the Josephson current in a model $c$–axis YBCO/Pb junction. We have assumed that the YBCO is made up of alternating layers of CuO$_2$ planes and CuO chains, stacked in the $z$–direction, and that the layer adjacent to the junction is a CuO$_2$ plane. We take the pairing interaction in the YBCO to have $d_{x^2−y^2}$ symmetry. For an incoherent junction the tunneling current is sensitive to the symmetry of the superconducting condensate (although not of the pairing interaction), and we find that distortions of the condensate due to the chains are sufficient to yield nonzero Josephson currents. The currents
are an order of magnitude smaller than observed experimentally. For a specular junction, the Josephson current is insensitive to the symmetry of the condensate because the tunneling matrix element is strongly influenced by the normal state band structure. In our model, the Josephson current is due to one small region of the Brillouin zone over which the gap is roughly constant. The calculated currents for a specular junction are of the same order of magnitude as those found experimentally by Sun et al. [2].
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FIGURES

FIG. 1. Band structure of YBCO. In (a) we show the normal state Fermi surface for the dispersion given in Eq. (11). The Fermi surface has two different pieces since the unit cell consists of a chain and a plane. The Fermi surfaces are shown for a range of chain–plane coupling values ($0 < t < 50$ meV). In the absence of chain–plane coupling ($t = 0$), the Fermi surfaces cross. As $t$ is increased, the Fermi surfaces are pushed apart. The dashed line is the line along which $\Delta_k$ vanishes. In (b) and (c) we plot the quasiparticle excitation energies $E_{\pm}$ [Eq. (8b)] along $k_y = 0$ and $k_y = 8k_x/3$ respectively. We have taken $t = 40$ meV for these curves and have plotted $t = 0$ limits of $E_{\pm} \left[ (\xi_1^2 + \Delta_k^2)^{1/2} \right]$ and $|\xi_x|$ for comparison. At temperatures lower than the $T_c$ of Pb, thermal excitation of quasiparticles in the YBCO is limited to the nodes of $E_-$. All results presented in this paper are for $\sigma_1 = 100$ meV, $\sigma_2 = 60$ meV, $\mu_1 = -80$ meV, $\mu_2 = 40$ meV.

FIG. 2. Critical voltage, $J_cR_n$, for an incoherent junction. We show the dependence of $J_cR_n(T = 0)$ on the chain–plane coupling parameter $t_0$. For small $t_0$ we find the expected quadratic increase in the critical voltage as the coupling distorts the gap away from $d_{x^2-y^2}$. At larger $t_0$, the coupling to the chains weakens the condensate, as well as distorting its structure, leading to a maximum in the curve. This curve shows that, for the simple model of incoherent tunneling, distortion of the condensate by the chains cannot account for the experimentally measured values of $J_cR_n \sim O(0.5 \text{ mV})$. The inset shows the temperature dependence of the critical voltage for $t_0 = 10$ meV. The curve increases slightly at low $T$. This stems from the multiband nature of the YBCO and the antisymmetry of the order parameter.
FIG. 3. Critical voltage, $J_c R_n$, for specular tunneling. Here the tunneling matrix element is chosen to conserve the component of the wavevector parallel to the junction. Furthermore, the tunneling matrix element is weighted in favour of particles with a large perpendicular velocity [Eq. (18)]. In (a), we show the temperature dependence of $J_c R_n$ for our multiband $d$–wave model (solid line), and for the simple $s$–wave model of Ambegoakar and Baratoff (dashed line). In order to make the $T = 0$ values of $J_c R_n$ agree, we have taken $2\Delta/T_c \sim 0.12$ in the $s$–wave model. The most important difference between this figure and Fig. 2 is that critical current is a full order of magnitude larger here. In (b), both $J_c R_n(T = 0)$ and $J_c(T = 0)$ are plotted as functions of $t_0$. The magnitude of $J_c(T = 0)$ is arbitrary since the tunneling probability, $P$, has not been specified. The critical voltage is nonvanishing as $t_0 \to 0$ because $R_n$ diverges.
\[ k = (k_x^2 + k_y^2)^{1/2} \]
