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c-axis Josephson tunnelling in twinned $YBa_2Cu_3O_{7-\delta}$ (YBCO) crystals

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Abstract. Josephson tunnelling between $YBa_2Cu_3O_{7-\delta}$ and Pb with the current flowing along the *c*-axis of the $YBa_2Cu_3O_{7-\delta}$ is presumed to arise from an s-wave component of the superconductivity in $YBa_2Cu_3O_{7-\delta}$. Experiments on multi-twin samples are not entirely consistent with this hypothesis. The sign changes of the s-wave order parameter across the N_T twin boundaries should give cancellations, resulting in a small ($\sqrt{N_T}$) tunnelling current. The actual current is larger than this. We present a theory of this unexpectedly large current based upon a surface effect: disorder-induced suppression of the d-wave component at the (001) surface leads to s-wave coherence across the twin boundaries and a non-random tunnelling current. We solve the case of an ordered array of d + s and d − s twins, and estimate that the twin size at which s-wave surface coherence occurs is consistent with typical sizes observed in experiments. In this picture, there is a phase difference of $\pi/2$ between different surfaces of the material. We propose a corner-junction experiment to test this picture.

1. Introduction

Understanding the nature of the order parameter is one of the main challenges in the theory of high-T_c superconductivity. One of the most fundamental issues is the competition between s waves and d waves. d waves are definitely the rule for high-T_c systems, yet there is strong evidence that the electron-doped NdCeCuO material is of s-wave type. At a microscopic level, this suggests that the mean-field pairing interaction has two eigenvalues which vie for dominance. Understanding this competition would provide insight into the pairing mechanism.

In this regard $YBa_2Cu_3O_{7-\delta}$ (YBCO) is of particular interest. In other systems, the square symmetry forces the ordering to be of pure d-wave or pure s-wave type. The presence of one most probably prevents the emergence of the other because of repulsive terms in the free energy, and the competition has a clear winner. In contrast, YBCO has orthorhombic symmetry. This makes it inevitable that d waves and s waves are always mixed [1]. Josephson tunnelling experiments with current flowing mainly in the *a*–*b* plane [2] have made it clear that the dominant component is a d-wave one, but a substantial body of work has also demonstrated the existence of Josephson tunnelling along the *c*-axis from YBCO to a Pb electrode, indicative of an s-wave component [3–6]. It is to be hoped that these latter experiments, if carefully analysed, can tell us about the strength of the s-wave admixture in the order parameter.

We shall first review the experimental and theoretical situation concerning *c*-axis tunnelling, concluding that there are major theoretical puzzles still to be resolved. Then we shall present a new model of the phenomena which we argue is in agreement with the data as they stand, and show how to test the model more thoroughly.

c-axis tunnelling from YBCO to Pb was first observed in twinned crystals etched with Br [3], with an $I_c R_n$ product of as much as 10% of the known gap of about 30 meV. This strongly suggested the presence of an s-wave component of the superconductivity of YBCO, as a pure d-wave current would average to zero over the Fermi surface. However, another possibility was that the current was due to second-order tunnelling of the d-wave component [7]. This hypothesis predicts the presence of Shapiro steps in the conductivity in units of $hf/4e$, where f is the frequency of the incident radiation. This was ruled out in subsequent microwave experiments [6]. Finally, the question of tunnelling through step walls at the surface arises, particularly if it is deeply etched. This would be a process in which the current actually flows in the *a–b* direction. However, the fabrication of *a–b* junctions [4] and the observation of tunnelling *in situ* without etching [8] appears to have laid this possibility to rest. The presence of a non-zero s-wave component in YBCO must now be accepted.

Is it reasonable to accept the 10% estimate of s to d which comes from the $I_c R_n$ product at face value? Clearly not, for the following reason. A twinned sample should have a relative population of twins of the two possible orientations given by statistical considerations. The d-wave component must remain coherent through the sample, as is shown by the corner-junction experiments [2]. Because the change in orientation reverses the relative sign of s and d we should have roughly equal areas of d+s and d−s superconductivity in the sample, in which case the net current should be zero. More precisely, the net current should be proportional to $I_c\sqrt{N_T}$, where I_c is the critical current of a single twin and N_T is the total number of twins. If we accept this argument, then the actual proportion of s to d would be higher than 10%. This would move the nodes in the gap well away from the diagonal in the Brillouin zone. This would be inconsistent with tricrystal experiments [9]. Furthermore, comparison of Josephson currents in single crystals to twinned crystals show similar R_n-values and I_c-values which range from 0.5 to 1.6 mA for single crystals and from 0.1 to 0.9 mA for twinned samples [4]. These numbers are subject to the objection that one cannot be sure that the tunnelling matrix elements are not extremely sensitive to the sample preparation method. Nevertheless, in view of the fact that R_n does not vary wildly from sample to sample, they suggest that a purely statistical analysis of twin populations with a resulting small imbalance of d + s and d − s is not a viable explanation of the data.

The dilemma was deepened by experiments on crystals with much larger twins, large enough that junctions could be formed which straddled either one or even zero twin boundaries [5]. These showed that the direction of current definitely did change sign across the twin boundary, a fact which can be established unambiguously by investigating the current as a function of field in the plane of the junction. This observation was consistent in all eight samples studied. Also, no such sign changes were observed in the absence of a boundary. These experiments therefore clearly confirm the mechanism of an s-wave component controlled by the orthorhombic distortion, without offering any explanation of the large current in heavily twinned samples. One further observation in these experiments may offer a clue, however. The current at zero applied field in single-boundary samples was consistently higher than calculated by looking at the relative sizes of the two twins. We will return to this point below.

Summarizing the experiments, we may say that an s-wave component which changes sign across boundaries is clearly present. If it always changes sign, then we cannot explain the data on twinned samples using purely statistical arguments. One possibility is that the twin populations are not equally likely. For example, if the twinning takes place under uniaxial stress, then one orientation would be favoured. Experiments which correlate microstructure with Josephson current are needed to rule this out [4]. However, given the size of the Josephson effect in twinned samples, it seems to us that this explanation is somewhat implausible.

The most detailed theory of c-axis tunnelling proposed to date is that offered by Sigrist *et al* [10]. Their picture involves no net tunnelling from the twins themselves. A time-reversal-breaking state at the twin boundary is predicted which results in a net Josephson current coming from the twin boundaries. This would give a Josephson current which is proportional to the number of boundaries for a fixed surface area. This is not observed, though again one must keep in mind that different samples must be compared to make any such statement, and variations in important microscopic parameters cannot be controlled in such comparisons. In addition, however, the theory predicts a current which has maximum asymmetry (as a function of in-plane angle) when the applied magnetic field is parallel to the boundary. This is an experiment in which the unknown matrix elements are held fixed. This prediction is in conflict with the experimental observations, which are symmetric at parallel orientation [6].

A quite different proposal was made by Xu *et al* [11]. These authors postulate a bulk d + i s state. In this theory, however, the s component does not change sign across the boundary, which does not agree with the measurements on single-boundary samples in a parallel field.

We present an alternative explanation in which the non-zero tunnelling current is the result of a surface effect. YBCO is notorious in photoemission experiments for not showing a gap. This proposal is inspired by the fact that photoemission experiments (with resolutions of order 10 meV or less) have also never succeeded in 'seeing' a gap at the (001) surface in this material (in contrast to $Bi_2Sr_2CaCu_2O_{8+x}$). This shows that the magnitude of the gap at this particular surface is much reduced. Furthermore, if this reduction is due to disorder, such as surface scattering, one would expect the d-wave component to be much more suppressed than any s-wave admixture. A similar suppression could result from an oxygen-vacancy concentration gradient. This suppression of the d-wave component of the order parameter as we approach the (001) surface of the YBCO in the context of c-axis tunnelling is one of two central hypotheses of our model and was first suggested by Bahcall [12]. The second crucial ingredient is new: the d-wave surface suppression results in a coherent s-wave surface layer and hence an enhanced Josephson tunnelling current in highly twinned samples without a very large admixture of s waves in the bulk.

2. Calculational method

Our calculation method will be essentially of the Ginzburg–Landau (GL) type, though we will base this on a tunnelling Hamiltonian approach. For many tunnelling experiments on unconventional superconductors, this is not adequate (see, for example, reference [13]). For example, if one wishes to calculate I–V characteristics, then consideration of Giaever tunnelling as well as Josephson tunnelling is required, and the GL method, which applies only in equilibrium, is not sufficient. Another important possibility in unconventional superconductors is the appearance of surface bound states [14], which is of course not included in the GL method. This phenomenon occurs at the (110) surface but not at the (001) surface of a $d_{x^2-y^2}$ superconductor. Thus we believe our method to be perfectly adequate for Josephson tunnelling through the (001) surface, the only application we have in mind.

Hence we consider a Hamiltonian:

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_T \tag{1}$$

where $\mathcal{H}_0$ is the sum of the BCS Hamiltonians for the YBCO and the Pb systems and the tunnelling Hamiltonian is

$$\mathcal{H}_T = \sum_{\vec{k},\vec{p},s} [T(\vec{k}, \vec{p}) a^{\dagger}_{\vec{k}s} b_{\vec{p},s} + \text{h.c.}]. \tag{2}$$

Here $\vec{k}s$ and $\vec{p}s$ are the momentum eigenstates in the YBCO and Pb, respectively, and a, b are the corresponding destruction operators. This equation defines the matrix element for tunnelling from $\vec{k}$ to $\vec{p}$. The Josephson current is then

$$I_J = -e\langle 0|\frac{\mathrm{d}N}{\mathrm{d}t}\frac{1}{E_0 - \mathcal{H}_0}\mathcal{H}_T|0\rangle - e\langle 0|\mathcal{H}_T\frac{1}{E_0 - \mathcal{H}_0}\frac{\mathrm{d}N}{\mathrm{d}t}|0\rangle \tag{3}$$

where the number operator is

$$N = \sum_{\vec{k}s} a^{\dagger}_{\vec{k}s} a_{\vec{k}s}. \tag{4}$$

We calculate this in a system where the gap can vary in space along the surface of the YBCO. If the spatial variations are not too rapid on the scale of a coherence length, we obtain the following result at zero temperature:

$$I_J = \frac{-2e}{\hbar}\int \mathrm{d}^2R \sum_{\vec{k},\vec{p}} \frac{|T(\vec{k},\vec{p})|^2 \Delta_{\mathrm{YBCO}}(\vec{R},\vec{k})\Delta_{\mathrm{Pb}}(\vec{p})}{E_{\vec{k}}E_{\vec{p}}(E_{\vec{k}} + E_{\vec{p}})}. \tag{5}$$

In this expression the integral runs over the surface, Δ_{YBCO} and Δ_{Pb} are the gap functions, and the E are the quasiparicle energies. $E_{\vec{k}}$ can also depend on $\vec{R}$ in our picture.

Two limiting cases for $|T(\vec{k},\vec{p})|^2$ are of interest. If the surface randomizes the momentum, then $|T(\vec{k},\vec{p})|^2$ is a constant. If the surface conserves parallel momentum components, then

$$|T(\vec{k},\vec{p})|^2 \sim \delta(k_x - p_x)\delta(k_y - p_y).$$

In either case, if $\Delta_{\mathrm{YBCO}}(\vec{R},\vec{k})$ is purely of d-wave type, then $I_J = 0$ because of the integration over $\vec{k}$. If, on the other hand, there is an admixture of the s wave (taken to be independent of $\vec{k}$, though this assumption is not strictly necessary), we can write

$$\Delta_{\mathrm{YBCO}}(\vec{R},\vec{k}) = \Delta_{\mathrm{d}}(\vec{R},\vec{k}) + \Delta_{\mathrm{s}}(\vec{R},\vec{k}). \tag{6}$$

We obtain

$$I_J = \frac{-2e}{\hbar}\int \mathrm{d}^2R \sum_{\vec{k},\vec{p}} \frac{|T(\vec{k},\vec{p})|^2 \Delta_{\mathrm{s}}(\vec{R})\Delta_{\mathrm{Pb}}(\vec{p})}{E_{\vec{k}}E_{\vec{p}}(E_{\vec{k}} + E_{\vec{p}})} \tag{7}$$

and from this follows the critical current

$$I_c = \frac{2}{eR_n}\int \mathrm{d}^2R\, \frac{\Delta_{\mathrm{s}}(\vec{R})\Delta_{\mathrm{Pb}}}{\Delta_{\mathrm{s}}(\vec{R}) + \Delta_{\mathrm{Pb}}} K\left(\frac{|\Delta_{\mathrm{s}}(\vec{R}) - \Delta_{\mathrm{Pb}}|}{\Delta_{\mathrm{s}}(\vec{R}) + \Delta_{\mathrm{Pb}}}\right). \tag{8}$$

Here K is the complete elliptic integral of the first kind, and the normal-state junction resistance R_n is given by

$$\frac{1}{R_n} = \frac{\pi e^2}{\hbar A} N_{\mathrm{YBCO}} N_{\mathrm{Pb}} \langle |T(\vec{k},\vec{p})|^2\rangle \tag{9}$$

where N_{YBCO} and N_{Pb} are the respective densities of states at the Fermi energy, and $\langle |T(\vec{k},\vec{p})|^2\rangle$ is the average value of the tunnelling matrix element. A is the area of the junction. Equation (8) forms the basis of our work. As long as

$$x \equiv |\Delta_{\mathrm{s}}(\vec{R}) - \Delta_{\mathrm{Pb}}|/(\Delta_{\mathrm{s}}(\vec{R}) + \Delta_{\mathrm{Pb}})$$

is not very close to unity, we may take $K(x) \approx \pi/2$ and the critical current is proportional to the spatial average of $\Delta_{\mathrm{s}}(\vec{R})$. It remains to calculate $\Delta_{\mathrm{s}}(\vec{R})$, the problem to which we now turn.

3. Double-twin model

Twinned samples are disordered on the μm scale, the twin boundaries running predominantly along the diagonal of the *a–b* plane. It is reasonable then to approximate the disordered sample by an array of straight twin boundaries running across the entire sample, which is considered to be semi-infinite. We concern ourselves in this paper with the ordered case in which all twins are of the same width and alternate between d + s and d − s. In real samples the twins have varying widths, but we have verified numerically that the basic results are unaffected by neglecting the disorder in the widths. The solution of the ordered model should be periodic with a period of two twins. Therefore, we solve the case of two twins with periodic boundary conditions. The twin boundary occupies the half-plane defined by $x = 0$ and $z \leqslant 0$. The plane $z = 0$ is the (001) surface of the YBCO sample. The model is illustrated schematically in figure 1.

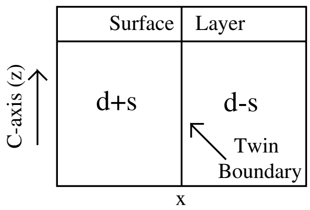

Figure 1. The ordered case where all twins are of equal width is equivalent to a d + s and a d − s twin with wrap-around boundary conditions. Near the (001) surface, there is a layer in which the d component of the order parameter is highly suppressed.

We shall write the bulk free-energy density in terms of the two order parameters Ψ_d and Ψ_s. Spatial variation is allowed only along the x-direction, (normal to the twin boundary), and along the z-direction (normal to the surface). The free-energy density is given by

$$\begin{aligned} f = {} & \alpha_d(z)|\Psi_d|^2 + \frac{\beta_d}{2}|\Psi_d|^4 + K_{dx}|\partial_x\Psi_d|^2 + K_{dz}|\partial_z\Psi_d|^2 \\ & + \alpha_s|\Psi_s|^2 + \frac{\beta_s}{2}|\Psi_s|^4 + K_{sx}|\partial_x\Psi_s|^2 + K_{sz}|\partial_z\Psi_s|^2 \\ & + \alpha_{sd}(x)(\Psi_s^*\Psi_d + \mathrm{c.c}) + \beta_{sd}|\Psi_s|^2|\Psi_d|^2. \end{aligned} \tag{10}$$

Some of the important physical ideas behind our model are displayed by this equation. α_d is a function of position in order to enforce the condition that the d-wave component is suppressed near the surface. Thus $\alpha_d \to \alpha_{d0} < 0$, a negative constant, as $z \to -\infty$, deep in the bulk. α_d increases toward 0 as $z \to 0$ at the surface. α_{sd} is the s–d coupling parameter which is a negative constant deep in the d + s twin and positive constant deep in the d − s twin. $\alpha_{sd}(x) = -\alpha_{sd}(-x)$.

The β_{sd}-term is the s–d repulsion mentioned in the introduction. We will neglect it in the calculations and have included it here only in order to stress that a large positive β_{sd} suppresses all s–d mixing in the absence of the bilinear α_{sd}-term. If this term is present, as it is here because of the orthorhombic distortion, then the size of the s admixture is controlled by α_{sd}/α_d.

We must also include the free energy of the twin boundaries. Any x-axis variation of Ψ_s and Ψ_d will take place within a distance of the order of a coherence length about the twin boundary. Since $\xi_{ab} \approx 20$ Å is very small compared to the average twin width (0.1 to 10 μm) we conclude that the detailed structure of the twin boundary is not very important. We will assume a very thin boundary and thus take α_{sd} to be piecewise constant. This is in direct contrast to the Sigrist *et al* model in which the current comes from the twin boundaries. In our model the current comes from the twins. We therefore approximate the free energy of the twin boundary by a Josephson-type coupling:

$$f_{TB} = -J_s|\Psi_s^+||\Psi_s^-|\cos(\phi_s^+ - \phi_s^-) - J_d|\Psi_d^+||\Psi_s^-|\cos(\phi_d^+ - \phi_d^-) \tag{11}$$

where J_s and $J_d > 0$. We can also now drop the x-axis gradient terms in the bulk free energy. Any x-axis variation in the order parameters takes place near the twin boundary and has been included in the boundary energy.

The problem has been reduced to two one-dimensional twins which are Josephson coupled. However, only one twin is actually required. As the surface of the YBCO is approached, the *magnitude* of Ψ_d and Ψ_s should vary in exactly the same way in both the d + s and d − s twins. Only the phases ϕ_s and ϕ_d are different. But while the phases differ between twins, they are not entirely independent. We set $\phi_d = \phi_s = 0$ in the bulk of the d + s twin, and $\phi_d = 0$, $\phi_s = \pi$ in the bulk of the d − s twin. As the (001) surface is approached, variation in ϕ_s^+ and ϕ_s^- should be symmetric about $\pi/2$, while ϕ_d^+ and ϕ_d^- will be symmetric about 0. This allows the boundary energy to be rewritten entirely in terms of the phases in the d + s twin:

$$f_{TB}^{\mathrm{d+s}}(z) = -J_d|\Psi_d(z)|^2\cos(2\phi_d(z)) + J_s|\Psi_s(z)|^2\cos(2\phi_s(z)). \tag{12}$$

ϕ_s and ϕ_d in the d − s twin can be deduced immediately, and the problem is now entirely one dimensional.

4. Solution

We will solve for the order parameters in the d + s twin. The solution for the d − s twin follows immediately. Our one-dimensional free-energy density is

$$f(z) = w\left\{\alpha_d(z)|\Psi_d|^2 + \frac{\beta_d}{2}|\Psi_d|^4 + \alpha_s|\Psi_s|^2 + \frac{\beta_s}{2}|\Psi_s|^4 + K_{dz}|\partial_z\Psi_d|^2 + K_{sz}|\partial_z\Psi_s|^2 + \alpha_{sd}(x)(\Psi_s^*\Psi_d + \mathrm{c.c})\right\} + -J_d|\Psi_d|^2\cos(2\phi_d) + J_s|\Psi_s|^2\cos(2\phi_s) \tag{13}$$

where w is the width of a single twin. Performing the usual minimizations, we get

$$\frac{\delta f}{2\,\delta|\Psi_d|} = w\left\{\alpha_d(z)|\Psi_d| + \beta_d|\Psi_d|^3 + \alpha_{sd}|\Psi_s|\cos(\phi_d - \phi_s) + K_{dz}\left(-\frac{1}{2}\,\partial_z^2|\Psi_d| + |\Psi_d|^2(\partial_z\phi_d)^2\right)\right\} - J_d|\Psi_d|\cos(2\phi_d) = 0 \tag{14}$$

and

$$\frac{\delta f}{2\,\delta\phi_d} = w\left\{-\alpha_{sd}|\Psi_d||\Psi_s|\sin(\phi_d - \phi_s) - \frac{1}{2}K_{dz}|\Psi_d|^2\,\partial_z^2\phi_d\right\} + J_d|\Psi_d|^2\sin(2\phi_d) = 0. \tag{15}$$

The analogous s-wave equations are

$$\frac{\delta f}{2\,\delta|\Psi_s|} = w\left\{\alpha_s|\Psi_s| + \beta_s|\Psi_s|^3 + \alpha_{sd}|\Psi_d|\cos(\phi_s - \phi_d) + K_{sz}\left(-\frac{1}{2}\,\partial_z^2|\Psi_s| + |\Psi_s|^2(\partial_z\phi_s)^2\right)\right\} + J_s|\Psi_s|\cos(2\phi_s) = 0 \tag{16}$$

and

$$\frac{\delta f}{2\,\delta\phi_s} = w\left\{-\alpha_{sd}|\Psi_d||\Psi_s|\sin(\phi_s - \phi_d) - \frac{1}{2}K_{sz}|\Psi_s|^2\,\partial_z^2\phi_s\right\} - J_s|\Psi_s|^2\sin(2\phi_s) = 0. \tag{17}$$

In general, these equations must be solved numerically, but it is instructive to first consider the limit $K_{dz} = K_{ds} = 0$, which may be obtained analytically. If we consider equations (6) and (8) we see that

$$J_d|\Psi_d|^2 \sin(2\phi_d) = J_s|\Psi_s|^2 \sin(2\phi_s) = w\alpha_{sd}|\Psi_s||\Psi_d| \sin(\phi_s - \phi_d). \quad (18)$$

ϕ_s and ϕ_d are between 0 and $\pi/2$. There are only the two obvious solutions: $\phi_d = \phi_s = 0$ or $\pi/2$.

The particular solution which minimizes the free energy is dependent upon the relative strengths of the s and d intertwin Josephson couplings, i.e., the ratio

$$R = J_d|\Psi_d|^2/J_s|\Psi_s|^2.$$

If $R > 1$, then $\phi_s = \phi_d = 0$. If $R < 1$, $\phi_s = \phi_d = \pi/2$. This is in the d + s twin. In the d − s twin, if $R > 1$, we have $\phi_d = 0$, $\phi_s = \pi$. If $R > 0$, then $\phi_d = -\pi/2$ and $\phi_s = \pi/2$. The magnitudes are obtained from the coupled set of equations

$$\begin{aligned} |\Psi_s| &= -\frac{1}{|\alpha_{sd}|}(\alpha_d(z)|\Psi_d| + \beta_d|\Psi_d|^3) \\ |\Psi_d| &= -\frac{1}{|\alpha_{sd}|}(\alpha_s|\Psi_s| + \beta_s|\Psi_s|^3) \end{aligned} \quad (19)$$

where we have assumed that the intertwin coupling has little effect on the magnitude of the order parameters, that is $J_s \ll w|\alpha_s|$ where w is the twin width. The exact form of $|\Psi_s|$ and $|\Psi_d|$ will depend on the $\alpha_d(z)$ chosen.

The main effect of the finite gradient terms $K_{s,d}|\partial_z\Psi_{s,d}|^2$ in the free energy is to smooth out the variation in the order parameters as the surface is approached. We expect the order parameter magnitudes to be only slightly affected by the introduction of the gradient terms. Variation in $|\Psi_d|$ and $|\Psi_s|$ should depend predominantly on $\alpha_d(z)$, since $K_d \ll |\alpha_d|$, etc. The effect on the phases is more dramatic. For relatively narrow twins, ϕ_s and ϕ_d now undergo a smooth transition from $\phi_s = \phi_d = 0$ in the bulk of the d + s twin to $\phi_s = \phi_d = \pi/2$ at the surface. In the d − s twin, ϕ_s changes from π to $\pi/2$ at the surface and ϕ_d from 0 to $-\pi/2$. The order parameter magnitudes and phases for a model $\alpha_d(z)$ are shown in figure 2.

The degree of smoothing depends upon the strength of the gradient term versus that of the coupling across the twin boundary. The dominant factor in this competition between the gradient and the intertwin coupling energy is the twin width. For very wide twins, the change in surface phase is diminished and may be eliminated altogether.

The maximum *c*-axis Josephson current is given by

$$\frac{J_{max}}{A} = \frac{J_0}{2}\{\sin(\phi_{Pb} - \phi_s^{d+s}) + \sin(\phi_{Pb} - \phi_s^{d-s})\} = J_0 \sin(\phi_s^{d+s}) \quad (20)$$

where A is the junction area and ϕ_{Pb} has been chosen to yield the maximum Josephson current. For very large twins it is not energetically favourable for the phase change to occur. The s-wave phase at the surface alternates between 0 and π across twin boundaries and no net Josephson current flows. As the twins become narrower, a threshold is reached where the s-wave phases start to shift towards $\pi/2$ at the surface. The s-wave surface phase alternates between ϕ_s^{d+s} and $\phi_s^{d-s} = \pi - \phi_s^{d+s}$. Some Josephson coupling is now possible. For very narrow twins ϕ_s is coherent across the entire surface of the crystal, and the maximum Josephson current flows. The current *saturates*, and further reduction of twin size has no effect on the current. This is illustrated in figure 3.

The saturation is one important phenomenological difference between our model and that of Sigrist *et al*.

We want an estimate of the average twin width at which s-wave surface coherence begins in terms of experimentally measurable quantities. Roughly speaking, this threshold will occur

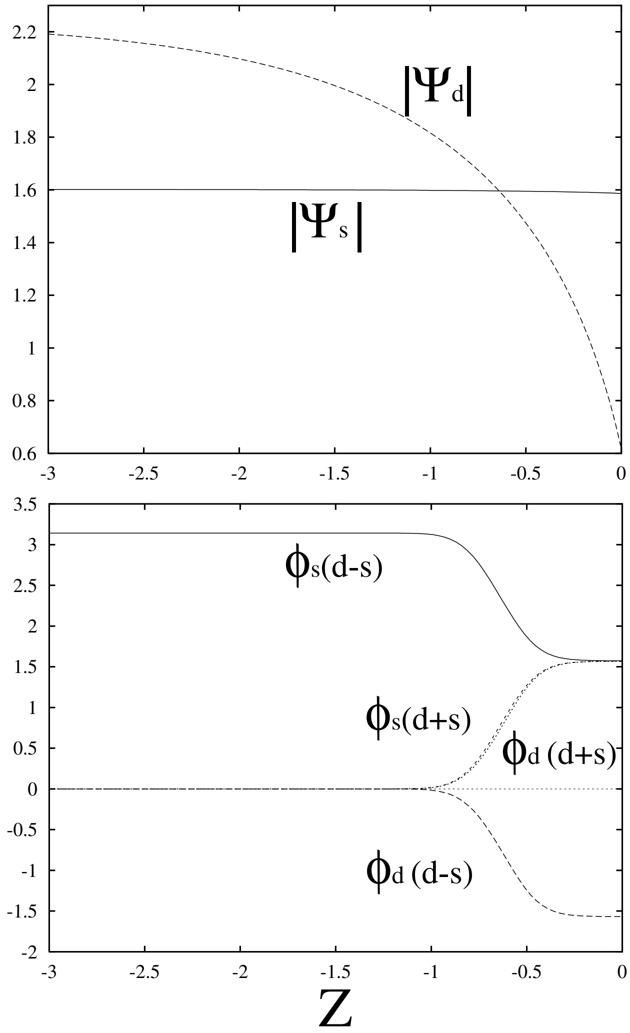

Figure 2. Order parameter magnitudes and phases near the (001) surface ($z = 0$). $\alpha_d(z) = -0.95(1 - e^z) + 0.05$, $\alpha_s = -0.5$, $\beta_d = \beta_s = 0.2$, $K_d = K_s = 10^{-6}$, $|\alpha_{sd}| = 0.01$, $J_d = J_s = 0.005$. In the bulk, ϕ_d is coherent across the twin boundary. At the surface, ϕ_s is coherent and is out of phase with the bulk ϕ_d by $\pi/2$.

when the strength of the s-wave coupling between twins is equal to the gradient energy involved in rotating the s-wave phase by $\pi/2$ at the surface. We will assume an very simple model with a surface layer of depth s in which $|\Psi_d| = |\Psi_d^0|$ for $z < -s$ and $|\Psi_d| = 0$ for $-s < z < 0$. $|\Psi_s|$ is assumed constant for all z.

The first task is to get some idea of the strength of s-wave coupling across the twin boundary. If we consider the situation far from the surface we may take $|\Psi_d(z = -\infty)|$ to be large and fixed. An effective free energy may then be written down for Ψ_s and an Euler–Lagrange equation for the variation in Ψ_s with respect to x derived:

$$\alpha_s \Psi_s + \alpha_{sd} \Psi_d - K_s \frac{\partial^2 \Psi_s}{\partial x^2} = 0. \tag{21}$$

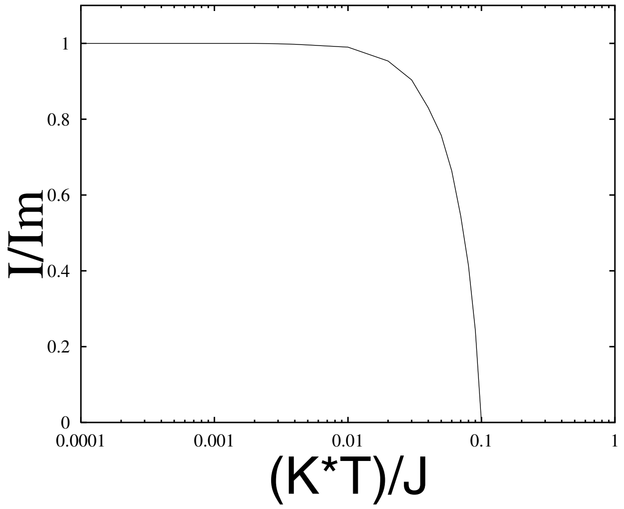

Figure 3. Net Josephson current versus twin size. The Ginzburg–Landau parameters are as for figure 2. $J = J_s = J_d$ and $K = K_s = K_d$. T is the twin size.

If we assume a step function boundary where $\alpha_{sd}(x) = -\mathrm{sgn}(x)\alpha^0_{sd}$, then we have the solution

$$\Psi_s(x) = \mathrm{sgn}(x)\Psi^0_s(1 - \mathrm{e}^{-|x|\xi_s}) \tag{22}$$

where Ψ^0_s is the bulk value. The result for the free energy per unit area of the twin boundary is

$$\frac{F_b}{A} = \xi_s\alpha_s|\Psi^0_s|^2. \tag{23}$$

The c-axis gradient energy is also required and is roughly

$$\frac{F_g}{A} = K_s|\Psi_s|^2\left(\frac{\pi/2}{s}\right)^2 w \tag{24}$$

where w is the twin width. Noting that $K_s/\alpha_s = \xi^2_c$ and setting $F_g = F_b$ we obtain

$$w = \frac{\xi_{ab}}{\xi^2_c}s^2. \tag{25}$$

For a surface layer with a depth of 100 Å (about eight unit cells), we obtain a twin width of approximately 1 μm. We emphasize that this is merely an order-of-magnitude estimate. In addition, it is not clear exactly how deep such a surface layer should be. However, the resulting twin width is not unreasonable. A highly twinned sample of 0.5 mm may have more than 10^3 twins, resulting in an average twin width of a few tenths of microns. Thus while we expect no net Josephson current in a lightly twinned sample, our model predicts the net Josephson current observed in more heavily twinned crystals.

5. Proposed experiment

Our model predicts a non-zero Josephson current resulting from a surface effect. For samples with relatively large twins, we expect a $\mathrm{d}+\mathrm{s}/\mathrm{d}-\mathrm{s}$ alternation between twins at the surface and no net Josephson current. This explains why experiments on two twin crystals show a sign change in the Josephson coupling to Pb across the twin boundary [5]. In a sample with many smaller twins, however, the coupling between twins wins out and a coherent s-wave surface layer results. We expect this to take place in samples where the average twin width is less than a few micrometres. The s-wave surface layer is $\pi/2$ out of phase with the bulk d-wave phase.

We emphasize this fact because the $\pi/2$ phase shift is experimentally verifiable. A YBCO–Pb corner-junction-type experiment with one junction on the (100) surface and the other on the (001) surface of a *highly twinned* YBCO sample should be able to detect this $\pi/2$ phase shift, as was previously suggested by Sigrist *et al* [10]. We give a schematic diagram of the proposed experimental configuration in figure 4. The current maximum as a function of field will be shifted by a quarter of a flux quantum. The Josephson coupling to the Pb at the (100) junction is predominantly due to the YBCO d-wave component since d-wave suppression is not expected at this surface. Since the *c*-axis Josephson coupling results from the smaller s-wave component, it is much weaker than the *a*-axis coupling. The (001) junction should therefore have a much larger area than the (100) junction in order to minimize any DC offset of the interference pattern.

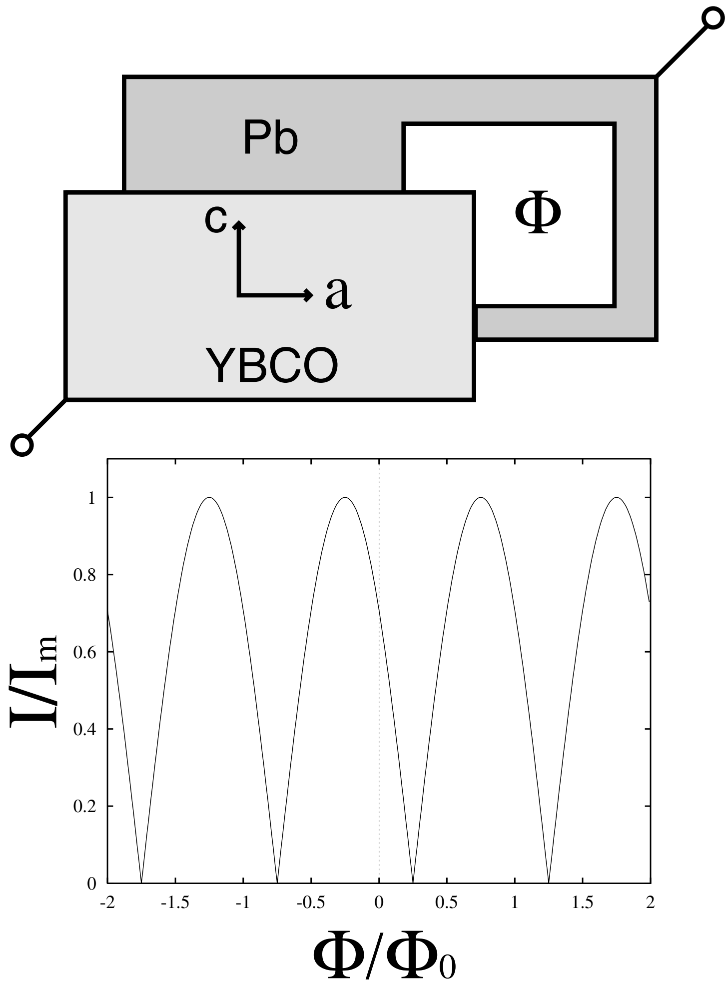

Figure 4. A schematic diagram of the proposed YBCO–Pb SQUID experiment. One junction is on the (100) surface of the YBCO, the other on the (001) surface. The $\pi/2$ shift between the bulk d-wave phase and the (001) surface s-wave phase shifts the current maximum by a quarter of a flux quantum.

6. Conclusions

The present theory can reconcile the puzzles mentioned at the outset. The surprisingly large value of $I_c R_n$ is ascribed to the partial coherence of the s-wave component at the surface. The fact this coherence is only partial gives a reasonable account of the overall differences between single-crystal and twinned samples. The fact that single-boundary junctions always show a change in sign of the s component is also consistent: in this case the twins are larger. These experiments also show excess current at zero applied magnetic field. This would be consistent with some *partial* coherence of the s component across the boundary, as the larger (stronger) of the two twins appears to control the weaker one. Hence we believe that the theory can account for all observations. The experiment of the previous section would be a critical test of the theory. Experiments in which the relative twin populations are precisely controlled would serve to rule out the alternative explanation in which the current is due to accidental anisotropy introduced in the growth process.

One important qualitative conclusion about the underlying physics of the bulk can be drawn from this picture: s waves compete with d waves in YBCO. If our model is correct, then the naive estimate of 10% admixture of the s wave as a proportion of the d wave remains roughly correct. Expressed in the language of equation (10), we have that

$$|\Psi_s|/|\Psi_d| \backsim \alpha_{sd}/(\alpha_s - \alpha_d) \backsim 0.1$$

at low temperatures. If s waves were very strongly suppressed by a large positive α_s, they would not be so easily induced by the lattice distortion.

The present theory predicts that only those materials with orthorhombic distortion should show c-axis tunnelling. Recently, c-axis Josephson tunnelling between $Ba_2Sr_2CaCu_2O_{8+x}$ and Pb [15] has been observed in spite of the absence of an orthorhombic distortion in this material. However, due to the fact that $I_c R_n \sim 1\ \mu$eV, orders of magnitude less than the gap value, we believe that this interesting effect is physically different from that seen in the YBCO experiment.

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