I. INTRODUCTION

The symmetry of the order parameter in the cuprates is the subject of much current debate. While several experimental techniques such as ARPES [1–4] and CTS [5] probe the magnitude of the superconducting order parameter Josephson tunnelling is, perhaps, the only observable phenomena which directly probes the phase of the superconducting order parameter as well as, indirectly, its magnitude.

The focus of the debate has been upon whether the order parameter has $s$-wave (even under a 90° rotation) or $d$-wave (odd under a 90° rotation) symmetry. Since most experiments are performed upon orthorhomic materials in which the $s$- and $d$-wave symmetries belong to the same irreducible representation there is no clear distinction between them and, rather than the symmetry of the order parameter, the discussion should focus on whether there are nodes present in the order parameter which cross the Fermi surface.

Although the $s$- and $d$-wave representations of the tetragonal systems mix freely in orthorhomic systems we can still speak of the “$s$” and “$d$” parts of the order parameter if what we mean are, respectively, the parts which are odd and even under a 90° rotation. It would, however, be highly unusual for one of these components to be present in an orthorhomic superconductor without the other being present as well. Further, if the odd, or $d$, part is dominant then nodes which cross the Fermi surface will be present in the order parameter (what we call a $(d + \epsilon s)$-wave order parameter) while if the even, or $s$, part is dominant the nodes, if they are present, will not cross the Fermi surface (what we call an $(s + \epsilon d)$-wave order parameter). It is possible for an order parameter that is even under a 90° rotation (i.e., $s$-wave) to have nodes but we consider this situation unlikely and we will not examine this possibility here.

Several corner junction YBCO-Pb tunnelling experiments [7–9] are cited as strong evidence for the order parameter in YBCO having $d$-wave type symmetry. Other tunnelling experiments which contain only YBCO in a bi- and tri-crystal rings [10–12] also give strong indications of order parameters with $d$-wave type symmetry. Both of these types of experiments have the plane of the junctions perpendicular to the $a$-$b$ plane – what we refer to as “edge junction” experiments. It is the observation of $\pi$ phase shifts in the corner junctions and half flux quanta in the ring experiments that is the strong evidence for the order parameter in YBCO having $d$-wave type symmetry. [13] Note that for the observation of $\pi$ phase shifts there is no difference between a $d$-wave order parameter and a $(d + \epsilon s)$-wave order parameter.

The results of these edge junction experiments are independent of the presence of twins in these materials. [14] This indicates that the order parameter is phase-locked across the twin boundaries, although calculations indicate [15,16] that the magnitudes (as well as the relative magnitudes and perhaps the relative phase as well) of the $d$ and $s$ may change in the twin boundary. Although this phase-locking is not unexpected it may have other consequences.

There is a second class of YBCO-Pb tunnelling experiments in which the plane of the junction is parallel to the $a$-$b$ plane – what we refer to as “c-axis junction” experiments. [17,18] The presence of a current in these experiments is cited as evidence against a $d$-wave order parameter in the literature [19,20] as well as articles for more general physics audiences. [21] In fact, due to the orthorhombic symmetry of these materials the order parameter will have $(d + \epsilon s)$-wave symmetry and a $c$-axis tunnelling current of reduced magnitude is expected in untwinned materials. [22]
to the $\epsilon$s part of the order parameter but is also caused by the $d$ part of the order parameter due to the orthorhombicity of the Fermi surface, a fact that appears not to be widely appreciated.

While there is quite a large variation in the maximum resistance-tunnelling current product, $I_c R_N$, observed in these $c$-axis tunnelling experiments, $I_c R_N$ in the untwinned samples is, on average, about twice that in the twinned samples. The argument that a finite $c$-axis YBCO-Pb tunnelling current is evidence against a $d$-wave order parameter is based upon the intuitive assumption that in the presence of twins any orthorhombicity in a phase-locked order parameter will average out over the junction area. In fact, theory clearly shows that this would be an unusual condition and that one twin should be significantly more abundant than the other. An experiment which measures the relative abundance of the two twins by comparing the intensities of the (200) and (020) diffraction peaks indicates that one of the two twins is, depending upon the specific sample, 2-3 times more abundant than the other.

If the ratio of the two possible twin orientations is $n:m$ and if the current-resistance product, $I_c R_N(T = 0)$, is $I_c R_N^{(c)}$ for an untwinned junction then for the twinned sample the current should be:

$$I_c R_N^{(\text{twin})} = \left| \frac{n-m}{n+m} \right| I_c R_N^{(c)}.$$  \hspace{1cm} (1)

This is consistent with the experimental observation of Sun et al. in which the Josephson tunnelling current in untwinned $c$-axis YBCO-Pb is about double that observed in twinned junctions if the ratio of twins is approximately 3:1.

In Section II we present a bcs formalism for a model system in which a tetragonal CuO$_2$ plane layer is coupled to an orthorhombic CuO chain layer and give the equation for the resistance-tunnelling current product, $I_c R_N$. In section III we present the results of some representative calculations as well as some experimental results on the relative abundances of the two twin orientations. In section IV we make some concluding statements.

\section*{II. FORMALISM}

For a bilayer system (ie, $\alpha = 1, 2$) the coupled bcs equations are:

$$\Delta_{1,1} = \frac{1}{\Omega} \sum_q (V_{k,q,12} \chi_{q,1} + V_{k,q,12} \chi_{q,2})$$

$$\Delta_{2,2} = \frac{1}{\Omega} \sum_q (V_{k,q,12} \chi_{q,1} + V_{k,q,22} \chi_{q,2}),$$  \hspace{1cm} (2)

where we have taken $V_{k,q,12} = V_{k,q,21}$ and:

$$\chi_{q,\alpha} \equiv \langle q \uparrow, \alpha | q \downarrow, \alpha \rangle$$

$$= \frac{\Delta_{q,\alpha}}{2E_{q,\alpha}} \tanh \left( \frac{E_{q,\alpha}}{2k_B T} \right);$$

is the the pair susceptibility, with:

$$E_{k,\alpha} = \sqrt{\epsilon_{k,\alpha}^2 + \Delta_{k,\alpha}^2},$$

where $\epsilon_{k,\alpha}$ are the band energies in the normal state. Note that we have taken $\langle q \uparrow, 1 \downarrow | q \downarrow, 1 \uparrow \rangle = 0$, ie there is no pairing between electrons in different planes although other workers do not make this assumption.

We note that this set of equations is invariant under substitution $\{\Delta_{k,12}, V_{k,q,12}\} \to \{-\Delta_{k,21}, -V_{k,q,12}\}$ which means that the overall sign of $V_{k,q,12}$ only affects the relative sign of the order parameters in the two layers and not their magnitudes. This is interesting because it means that the effect on $T_c$ of having an interlayer interaction is independent of whether this interaction is attractive or repulsive, although the $c$-axis Josephson tunnelling current still depends upon the relative sign of the interlayer interaction.

The $c$-axis Josephson junction resistance-tunnelling current product, $I_c R_N(T)$, through a superconductor-insulator-superconductor junction for incoherent $c$-axis tunneling is given by the relation:

$$I_c R_N(T) = \frac{2\pi T N^{(\text{Pb})}(0) N^{(\text{YBCO})}(0) \pi^2}{\sum_n A^{(\text{Pb})}(\omega_n) A^{(\text{YBCO})}(\omega_n)}$$  \hspace{1cm} (3)

where:

$$A^{(\cdot)}(\omega_n) \equiv \frac{1}{\Omega} \sum_k \frac{\Delta^{(\cdot)}_k}{(\epsilon_k^{(\cdot)})^2 + (\Delta^{(\cdot)}_k)^2 + (\omega_n)^2},$$  \hspace{1cm} (4)

in which the superscript $(\cdot)$ indicates on which side of the junction the dispersion and order parameter are on, the sum over $\omega_n \equiv \pi T (2n - 1)$ is for all Matsubara frequencies, $R$ is the resistance of the junction and $N^{(\cdot)}(0)$ is the normal state electronic DOS given by:

$$N^{(\cdot)}(\omega) \equiv \frac{1}{\Omega} \sum_k \delta(\epsilon_k^{(\cdot)} - \omega)$$

$$= \lim_{T \to 0} \frac{1}{\pi \Omega} \sum_k \frac{\Gamma}{(\epsilon_k^{(\cdot)} - \omega)^2 + \Gamma^2}.$$  \hspace{1cm} (5)

Since the DOS and $\Delta^{(\text{Pb})}_k$ for lead are constant the sum in Eq. 4 can be performed and $A^{(\text{Pb})}(\omega_n)$ is given by:

$$A^{(\text{Pb})}(\omega_n) = \frac{\Delta^{(\text{Pb})}_k}{\sqrt{(\Delta^{(\text{Pb})}_k)^2 + (\omega_n)^2}}.$$  \hspace{1cm} (6)

If the tunneling were coherent the matrix element would have a $(k - k')$ dependence, and the sums over $k$-space wouldn’t be separable.
III. RESULTS

We use the same band structure as in our previous work on the penetration depth of a coupled chain-plane bilayer in which we assume tetragonal symmetry for the electron dispersion in the CuO$_2$ plane with first and second neighbour hopping, while the chains are quasi-one dimensional with very different hopping probabilities in the x- and y- directions (the chains are along the y-direction). For the pairing potential, $V_{k,q,\alpha\beta}$, which appears in the coupled BCS equations and which determines the superconductivity, we use a nearly antiferromagnetic Fermi liquid model with magnetic susceptibility $\chi_m$ which appears in the coupled BCS equations and which determines the superconductivity, we use a nearly antiferromagnetic Fermi liquid model with magnetic susceptibility $\chi_m$ which appears in the coupled BCS equations (2) and which determines the superconductivity, we use a nearly antiferromagnetic Fermi liquid model with magnetic susceptibility $\chi_m$ which appears in the coupled BCS equations (2) and which determines the superconductivity, we use a nearly antiferromagnetic Fermi liquid model with magnetic susceptibility $\chi_m$. Our results are not specific to this interaction – any interaction which would result in a d-wave order parameter in the CuO$_2$ plane layer will give a $(d+\epsilon s)$-wave order parameter when the CuO$_2$ planes are coupled to the CuO chain layers.

No pairing interaction is assumed to act directly in the chain band, i.e. $g_{22} = 0$, so that the superconductivity in the chains is entirely due to the $g_{12} = g_{21} \neq 0$. This parameter ($g_{12}$) is fixed to get a critical temperature value of 100K for a chosen value of the in plane pairing, $g_{11}$. In Fig. 1, we show results for the gap value $\Delta_{k,1}$ in the planes (Fig. 1a) and for $\Delta_{k,2}$ in the chains (Fig. 1b) as a function of $k$ in the first Brillouin zone. The order parameters result from a numerical solution of equations (2). For the runs shown in Fig. 1, $\{g_{11}, g_{12}, g_{22}\} = \{26.2, 10.0\}$ and $T_c = 100$K.

On the right hand side of Fig. 1, we have decomposed the order parameters into d-wave (c) and (d) and s-wave (e) and (f) components for the plane and chain, respectively. While the main component is certainly the d-wave part, the s-wave admixture is, nevertheless, significant in magnitude in both the chain and plane bands.

A useful representation of these gap results is to show the contours of gap zeros on the same plot as the Fermi surface. This is presented in the series of frames shown in Fig. 2. The top frames apply to the plane while the bottom frames apply to the chains. In all cases, (a), (c), (e) for the planes and (b), (d), (f) for the chains, the same Fermi surface (dashed curves) was used. By choice, the Fermi contour have tetragonal symmetry in the top figure while the chain Fermi surface is a quasi straight line along $k_x$, as is expected for chains along the y-direction in configuration space. The pictures are for three different values of pairing potential. The first set of two frames (a) and (b) are for $\{g_{11}, g_{12}, g_{22}\} = \{29.9, 5.0\}$, i.e. very little coupling between chains and planes (off diagonal large small). In this case, the gap in the plane is nearly pure d-wave as is also the induced gap in the chains. The zero gap contours are given by the solid line and would be the main diagonals in a pure d-wave system. As the coupling $g_{12}$ is increased $\{g_{11}, g_{12}, g_{22}\} = \{26.2, 10.0\}$, a significant s-wave component gets mixed into both solutions and the gap nodes move off the main diagonals of the Brillouin zone (This is the solution that is plotted in Fig. 2). The gap nodes still cross the Fermi surfaces in both chains and planes. As the coupling is further increased to $\{g_{11}, g_{12}, g_{22}\} = \{9.18, 20.0\}$, Fig. 2 (c) and (d), the gap nodes move far off the diagonal and for the chains they no longer cross the Fermi surface so that there is a finite minimum value of the gap on this sheet of the Fermi surface.

Calculation of the product of Josephson current times resistivity given in equation (3) for a YBCO-I-Pb tunnel junction gives for the intermediate case $\{g_{11}, g_{12}, g_{22}\} = \{26.2, 10.0\}$ the tunnelling current, $I_c R_N(T = 0)$, is 0.2-0.3 meV for the plane layers and ±(2-3) meV for the chain layers. The relative sign depends upon whether the interlayer interaction, $g_{12}$, is attractive or repulsive. These values for chain and plane tunnelling current, $I_c R_N$, are upper and lower bounds and note that the expected value should be somewhere in between since the $I_c R_N(T = 0)$ values are dependent upon the amount of tunnel junction area which is covering the uppermost chain or plane layer.

The order of magnitude difference obtained between plane and chain layer for the $I_c R_N(T = 0)$ product is understood as follows. For a given Matsubara frequency, $\omega_n$ in equation (4), the contribution to the sum over $k$, which ranges over the entire Brillouin zone, is strongly peaked about the Fermi surface because the denominator in (3) becomes smallest in this case. This is seen clearly in Fig. 2 where we show the integrand of equation (4), again for the intermediate case, as a function of $k$, in the first Brillouin zone for planes (a) and chains (b), respectively for a particular Matsubara frequency, $\omega_n = 50$meV. It is clear that in the plane layer the positive and negative parts largely cancel each other. They would, in fact, give exactly zero if the gap had pure d-wave symmetry. The situation for the chains is completely different because the Fermi surface now does not have tetragonal symmetry and even if the gap was pure d-wave there would not be a large degree of cancellation between the positive and negative regions. Thus, we note the important result that the main part of the Josephson current coming from the chains is due to the d-wave part of the gap function and would still be large if we did not account for the s-wave admixture. Thus, in an experiment on an untwinned single crystal of YBCO the Josephson current coming from the chain part of the Fermi surface is sampling mainly the d-wave part of the gap and therefore, such experiments do not reflect directly the s-wave admixture.

It has been argued that for twinned samples, the c-axis Josephson current will cancel because of the cancellation between a- and b-twins. This argument would apply equally well to our work, since we should then average...
over pictures as shown in Fig. 3(b) with opposite phases (a- and b-twins). However, we do not expect twins to be present in equal numbers, and the expected cancellation will not occur.

High resolution x-ray scattering measurements have been carried out on a small single crystal of YBa$_2$Cu$_3$O$_{6.93}$ for the purpose of investigating its twin structure. Measurements were made with an 18kW rotating anode x-ray source and a double-axis diffractometer using a perfect Ge(111) monochromator with sufficient resolution to cleanly separate Cu K$_{\alpha 1}$ from Cu K$_{\alpha 2}$ radiation. Full details will be given in a separate publication.

The crystal under study was grown by the UBC group and had approximate dimensions of $1 \times 1 \times 0.03$ mm$^3$, with the c-axis oriented along the thin dimension. The crystal was sufficiently thin that scattering within the orthorhombic basal plane (such as (2,0,0) and (0,2,0)) could be performed in transmission geometry and such measurements thus probe the bulk of the crystal. Representative longitudinal scans of the (2,0,0) and (0,2,0) Bragg peaks are shown for both twin domains in Figure 4. As is clear from this figure, one twin domain has a peak intensity which is more than an order of magnitude stronger than the other. This leads naturally to an interpretation of the twin structure in the crystal in terms of a majority and a minority domain. Also, as would be expected in this scenario, the minority phase lineshape is very noticeably broader than that of the majority phase, whose lineshape appears to be approximately resolution limited. This is shown in the inset to Figure 4, where the same data is plotted on a linear intensity axis, and has been scaled so that the peak intensity of the two domains coincide.

The majority and minority phase domain distribution in this crystal was found to be inhomogeneous. X-ray scattering measurements were performed with a very narrow ($\sim 0.05$ mm) incident beam to allow measurements which probe different regions of the crystal. The twin structure was investigated as the sample was translated through the narrow beam along the majority phase axis. This investigation yielded results which ranged from completely untwinned on one extreme edge of the crystal to an approximate 1 to 1 ratio of the volume fraction of majority to minority domains on the other edge. Interior regions of the crystal yielded some intermediate value of this ratio. We estimate the average ratio of the volume fraction occupied by the majority and minority twin domains for the entire sample to be about 2-3 to 1. While these measurements reveal a complex inhomogeneous morphology to the twin structure, it is certainly clear that macroscopic regions of the crystal exist in which one domain predominates over the other.

IV. CONCLUSIONS

For c-axis incoherent YBCO-I-Pb Josephson tunnelling junctions, the d-wave component of the gap parameter can contribute very significantly because of the orthorhombic nature of the chain Fermi surface which emphasizes the contributions to the Josephson current from those parts of the Brillouin zone along the Fermi surface. The s-component of the gap in the chains and planes will also contribute but this may be less important so that such experiments on untwinned samples do not probe directly the s-wave admixture of a predominantly d-wave gap function.

We argue that the observation of a c-axis tunnelling current in the experiments of Sun et al. [11] and Tanaka et al. [15] on twinned samples can also be understood within our theory because we do not expect equal numbers of a- and b-twins in their experiments.

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FIG. 1. The order parameter in the first Brillouin zone for (a) the plane layers and (b) the chain layers. Beside are the projections of the $d$ components, (c) and (d), and the $s$ components, (e) and (f). The vertical scale in all frames is the same. Note that the relative phase of the $d$-components in the two layers are the same while that of the $s$-components are opposite; this is caused by the interlayer interaction, $V_{k,q,12}$, being negative (i.e., repulsive).

FIG. 2. The Fermi surface (dashed curves) and gap nodes (solid curves) for a CuO$_2$ plane layer (top frames) and a CuO chain layer (bottom frames) for three different interlayer interaction strengths (left, middle and right frames). As the strength of the interlayer interaction, $g_{12}$, is increased (left to right frames) the proportion of the $s$-component in both layers increases. If the interlayer interaction were further increased the gap nodes would leave the Brillouin zone altogether and the order parameter would become $s$-like. Note that the Fermi surface in the CuO$_2$ plane layer is tetragonal but that the gap node is orthorhombic.

FIG. 3. The $k$-space integrand of $A^{\text{YBCO}}(\omega_n)$ (see Eq. 3) for (a) the CuO$_2$ plane layer and (b) the CuO chain layer. In the plane layer the positive and negative parts mostly cancel and the resulting current is small while in the chain layer only a very small amount of the integrand, $A^{\text{YBCO}}(\omega_n)$, is negative and the resulting current is large. This effect is due to the different Fermi surfaces in the two layers.
FIG. 4. Representative longitudinal x-ray scattering scans through the (2,0,0) and (0,2,0) Bragg peaks of the YBa$_2$Cu$_3$O$_{6.93}$ single crystal are shown on a logarithmic scale. It is clear that the peak intensity of the majority phase twin domains are at least an order of magnitude stronger than that of the corresponding minority phase domain. The inset shows the same data, but now on a linear intensity axis, and scaled so that the peak intensities for the two domains coincide. The Bragg features of the minority twin domains are clearly much broader than those of the majority phase domains.