Angular dependence of the Josephson critical current in *c*-axis twist junctions of high-temperature superconductors

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We have investigated theoretically the case of a highly anisotropic layered superconductor consisting of two identical parts that are twisted with respect to each other by an angle ϕ_0 about the c axis. This work was motivated by recent high-quality c-axis twist Josephson junctions prepared with $Bi_2Sr_2CaCu_2O_{8+\delta}$ by Li *et al.* Our interest lies in studying whether the Josephson critical voltage I_cR_n measured along the c axis in high-temperature superconductors as a function of ϕ_0 could give valuable information regarding the orbital symmetry of the superconducting order parameter. We assume both coherent and incoherent interlayer tunneling processes, and ordinary intralayer impurity scattering. We have derived and studied the effective Lawrence-Doniach model appropriate for the cases of pure s-wave and $d_{x^2-y^2}$-wave order parameters, a dominant $d_{x^2-y^2}$ and subdominant d_{xy} mixed order parameter, and a dominant $d_{x^2-y^2}$ with a subdominant s-wave mixed order parameter. Our results suggest that Josephson tunneling across the c-axis twist junctions can indeed be a useful tool for probing the superconducting order-parameter symmetry. Further experiments to clarify the situation are suggested. [S0163-1829(98)05226-6]

I. INTRODUCTION

In recent years, there has been a raging controversy regarding the orbital symmetry of the superconducting order parameter in the high-temperature superconductors. Many experiments[1–3] were interpreted in terms of a $d_{x^2-y^2}$-wave order parameter predicted by theories involving a repulsive pairing interaction,[4] but many others[5–10] were interpreted in terms of a more conventional s-wave order parameter, as obtained in the standard BCS theory based upon rather isotropic, attractive pairing mediated by phonons or other such bosons. In the last year or so, an increasing number of these experiments appear to have been easiest to explain from a predominant $d_{x^2-y^2}$-wave order parameter, most likely accompanied by a subdominant s-wave order parameter.[11] However, nearly all of the important experiments purporting to provide evidence regarding the orbital symmetry of the order parameter were performed on the single material $YBa_2Cu_3O_{7-\delta}$ (YBCO). Unfortunately, YBCO is always distinctly orthorhombic, due to the inescapable presence of the conducting CuO chains. Hence, both the s-wave and the $d_{x^2-y^2}$-wave order parameters belong to the same representation of the relevant crystal group C_{2v}, and can mix freely at all temperatures T. Thus, before one becomes too prejudiced by the apparent results on a single material, one ought to examine the available experimental evidence that might be relevant to this question in a different material.

To date, the only other materials for which Josephson junction experiments, which are the most sensitive experiments to determine the phase of the order parameter, have been performed are the single experiment on $Tl_2Ba_2CuO_{4+\delta}$ (Tl2201) (Ref. 12) and a few on $Bi_2Sr_2CaCu_2O_{8+\delta}$ (Bi2212).[13–17] Until recently, Tl2201 was thought to have a crystal structure that was tetragonal, but very recent neutron-diffraction results have determined that most samples of Tl2201 are rather orthorhombic, as is YBCO.[18] Although there has never been any consensus on the actual crystal structure of Bi2212,[19] most samples are thought to be orthorhombic. However, in this case the orthorhombicity is different, with a distortion along the diagonal between the crystal a and b axes.[20] Such a distortion would not lead to the coexistence of a $d_{x^2-y^2}$-wave order parameter with either an s-wave or a d_{xy}-wave order parameter, except below a second phase transition, since these order parameters are manifestations of different representations of the crystal group.

In Bi2212, the only published experiments relevant to the order-parameter symmetry of which we are aware were made by Josephson tunneling into the ab plane and into a mixed c-axis, ab-plane configuration, and by scanning tunneling microscopy (STM) onto the top (c-axis) surface.[17,21–23] These experiments led to inconsistent conclusions, with STM measurements appearing to give ''d-wave-like'' results when the tip was above a (nominally semiconducting) BiO layer, but ''s-wave-like'' results when it was above a (superconducting) CuO_2 layer. While apparent Josephson tunneling into the c-axis did not produce any measurable I_cR_n, Josephson tunneling into the ab-plane gave a very large I_cR_n value, which has recently also been seen consistently in c-axis point-contact measurements,[24] although the direction of the Josephson currents in that latter experiment was unknown. In addition, angle-resolved photoemission spectroscopy (ARPES) experiments on Bi2212 have been interpreted as being consistent with an order parameter of the $d_{x^2-y^2}$ form.[25,26] We remark that ARPES experiments are insensitive to electronic properties of the sample arising from states physically deeper than about 10 Å from the surface. Al-

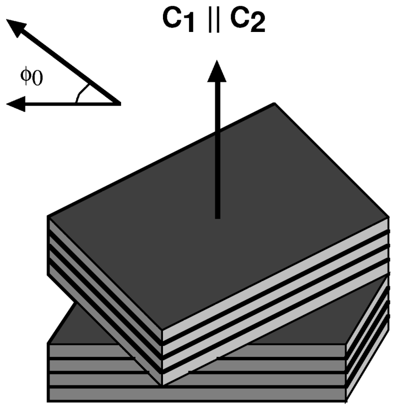

FIG. 1. Sketch of the twisted bicrystal. A single crystal is cleaved in a plane normal to the c axis; the two cleaved sections are rotated by an angle ϕ_0 with respect to each other, and then fused together as pictured.

though one cannot determine the phase of the order parameter through ARPES experiments, one would have to conclude from the data that the order parameter was locked onto the crystal lattice on the top atomic layer normal to the c axis, provided that the ARPES experiments are indeed measuring the superconducting and not some other order parameter such as that pertaining to a charge-density wave or spin-density wave.[27]

Very recently, some preliminary results relevant to the symmetry of the order parameter in Bi2212 have become available.[13–15] In these experiments, a high-quality single crystal of Bi2212 was cleaved mechanically between neighboring BiO layers; the two cleaved surfaces were then rotated by an angle ϕ_0 with respect to each other and heat treated to fuse them back together, as pictured in Fig. 1. Miraculously, transmission electron microscope studies showed that the fused boundary appeared in many samples to be essentially perfect. To measure the I_c across the twist boundary, the authors attached two current leads far from the twist, and four voltage leads near it. Due to the large values of I_c at low T, it was necessary to apply a substantial magnetic field along the c axis to reduce I_c. The $I_c(\phi_0)$ they obtained were identical to those obtained for single-crystal Bi2212, without any twist boundaries, and were essentially independent of ϕ_0.[13] For T close to the transition temperature T_c it is possible to measure I_c without applying a magnetic field. First results also show no significant variation of I_c with the twist angle ϕ_0.[16] These observations appear to be incompatible with d-wave pairing.

Unfortunately, the dependence of I_c upon the junction area A and on the current distribution, which could be very inhomogeneous, is presently unknown. However, we expect that ambiguities inherent in the present experiments, which were designed to study the weak link behavior of the grain boundary and not the symmetry of the order parameter, will be removed in the future. In this paper we therefore study the problem of the critical supercurrent along the c axis in a highly anisotropic layered superconductor (i.e., Bi2212) with a c-axis twist junction angle ϕ_0. We restrict our considerations to the temperature regime near T_c, where the experiments can be performed in the absence of the complicating magnetic field, which we neglect. It is our aim to establish whether d-wave pairing can be ruled out conclusively by measuring the supercurrent through a c-axis twist junction. To achieve this aim it is necessary to take into consideration admixtures of order parameters with different symmetries in such a way that the interpretation of other experiments is not affected. If the pair state, locked onto the crystal lattice, had $d_{x^2-y^2}$ symmetry, it would be obvious that the supercurrent would vanish for $\phi_0=45°$. The presence of a subdominant order parameter with d_{xy} symmetry would allow the overall d-wave order parameter to rotate and thus compensate for the twist. A subdominant s-wave order parameter could dominate the supercurrent because of differences in the tunneling matrix elements.

In Sec. II, we shall introduce a weak-coupling model of unconventional superconductivity in a layered superconductor with some form of single-particle interlayer tunneling, and in Sec. III we shall discuss the resulting self-consistency equations for the case of two competing order parameters. In Sec. IV these equations are simplified by keeping only terms of cubic order in the order-parameter amplitudes and the effective Lawrence-Doniach[28] free energy for these two order parameters is evaluated. Section V contains an outline of the calculation of the Josephson current and the definition of the critical current that, in the presence of a complex order parameter, presents some difficulties. We also calculate the quasiparticle current for both coherent and incoherent tunneling in order to elucidate the problems involved in deriving a relation between the parameters in the Josephson critical current and the normal-state resistance when the tunneling takes place between two-dimensional superconductors. In Sec. VI solutions of the Lawrence-Doniach equations (Sec. IV) in the absence of the twist junction are given, which are required to fix the boundary conditions. When the order parameter is complex, the boundary conditions are established by the requirement that there must be no Josephson current along the c axis for the closed system. In Sec. VII the numerical results are presented and discussed. Greatest attention is given to the very interesting possibility of two purely real d-wave order parameters, where the sign of the subdominant d_{xy}-wave order parameter changes across the twist boundary. This solution is found when the bare transition temperature T_{cB} of the subdominant order parameter is very low. If T_{cB} is comparable to the transition temperature of the dominant order parameter, the competing order parameters are most likely out of phase with each other, their phases differing by $\pi/2$ in the bulk, far from the twist boundary. Our conclusions are presented in Sec. VIII.

II. MODEL

We assume that the system consists of $2N \gg 1$ layers, which are labeled with integers n such that $-N \leqslant n \leqslant -1$, $1 \leqslant n \leqslant +N$. The two sections $n \geqslant 1$ and $n \leqslant -1$ of the crystal are assumed to be rotated relative to one another by an angle ϕ_0, creating a [001] twist grain boundary between layers $n=1$ and $n=-1$. For simplicity, we treat each microscopic CuO_2 double layer of Bi2212 as a single conducting (or superconducting) layer. We assume that the charge carriers on these planes are fermions described by the standard Hamiltonian $\mathcal{H}$ of layered superconductors

$$\mathcal{H}=\mathcal{H}_0+\mathcal{H}_1+\mathcal{V}, \tag{1}$$

with

$$\mathcal{H}_0=\sum_{n,\sigma,\mathbf{k}} \psi^\dagger_{n\sigma}(\mathbf{k})\xi_0(\mathbf{k})\psi_{n\sigma}(\mathbf{k}), \tag{2}$$

$$\mathcal{H}_1=\sum_{\substack{n,n',\sigma,\mathbf{k},\mathbf{k}'\\ \langle nn'\rangle}} \psi^\dagger_{n,\sigma}(\mathbf{k})\ t_{n,n'}(\mathbf{k}-\mathbf{k}')\ \psi_{n',\sigma}(\mathbf{k}'), \tag{3}$$

$$\mathcal{V}=\sum_{n,\sigma,\mathbf{k},\mathbf{k}'} \psi^\dagger_{n,\sigma}(\mathbf{k})\psi^\dagger_{n,-\sigma}(-\mathbf{k})\lambda_n(\mathbf{k},\mathbf{k}')\times\psi_{n,-\sigma}(-\mathbf{k}')\psi_{n,\sigma}(\mathbf{k}'). \tag{4}$$

$\psi^\dagger_{n,\sigma}(\mathbf{k})$ $[\psi_{n,\sigma}(\mathbf{k})]$ creates (annihilates) a single quasiparticle with spin σ, wave vector $\mathbf{k}=(k_x,k_y)$, and energy $\xi_0(\mathbf{k})=\epsilon(\mathbf{k})-E_F$ relative to the Fermi energy E_F within the nth layer. $\mathcal{H}_1$ is the Hamiltonian describing single-particle tunneling between near-neighbor layers n and $n'=n\pm1$, denoted by $\langle nn'\rangle$, for which $t_{n',n}(\mathbf{k}'-\mathbf{k})=t^*_{n,n'}(\mathbf{k}-\mathbf{k}')$, and $\mathcal{V}$ is the generalized singlet intralayer pairing Hamiltonian. We take $c=\hbar=k_B=1$.

The tunneling matrix element $t_{n,n'}$ depends only upon the change in momentum $\mathbf{k}-\mathbf{k}'$, when umklapp processes can be neglected, as for free particles. We assume there are two types of interlayer tunneling processes, coherent tunneling and incoherent tunneling at the positions of ''electrical shorts.'' Here we treat both of these processes together. In coherent tunneling, the tunneling matrix element in real space is translationally invariant, so that in momentum space it preserves the wave vector parallel to the junction. The incoherent process occurs at random defects situated at the positions $\mathbf{R}^{nn'}_\mu$ between the adjacent layers n,n', at which the potential barrier for interlayer tunneling is reduced. The tunneling matrix elements are thus of the form

$$t_{n,n'}(\mathbf{k}-\mathbf{k}')=\delta_{n',n\pm1}\left[J\delta^{(2)}(\mathbf{k}-\mathbf{k}')+\sum_\mu \tau(\mathbf{k}-\mathbf{k}')\ e^{-i(\mathbf{k}-\mathbf{k}')\mathbf{R}^{nn'}_\mu}\right]. \tag{5}$$

Physical quantities are obtained by taking two-dimensional averages with respect to the random sites,[29] which we denote by $\langle\cdots\rangle$. In the first-order term, we can neglect the contribution from incoherent tunneling, since we already consider explicitly the coherent tunneling. For the second-order term, we obtain

$$\langle t_{n,n'}(\mathbf{k}-\mathbf{k}')t_{n',n''}(\mathbf{k}'-\mathbf{k}'')\rangle=\delta_{n',n\pm1}\delta^{(2)}(\mathbf{k}-\mathbf{k}'')\times[|J|^2\delta^{(2)}(\mathbf{k}-\mathbf{k}'')\delta_{n'',n'\pm1}+\delta_{n'',n}f_{\text{inc}}(\mathbf{k}-\mathbf{k}')]. \tag{6}$$

The averages of incoherent tunneling processes between different adjacent layer pairs vanish. The δ function outside the square brackets reflects the restoration of translational invariance upon averaging. We note that the incoherent tunneling function $f_{\text{inc}}(\mathbf{k}-\mathbf{k}')=\rho|\tau(\mathbf{k}-\mathbf{k}')|^2$, with ρ the density of incoherent tunneling sites, is ordinarily taken to be a constant, as was done by Ambegaokar and Baratoff.[30] As has been noted before, though, it is important to keep the momentum dependence when tunneling between d-wave superconductors is considered.[31–33] These authors considered tunneling along directions parallel to the conducting planes, but the arguments applicable to c-axis tunneling are very similar.

Thus, in order to have Josephson tunneling between the layers of a purported d-wave superconductor, we must require some amount of coherent tunneling,[34,35] or else we have to introduce some d-wave anisotropy to the incoherent tunneling amplitude.[33,36] We therefore assume in this work that the incoherent part of the second-order tunneling process in Eq. (6) can be expanded as

$$f_{\text{inc}}(\mathbf{k}-\mathbf{k}')=\frac{1}{N_{2D}(0)}\sum_{\ell=0}^{\infty}\frac{\cos[\ell(\phi_{\mathbf{k}}-\phi_{\mathbf{k}'})]}{2\pi\tau_{\perp\ell}}, \tag{7}$$

where $N_{2D}(0)$ is the two-dimensional density of states; for free particles, $N_{2D}(0)=m/(2\pi)$. We have introduced the incoherent pair tunneling rates $1/\tau_{\perp\ell}$. Generally one would expect $1/\tau_{\perp\ell}$ to decrease rapidly with increasing ℓ, with the s-wave term, corresponding to complete incoherence, being by far the largest.

We remark that Eq. (7) assumes that the single-quasiparticle tunneling matrix element only depends upon the tunneling angle $\phi_{\mathbf{k}}-\phi_{\mathbf{k}'}$. That is, we assume the tunneling amplitude does not depend upon the orientation of the quasiparticle relative to the underlying crystal lattice, but only upon the relative change in direction incurred upon interlayer tunneling. We thus expect the tunneling to be invariant under $\mathbf{k}\leftrightarrow\mathbf{k}'$. In this case, if one were to have added a phase shift $\delta^{n,n'}_\ell$ to the term $\ell(\phi_{\mathbf{k}}-\phi_{\mathbf{k}'})$ inside the argument of the cosine, one would be forced to add an equivalent term with $\delta^{n,n'}_\ell\to-\delta^{n,n'}_\ell$, in order to preserve the invariance under $\mathbf{k}\leftrightarrow\mathbf{k}'$. Thus, we set $\delta^{n,n'}_\ell=0$.

The pairing interaction $\mathcal{V}$ is treated in the mean-field approximation, which leads to the following ''impurity''-averaged self-consistency equation for the order parameter on the nth layer:

$$\Delta_n(\mathbf{k})=T\sum_{\omega,\mathbf{k}'}\lambda_n(\mathbf{k},\mathbf{k}')\mathcal{F}_{n,n}(\mathbf{k}',\omega). \tag{8}$$

The sum over Matsubara frequencies ω is cut off in the usual way at some frequency ω_D.

Assuming the interlayer tunneling process is ''weak,'' we expand the anomalous Green's function $\mathcal{F}_{n,n}(\mathbf{k},\omega)$ in powers of t. For coherent tunneling in the bulk of a layered superconductor, it is elementary to include the tunneling to all orders in t,[34,35] but when a surface (such as a twist boundary) is introduced, the order parameters on each layer are inequivalent, and the Fourier-transform technique does not work.[37,38] So, we have to rely on this expansion technique, although it is only valid for $t\ll T_c$ in the absence of intralayer scattering. To second order in the interlayer tunneling, one obtains

$$\begin{aligned}\mathcal{F}_{n,n}(\mathbf{k},\omega)=\mathcal{F}_n^0(\mathbf{k},\omega)+\sum_{\substack{n'\\ \langle nn'\rangle}}\sum_{\mathbf{k}'}&[|J|^2\delta^{(2)}(\mathbf{k}-\mathbf{k}')\\&+f_{\rm inc}(\mathbf{k}-\mathbf{k}')][\mathcal{F}_n^0(\mathbf{k},\omega)\mathcal{G}_{n'}^{0\dagger}(\mathbf{k}',\omega)\mathcal{G}_n^{0\dagger}(\mathbf{k},\omega)\\&+\mathcal{F}_n^0(\mathbf{k},\omega)\mathcal{F}_{n'}^{0\dagger}(\mathbf{k}',\omega)\mathcal{F}_n^0(\mathbf{k},\omega)\\&+\mathcal{G}_n^0(\mathbf{k},\omega)\mathcal{F}_{n'}^0(\mathbf{k}',\omega)\mathcal{G}_n^{0\dagger}(\mathbf{k},\omega)\\&+\mathcal{G}_n^0(\mathbf{k},\omega)\mathcal{G}_{n'}^0(\mathbf{k}',\omega)\mathcal{F}_n^0(\mathbf{k},\omega)].\end{aligned}\tag{9}$$

The bare BCS-type Green's functions are given by

$$\mathcal{G}_n^0(\mathbf{k},\omega)=\frac{-[i\omega+\xi_0(\mathbf{k})]}{\omega^2+\xi_0^2(\mathbf{k})+|\Delta_n(\mathbf{k})|^2},$$
$$\mathcal{F}_n^0(\mathbf{k},\omega)=\frac{\Delta_n(\mathbf{k})}{\omega^2+\xi_0^2(\mathbf{k})+|\Delta_n(\mathbf{k})|^2},\tag{10}$$

$\mathcal{F}^{0\dagger}(\mathbf{k},\omega)=[\mathcal{F}^0(\mathbf{k},\omega)]^*$, and $\mathcal{G}^{0\dagger}(\mathbf{k},\omega)=[-\mathcal{G}^0(\mathbf{k},\omega)]^*$. The important term in Eq. (9) is the third term, which explicitly couples $\mathcal{F}_n^0$ to $\mathcal{F}_{n'}^0$ in linear order, and leads to the linear coupling of the order parameters on adjacent layers, the Josephson tunneling term in the Lawrence-Doniach model.

III. GAP EQUATIONS

The gap equation is obtained by inserting the anomalous Green's function from Eq. (9) into Eq. (8). Depending on the range over which the twist grain boundary affects the intralayer order parameters, we need to solve a rather large number of coupled two-dimensional nonlinear integral equations. (The total number of layers considered in most of our numerical calculations was 160.) This problem is so formidable that one needs to make some simplifying assumptions to make it amenable to numerical solution.

First, we assume that all the functions in Eq. (8) with the exception of the Green's functions vary weakly with energy $\xi_0(\mathbf{k})$. We can thus replace $\mathbf{k}$ and $\mathbf{k}'$ in the arguments of Δ_n, λ_n, and $f_{\rm inc}$ by the angles $\phi_{\mathbf{k}}$ and $\phi_{\mathbf{k}'}$ that specify the orientations of the Fermi momenta in the two-dimensional Brillouin zone. We then make use of the standard approximation $A^{-1}\Sigma_{\mathbf{k}}\rightarrow N_{2D}(0)\int(d\phi_{\mathbf{k}}/2\pi)\int_{-\infty}^{+\infty}d\xi_0$, where A is the area of a layer. After integrating over ξ_0, we obtain

$$\begin{aligned}\Delta_n(\phi_{\mathbf{k}})=\pi TN_{2D}(0)\sum_\omega\int_0^{2\pi}\frac{d\phi_{\mathbf{k}'}}{2\pi}\lambda_n(\phi_{\mathbf{k}},\phi_{\mathbf{k}'})\Bigg\{&\frac{\Delta_n(\phi_{\mathbf{k}'})}{D_n(\omega,\phi_{\mathbf{k}'})}+\sum_{\substack{n'\\ \langle nn'\rangle}}\Bigg[|J|^2\Gamma_{\rm coh}(\omega,\Delta_n(\phi_{\mathbf{k}'}),\Delta_{n'}(\phi_{\mathbf{k}'}))\\&+2\pi N_{2D}(0)\int_0^{2\pi}\frac{d\phi_{\mathbf{k}''}}{2\pi}f_{\rm inc}(\phi_{\mathbf{k}'}-\phi_{\mathbf{k}''})\Gamma_{\rm inc}(\omega,\Delta_n(\phi_{\mathbf{k}'}),\Delta_{n'}(\phi_{\mathbf{k}''}))\Bigg]\Bigg\},\end{aligned}\tag{11}$$

where

$$D_n(\omega,\phi_{\mathbf{k}})=[\omega^2+|\Delta_n(\phi_{\mathbf{k}})|^2]^{1/2}.\tag{12}$$

In Eq. (11), $\Gamma_{\rm coh}$ and $\Gamma_{\rm inc}$ are the coherent and incoherent parts of the second-order interlayer tunneling processes, respectively. The exact forms of $\Gamma_{\rm coh}$ and $\Gamma_{\rm inc}$ are given in the Appendix.

Second, we approximate the pairing interaction λ_n by a sum of separable terms:

$$\lambda_n(\phi_{\mathbf{k}},\phi_{\mathbf{k}'})=\sum_i\lambda_i\varphi_n^{(i)}(\phi_{\mathbf{k}})\varphi_n^{(i)}(\phi_{\mathbf{k}'}),\tag{13}$$

where the basis functions $\{\varphi_n^{(i)}(\phi_{\mathbf{k}})\}$ are chosen in accordance with the symmetry of the system. Since the order parameters are expected to lock onto the lattice, the arguments of the basis functions have to be shifted by $+\phi_0/2$ $(-\phi_0/2)$ for positive (negative) values of n when there is a single twist grain boundary between layers $+1$ and -1 with twist angle ϕ_0. Otherwise, the basis functions are independent of the layer index. For this type of pairing interaction, the momentum dependence of the order parameter is of the form

$$\Delta_n(\phi_{\mathbf{k}})=\sum_i\Delta_n^{(i)}\varphi_n^{(i)}(\phi_{\mathbf{k}}),\tag{14}$$

where the $\Delta_n^{(i)}$ are C numbers, which we calculate.

Before we can proceed any further we need to specify the basis functions $\varphi_n^{(i)}(\phi_{\mathbf{k}})$. At present the most popular choice for tetragonal high-T_c materials is $\varphi_n^{(d1)}(\phi_{\mathbf{k}})=\sqrt{2}\cos2\phi_{\mathbf{k}}$, corresponding to a d-wave state with $d_{x^2-y^2}$ symmetry, as the only nonvanishing contribution to the pairing interaction [Eq. (13)]. If, following Ambegaokar and Baratoff,[30] we assume the tunneling matrix elements to be momentum independent, so that $f_{\rm inc}=$const, then we see immediately from Eqs. (11) and (A2) that incoherent tunneling does not couple d-wave order parameters on neighboring planes. If $f_{\rm inc}$ has some momentum dependence, represented in Eq. (7) as a Fourier series, all terms with $\ell=2+4i$, i a nonnegative integer, will contribute to the coupling of states with $d_{x^2-y^2}$ symmetry. Of course, those with $i>2$ only contribute to the coupling of order Δ^6 and/or higher, so they are negligible in the Ginzburg-Landau regime. In the presence of a 45° twist, we must replace $\cos2\phi_{\mathbf{k}}$ by $\sin2\phi_{\mathbf{k}}$ on one of the layers. Then, neither coherent tunneling nor incoherent tunneling with the momentum dependence equation (7) can provide any coupling between the d-wave states across the twist grain boundary. It is clear that similar conclusions apply to the critical Josephson current I^{JC} to be discussed in more detail below.

One can escape these conclusions if, due to some more general momentum dependence of the pairing interaction, pairing channels with different symmetries are available. In particular, a combination of states with $d_{x^2-y^2}$ and d_{xy} symmetry,

$$\Delta_n(\phi_{\mathbf{k}})=A_n\sqrt{2}\,\cos(2\phi_{\mathbf{k}}\pm\phi_0)+B_n\sqrt{2}\,\sin(2\phi_{\mathbf{k}}\pm\phi_0),\quad (dd), \tag{15}$$

where the $+$ $(-)$ sign pertains to positive (negative) layer indices, can also be written as $C_n\sqrt{2}\,\cos[2\phi_{\mathbf{k}}\pm(\phi_0-\delta_n)]$, provided A_n and B_n are real and B_n changes sign across the twist grain boundary. We see that such a superposition of the two d-wave states will reduce the mismatch between the order parameters above and below the twist grain boundary and thus will lead to an increase in the coupling between layers and hence also in I^{JC}. If the two d-wave states were degenerate, the angles δ_n would be arbitrary and the order parameter could rotate freely in the plane. A complicating feature is that in the presence of two nearly degenerate pairing channels, weak-coupling theory predicts a time-reversal symmetry-breaking state like $A_n\sqrt{2}\,\cos(2\phi_{\mathbf{k}}\pm\phi_0)+iB_n\sqrt{2}\,\sin(2\phi_{\mathbf{k}}\pm\phi_0)$. Near the twist grain boundary and below the transition temperature of subdominant pair state we would, therefore, expect A_n and B_n to be both complex.

Another, more trivial explanation for a finite Josephson critical current at any twist angle would be the presence of a subdominant pair state with s-wave symmetry:

$$\Delta_n(\phi_{\mathbf{k}})=A_n\sqrt{2}\,\cos(2\phi_{\mathbf{k}}\pm\phi_0)+B_n,\quad (ds). \tag{16}$$

We will only consider the case that pairing takes place in at most two channels, so we can use A_n to designate the average amplitude of the dominant pair state and B_n to designate that of the subdominant pair state, which may have either $d_{x^2-y^2}$ or s symmetry. Since there appears to be no evidence for the presence of two or more order-parameter components in Bi2212 we shall study the variation of the order-parameter components and the Josephson critical current with layer index for several values of the temperature at which the transition to a two-component state takes place, including very low ones.

Even with these simplifying assumptions the numerical work required is considerable, because neither the angular integrals nor the sum over Matsubara frequencies can be performed analytically. As a first step we shall, therefore, take the approximations further and consider only the Ginzburg-Landau regime. To elucidate the qualitative effects that arise from the destruction of translational invariance along the c axis, this is probably sufficient. On the basis of the knowledge gained within the constraints of the Ginzburg-Landau approximation and in the light of available experimental data, one can then decide whether or not a full-scale weak-coupling calculation is worthwhile.

IV. LAWRENCE-DONIACH PHENOMENOLOGICAL MODEL

The Ginzburg-Landau theory of superconductivity has been generalized to layered materials by Lawrence and Doniach.[28] The corresponding equations for multicomponent unconventional pair states in the presence of a twist grain boundary are obtained by expanding the first term in Eq. (11) to third order in Δ_n while keeping only first-order contributions in Eqs. (A1) and (A2):

$$\Gamma_{\mathrm{coh}}(\omega,\Delta_n(\mathbf{k}'),\Delta_{n'}(\mathbf{k}'))=\frac{\Delta_{n'}(\mathbf{k}')-\Delta_n(\mathbf{k}')}{2|\omega|^3}, \tag{17a}$$

$$\Gamma_{\mathrm{inc}}(\omega,\Delta_n(\mathbf{k}'),\Delta_{n'}(\mathbf{k}''))=\frac{2[\Delta_{n'}(\mathbf{k}'')-\Delta_n(\mathbf{k}')]}{\omega^2}. \tag{17b}$$

The various frequency sums can now be performed:

$$\pi T\sum_{\omega}\frac{1}{\omega^2}=\frac{\pi}{4T}\equiv a_0(T), \tag{18a}$$

$$\pi T\sum_{\omega}\frac{1}{2|\omega|^3}=\frac{7\zeta(3)}{8\pi^2T^2}\equiv b_0(T), \tag{18b}$$

so that we obtain the following self-consistency equation:

$$\begin{aligned}\Delta_n(\phi_{\mathbf{k}})=N_{2D}(0)\int_0^{2\pi}\frac{d\phi_{\mathbf{k}'}}{2\pi}\lambda_n(\phi_{\mathbf{k}},\phi_{\mathbf{k}'})\Bigg\{&\Delta_n(\phi_{\mathbf{k}'})\ln\left(\frac{2\gamma\omega_D}{\pi T}\right)-b_0(T)\Delta_n(\phi_{\mathbf{k}'})|\Delta_n(\phi_{\mathbf{k}'})|^2\\&+\sum_{\substack{n'\\ \langle nn'\rangle}}|J|^2b_0(T)[\Delta_{n'}(\phi_{\mathbf{k}'})-\Delta_n(\phi_{\mathbf{k}'})]\\&+a_0(T)\sum_{\substack{n'\\ \langle nn'\rangle}}\int_0^{2\pi}\frac{d\phi_{\mathbf{k}''}}{2\pi}\pi N_{2D}(0)f_{\mathrm{inc}}(\phi_{\mathbf{k}'}-\phi_{\mathbf{k}''})[\Delta_{n'}(\phi_{\mathbf{k}''})-\Delta_n(\phi_{\mathbf{k}'})]\Bigg\},\end{aligned} \tag{19}$$

where we have introduced a cutoff ω_D for the divergent frequency sum. Inserting the two-component pair states Eq. (15) or Eq. (16) and using the expansion equation (7), the integrations with respect to $\phi_{\mathbf{k}''}$ and $\phi_{\mathbf{k}'}$ can be done. Linearizing the resulting equations and ignoring contributions from tunneling, one finds the bare transition temperatures T_{ci}^0:

$$\frac{1}{\lambda_i N_{2D}(0)}=\ln\left(\frac{2\gamma\omega_D}{\pi T_{ci}^0}\right) \tag{20}$$

with $i=A,B$. $\gamma=1.781$ is the exponential of Euler's constant. Using these relations to eliminate the coupling constants, the density of states, and the cutoff, we obtain as an intermediate step Eqs. (A3) in the Appendix.

The terms in these two equations are rearranged into two groups, one pertaining to layer n only, the other one representing coupling terms that vanish in the absence of the twist grain boundary, i.e., when the order parameters are identical on all the layers. Then the leading intralayer term will contain the factor

$$t_i=\ln(T/T_{ci})\approx(T-T_{ci})/T_{ci}, \tag{21}$$

where for either of the d-wave states, T_{ci} follows from

$$\ln(T_{ci}/T_{ci}^0)+a_0(T_{ci})[1/\tau_{\perp 0}-1/2\tau_{\perp 2}]=0. \tag{22}$$

$T_{ci}\approx T_{ci}^0-(\pi/4)\,[1/\tau_{\perp 0}-1/2\,\tau_{\perp 2}]$ represents the bulk transition temperature of a d-wave superconductor reduced from its ''bare'' value [Eq. (20)] by second-order incoherent tunneling.[39] This T_c reduction is mitigated by the d-wave part of the incoherent tunneling. Since d-wave scattering cannot enhance T_c, we require $1/[2\tau_{\perp 2}]<1/\tau_{\perp 0}$. This requirement appears reasonable in view of the fact that $f_{\rm inc}$ in Eq. (7) is positive definite. For the model considered by Graf *et al.*,[33] which emphasizes strong forward scattering, one finds $1/\tau_{\perp 2}\leqslant 1/\tau_{\perp 0}$. Ordinarily, however, we expect $1/\tau_{\perp 2}\ll 1/\tau_{\perp 0}$. The suppression of $\ell\neq 0$ superconductivity by nonmagnetic impurities[40,41] is obviously closely related, so that it is not surprising that Eq. (22) again describes the T_c reduction, provided the appropriately defined scattering times are sufficiently long. For the isotropic s-wave state considered here, incoherent tunneling does not lead to a T_c reduction (see the Appendix). In this paper we shall not consider the dependence of T_{ci} on $\tau_{\perp 0}$ and $\tau_{\perp 2}$ in any detail, instead we shall treat T_{cA} and T_{cB} as independent parameters.

After these remarks we can write down two sets of equations for the case that the pair state is a superposition of two d-wave states, Eq. (15):

$$0=t_AA_1+\tfrac{3}{2}\,b_0(T)[A_1|A_1|^2+\tfrac{2}{3}\,A_1|B_1|^2+\tfrac{1}{3}\,A_1^*B_1^2]$$
$$+\,\eta_d'(A_1-A_{-1}\cos 2\phi_0+B_{-1}\sin 2\phi_0)+\eta_d(A_1-A_2), \tag{23a}$$

$$0=t_BB_1+\tfrac{3}{2}\,b_0(T)[B_1|B_1|^2+\tfrac{2}{3}B_1|A_1|^2+\tfrac{1}{3}\,B_1^*A_1^2]$$
$$+\,\eta_d'(B_1-B_{-1}\cos 2\phi_0-A_{-1}\sin 2\phi_0)+\eta_d(B_1-B_2). \tag{23b}$$

For the superposition of d- and s-wave states, Eq. (16), we find

$$0=t_AA_1+\tfrac{3}{2}\,b_0(T)[A_1|A_1|^2+\tfrac{4}{3}\,A_1|B_1|^2+\tfrac{2}{3}A_1^*B_1^2]$$
$$+\,\eta_d'(A_1-A_{-1}\cos 2\phi_0)+\eta_d(A_1-A_2), \tag{24a}$$

$$0=t_BB_1+b_0(T)[B_1|B_1|^2+2B_1|A_1|^2+B_1^*A_1^2]$$
$$+\,\eta_s'(B_1-B_{-1})+\eta_s(B_1-B_2). \tag{24b}$$

Here, we have introduced the abbreviations

$$\eta_d=a_0(T)/(4\tau_{\perp 2})+|J|^2b_0(T), \tag{25a}$$

$$\eta_s=a_0(T)/(4\tau_{\perp 0})+|J|^2b_0(T). \tag{25b}$$

Writing η_d' and η_s' in front of the terms representing tunneling across the twist grain boundary we allowed for the possibility that tunneling matrix elements representing this process might be different. This possibility arises from the fact that the atomic orbitals entering in a microscopic calculation of the tunneling matrix elements would be rotated with the lattice. Depending on the anisotropy of the orbitals involved, their overlap will thus depend on the twist angle ϕ_0. In addition to this intrinsic effect, the quality of the interface could be different, especially if the samples were treated chemically or physically after cleavage and before fusing together to form the twist junctions. This possibility could be of great experimental importance, and will be discussed further in Sec. VIII.

Equations for an arbitrary set of neighboring planes n, $n\pm 1$ are obtained by setting $\phi_0=0$, $\eta=\eta'$, and by replacing the index 1 by n. Note, that Eqs. (23) are not symmetric with respect to the interchange of $+1$ and -1. To obtain the correct equations for A_{-1} and B_{-1} the sign of the twist angle ϕ_0 needs to be changed.

As anticipated, there is indeed no coupling for the $d_{x^2-y^2}$ state across a 45° twist grain boundary. However, if pairing in a d_{xy} state is possible, a linear coupling between these two pair states is caused by the twist that will lead to $B_1>0$ even for $T>T_{cB}$. No such linear coupling arises from a superposition of a d-wave and s-wave state. These conclusions are not altered when the coupling terms [Eqs. (A1) and (A2)] are expanded to third order, as one obtains the above forms of $\Gamma_{\rm coh}$ and $\Gamma_{\rm inc}$, multiplied by terms such as $|\Delta_n(\mathbf{k}')|^2$ and $|\Delta_{n'}(\mathbf{k}')|^2$, which are positive definite. Similarly, taking the perturbation theory with respect to the tunneling Hamiltonian to fourth order does not change the physics qualitatively. In particular, one does *not* get any linear Josephson coupling between s-wave and $d_{x^2-y^2}$-wave order parameters along the c axis.

In order to introduce dimensionless quantities and to reduce the number of parameters we normalize all order-parameter components with respect to

$$|A|^2=-\frac{2t_A}{3b_0(T)}\approx\frac{2}{3b_0(T_{cA})}\left(1-\frac{T}{T_{cA}}\right), \tag{26}$$

which is the solution of the above equations in the absence of the twist grain boundary and in the absence of additional pairing channels. We shall consider the regime $T_{cA}\geqslant T\geqslant 0.5T_{cA}$. For this temperature range we shall put the arguments in a_0 and b_0 [Eq. (18)] equal to T_{cA}, a constant, and use the approximation $t_A\approx T/T_{cA}-1$. The resulting approximate expression for the T dependence of $|A|^2$ actually agrees reasonably well at all temperatures with the result of the weak-coupling theory while the ''exact'' Ginzburg-Landau expression shows qualitatively different behavior at low T. We see from Eqs. (21), (23), and (24) that a small value of T_{cB} will give small real values for B_n. For $T_{cA} \geqslant T \gg T_{cB}$ we have $t_B \gg 1$ so that Eq. (23b) reduces to

$$B_1 = \frac{\eta_d'}{t_B} A_1 \sin 2\phi_0 \tag{27}$$

and $B_n \propto t_B^{-n}$. Using the approximate expression Eq. (21) would severely underestimate B_1 for $T_{cB} \leqslant T_{cA}$.

Writing X_n and Y_n for the normalized order-parameter components, Eqs. (23) are transformed into

$$0 = X_1 - X_1|X_1|^2 - \epsilon_d X_1|Y_1|^2 - 2\,\delta_d X_1^* Y_1^2 + \frac{\eta_d}{t_A}(X_1 - X_2) + \frac{\eta_d'}{t_A}(X_1 - X_{-1}\cos 2\phi_0 + Y_{-1}\sin 2\phi_0), \tag{28a}$$

$$0 = \frac{t_B}{t_A} Y_1 - \beta_d Y_1|Y_1|^2 - \epsilon_d Y_1|X_1|^2 - 2\,\delta_d Y_1^* X_1^2 + \frac{\eta_d'}{t_A}(Y_1 - Y_{-1}\cos 2\phi_0 - X_{-1}\sin 2\phi_0) + \frac{\eta_d}{t_A}(Y_1 - Y_2). \tag{28b}$$

The same transformations are applied to Eqs. (24).

As in the Lawrence-Doniach theory we have introduced here phenomenological parameters β, δ, ϵ which, in the weak-coupling theory developed above, have the values

$$\beta_d = \tfrac{3}{2}\,\beta_s = 1, \tag{29a}$$

$$\epsilon_d = \tfrac{1}{2}\,\epsilon_s = \tfrac{2}{3}, \tag{29b}$$

$$\delta_{d,s} = \tfrac{1}{4}\,\epsilon_{d,s}. \tag{29c}$$

Different values can result from strong-coupling effects.

From these equations one can construct a dimensionless Lawrence-Doniach free energy F_{LD} such that variations with respect to each of the order parameters and their complex conjugates reproduce the Lawrence-Doniach equations (28) as well as the equations for all other layers indices. Also, combinations of two d-wave states [Eq. (15)] can easily be treated simultaneously with the combination of d- and s-wave states [Eq. (16)]. We find

$$\begin{aligned} F_{LD} = &\sum_{n=1}^{N} (F_n + F_{-n}) \quad \text{(intralayer)} \\ &+ \sum_{n=1}^{N-1} (F_{n,n+1} + F_{-n,-n-1}) \quad \text{(interlayer coupling)} \\ &+ F_{-1,+1} \quad \text{(twist grain boundary coupling)}. \end{aligned} \tag{30}$$

with

$$F_n = -|X_n|^2 - \frac{t_B}{t_A}|Y_n|^2 + \tfrac{1}{2}\,|X_n|^4 + \beta_{d,s}\,\tfrac{1}{2}|Y_n|^4 + \epsilon_{d,s}|X_n|^2|Y_n|^2 + \delta_{d,s}(X_n^2 Y_n^{*2} + X_n^{*2} Y_n^2), \tag{31a}$$

$$-t_A F_{n,n+1} = \eta_d |X_n - X_{n+1}|^2 + \eta_{d,s}|Y_n - Y_{n+1}|^2, \tag{31b}$$

$$-t_A F_{-1,+1} = \begin{cases} \eta_d'(|[X_1 + X_{-1}]\sin\,\phi_0 - [Y_1 - Y_{-1}]\cos\,\phi_0|^2 + |[X_1 - X_{-1}]\cos\,\phi_0 + [Y_1 + Y_{-1}]\sin\,\phi_0|^2) & \text{for } dd, \\ \eta_d'(|X_1 - X_{-1}|^2\cos^2\phi_0 + |X_1 + X_{-1}|^2\sin^2\phi_0) + \eta_s'|Y_1 - Y_{-1}|^2 & \text{for } ds. \end{cases} \tag{31c}$$

For the dd case [Eq. (15)], $F_{-1,+1}$ can be obtained from an obvious generalization of the standard Lawrence-Doniach coupling energy

$$F_{-1,+1} \propto \eta_d' \int \frac{d\phi_{\mathbf{k}}}{2\pi} |\Delta_1(\phi_{\mathbf{k}}) - \Delta_{-1}(\phi_{\mathbf{k}})|^2. \tag{32}$$

However, such is not the case for the ds state. If it [Eq. (16)] is inserted in Eq. (32), one cannot obtain Eq. (31c) with the coupling parameters η_d' and η_s' different from one another.

F_{LD} remains the same if we change ϕ_0 from zero to $\pi/2$, provided the signs of X_n and Y_n for all $n \leqslant -1$ are changed. The same is true if we replace an arbitrary ϕ_0 by $\pi/2 - \phi_0$. To render $F_{-1,+1}^{(dd)}$ invariant, we also have to change the sign of ϕ_0 taking into account the fact that one is now rotating the sample sections in opposite directions. The effect of a twist grain boundary for tetragonal systems is thus seen to be symmetric with respect to the twist angle $\phi_0^{\max} = \pi/4$. Henceforth, we shall only consider the range $0 \leqslant \phi_0 \leqslant \pi/4$.

The free energy describing the twist grain-boundary coupling is not symmetric with respect to the interchange of layer indices in the dd case, unless $X_1 = X_{-1}$ and $Y_1 = Y_{-1}$. This choice, however, does not minimize $F_{-1,+1}$ for $\phi_0 \neq 0$. In order to justify the use of the pair state, Eq. (15), we have already argued that Re Y_n should be antisymmetric to alleviate the strain introduced by the twist grain boundary. In general, we have $F_{-1,+1}(\phi_0) = F_{+1,-1}(-\phi_0)$, consistent with our discussion below [Eq. (23)]. $F_{-1,+1}$ is, however, invariant if we substitute (X_{-1}^*, X_{+1}^*) for (X_{+1}, X_{-1}) and $(-Y_{-1}^*, -Y_{+1}^*)$ for (Y_{+1}, Y_{-1}). The intralayer terms F_n and terms describing the interlayer coupling on either side of the twist are obviously invariant under this substitution. We thus conclude that the solutions of the Lawrence-Doniach equations for the dd case have the symmetry

$$\begin{aligned} X_{-n} &= X_n^*, \\ Y_{-n} &= -Y_n^*, \end{aligned} \tag{33}$$

for all $1\leqslant n\leqslant N$. This conclusion can also be reached by studying the Lawrence-Doniach equations for the real and imaginary parts of the order parameters, for which the computer code was written, and it is supported by the results of our numerical calculations. For $\pi/2\geqslant\phi_0\geqslant\pi/4$, the minus sign would appear in the relation for the dominant order parameter. Using this symmetry, $F_{-1,+1}$ reduces to

$$F^{(dd)}_{-1,+1}=-\frac{4\eta'_d}{t_A}\{|X'_1\sin\phi_0-Y'_1\cos\phi_0|^2+|X''_1\cos\phi_0+Y''_1\sin\phi_0|^2\},\qquad(34)$$

where a prime (double prime) denotes the real (imaginary) part. We see that, with $X''_1=-Y''_1\tan\phi_0$ and $Y'_1=-X'_1\tan\phi_0$, $F^{(dd)}_{-1,+1}$ would vanish for any ϕ_0. No such cancellation can occur for $F^{(ds)}_{-1,+1}$ so that the only way to reduce this (positive) contribution to the free energy is to suppress the d-wave order parameter near the grain boundary, while the (isotropic) s-wave order parameter, unaffected by the presence of the twist grain boundary, should show the bulk behavior $Y_{-n}=Y_n$.

A complication can be expected in the dd case at temperatures $T<T_{cB}$ and for $\delta_d<0$. Then the subdominant order parameter is real and finite for all twist angles. To minimize $F^{(dd)}_{-1,+1}$ it would need to have the symmetry $Y_1=Y_{-1}$ for $\phi_0=0$ and $Y_1=-Y_{-1}$ for $\phi_0=\pi/2$.

V. CRITICAL CURRENT

Following the original work of Josephson[42] and that of Ambegaokar and Baratoff,[30] as described in detail by Mahan,[43] we calculate the time rate of change of the fermion number operator on layer n: $N_n=\Sigma_\sigma\Sigma_{\mathbf{p}}c^\dagger_{\mathbf{p}n\sigma}c_{\mathbf{p}n\sigma}$. Only tunneling to one of the two neighboring layers is considered because otherwise the tunnel current, defined as $I_n(t)=-e\langle\dot N_n\rangle(t)$, would vanish. $\langle\dot N_n\rangle(t)$ is evaluated using linear response theory with respect to the tunneling Hamiltonian, Eq. (3). The resulting dc Josephson current can be expressed most conveniently as a sum over Matsubara frequencies:

$$I^J_n=4e\ \mathrm{Im}\int\frac{d^2\mathbf{k}}{(2\pi)^2}\int\frac{d^2\mathbf{k}'}{(2\pi)^2}[|J|^2\delta^{(2)}(\mathbf{k}-\mathbf{k}')+f_{\mathrm{inc}}(\mathbf{k}-\mathbf{k}')]T\sum_\omega\mathcal{F}^0_n(\mathbf{k},\omega)\mathcal{F}^{0\dagger}_{n\pm1}(\mathbf{k},\omega),\qquad(35)$$

where the upper (lower) sign corresponds to $n\geqslant1$ ($n\leqslant-1$). The Josephson current I^J_0 across the twist is obtained from $\mathcal{F}^0_1\mathcal{F}^{0\dagger}_{-1}$. The commonly used step to revert to real frequencies requires some caution when the order parameter is complex because the spectral representation of the anomalous Green's function needs to be generalized. Inserting the bare Green's functions [Eq. (10)] and performing the integral with respect to energy ξ_0 gives for the case of coherent tunneling between neighboring layers,

$$I^{J,\mathrm{coh}}_n=2e[2\pi N_{2D}(0)]|J|^2\ \mathrm{Im}\int\frac{d\phi_{\mathbf{k}}}{(2\pi)}T\times\sum_\omega\frac{\Delta_n(\phi_{\mathbf{k}})\Delta^*_{n\pm1}(\phi_{\mathbf{k}})}{D_{n\pm1}(\mathbf{k},\omega)D_n(\mathbf{k},\omega)[D_{n\pm1}(\mathbf{k},\omega)+D_n(\mathbf{k},\omega)]},\qquad(36)$$

where $D_n(\mathbf{k},\omega)$ has been defined in Eq. (12). This expression with a layer index and $\phi_{\mathbf{k}}$-independent Δ was given previously.[35] If the tunneling is incoherent, the two Green's functions are integrated separately with respect to energy so that the corresponding expression is

$$I^{J,\mathrm{incoh}}_n=e[2\pi N_{2D}(0)]^2\ \mathrm{Im}\int\frac{d\phi_{\mathbf{k}}}{2\pi}\int\frac{d\phi_{\mathbf{k}'}}{2\pi}f_{\mathrm{inc}}(\mathbf{k}-\mathbf{k}')T\times\sum_\omega\frac{\Delta_n(\phi_{\mathbf{k}})\Delta^*_{n\pm1}(\phi_{\mathbf{k}'})}{D_n(\mathbf{k},\omega)D_{n\pm1}(\mathbf{k}',\omega)}.\qquad(37)$$

We see that in this case of a layered compound different assumptions with respect to the tunneling process lead to different temperature dependences of the Josephson current. These differences may be relevant to the intrinsic voltage steps observed in various high-temperature superconductors.[44,45] This is also true for c-axis break junctions between two layered superconductors with sufficiently weak intrinsic interlayer coherent tunneling,[46] as seen in recent experiments.[24] However, this is not the case when the Josephson effect between two half-spaces filled with three-dimensional superconductors is considered.[30,47] When one assumes the tunneling matrix element to be completely independent of momentum,[30] the result given above for incoherent tunneling with $f_{\mathrm{inc}}=\mathrm{const}$ is obtained. If momentum conservation parallel to the tunnel barrier is assumed,[47] one is still left with two integrations with respect to the momenta perpendicular to the barrier. Since those particles moving perpendicular to the barrier are most likely to tunnel, $k_\parallel$ is neglected in the arguments of the Green's functions so that integrating with respect to $k_\parallel$ simply leads to an effective tunneling matrix element.[47] The remaining integrals with respect to $k_\perp$ and $k'_\perp$ are, with the usual approximations, formally identical to the energy integrals evaluated in the case of incoherent tunneling.

In the Ginzburg-Landau regime we can approximate $D_n(\mathbf{k},\omega)$, Eq. (12), by $|\omega|$ so that the frequency sum in Eq. (36) and Eq. (37) can be performed. For the combination of two d-wave states given in Eq. (15) we find for the total Josephson current across the twist grain boundary

$$I^J_0=4eN_{2D}(0)\eta'_d\ \mathrm{Im}\{(A_1A^*_{-1}+B_1B^*_{-1})\cos2\phi_0-(A_1B^*_{-1}-B_1A^*_{-1})\sin2\phi_0\}.\qquad(38)$$

The corresponding result for the combination of a $d_{x^2-y^2}$ state and an s-wave state given in Eq. (16) reads

$$I^J_0=4eN_{2D}(0)\mathrm{Im}\{\eta'_dA_1A^*_{-1}\cos2\phi_0+\eta'_sB_1B^*_{-1}\}.\qquad(39)$$

The current between any other pair of neighboring layers is formally obtained from these equations by setting $\eta'_d=\eta_d$, $\eta'_s=\eta_s$, $\phi_0=0$, and by replacing $(1,-1)$ by any pair $(n,n\pm1)$ of positive (upper) or negative (lower) integers.

The order-parameter amplitudes A_n and B_n are calculated from Eq. (28) which describes a large but finite stack of Josephson coupled superconducting layers. Without attaching current leads, no net current can flow perpendicular to the layers so that I_n^J must vanish for all n. This means that the expression inside the braces must be real, even though A_n and B_n may be complex. We can thus interpret the expressions on the right-hand sides of Eq. (38) and Eq. (39) without the imaginary part being taken as the *critical Josephson current* I_n^{JC}.

The incoherent contribution to the s-wave channel I_0^{JC} is $eN_{2D}(0)[a_0(T)/\tau_{\perp 0}]B_1B_{-1}^*$, which is exactly the same as that obtained by Ambegaokar and Baratoff.[30] Calculating the quasiparticle current in the normal state within the same approximations and taking into account only incoherent tunneling we find

$$I_n^{qp}(\text{incoh}) = 2eN_{2D}(0)\frac{1}{\tau_{\perp 0}}eV, \tag{40}$$

so that $1/\tau_{\perp 0}$ can be expressed in terms of the normal-state resistance. Including coherent tunneling in the Ginzburg-Landau regime only changes the constant of proportionality between I_0^{JC} and $B_1B_{-1}^*$. However, according to Eqs. (36) and (37) we can expect different temperature dependencies of $I_0^{JC}(\text{coh})$ and $I_0^{JC}(\text{incoh})$ outside the Ginzburg-Landau regime. In particular, at $T=0$ one finds that $I_0^{JC}(\text{incoh})$ is proportional to the order-parameter amplitude[30] while $I_0^{JC}(\text{coh})$ turns out to be independent of this quantity. Calculations of the normal-state quasiparticle current from coherent tunneling between neighboring layers yields[43]

$$I_n^{qp}(\text{coh}) = \frac{eN_{2D}(0)|J|^2}{\pi^2}\frac{2\Gamma eV}{(eV)^2+(2\Gamma)^2}. \tag{41}$$

Conserving energy and momentum during the coherent tunneling process at finite voltages V requires the presence of some intralayer scattering, parametrized by a scattering rate Γ. Note that the coherent quasiparticle current is only Ohmic for $eV \ll \Gamma$.

If quasiparticle tunneling between two superconducting half-spaces across a planar interface is considered,[47] it is not necessary to invoke quasiparticle scattering in either of the superconductors. As in the case of Josephson tunneling discussed above, the additional degree of freedom represented by the momentum perpendicular to the tunneling barrier leads for two three-dimensional superconductors to a result for the quasiparticle tunneling current formally identical with that obtained from incoherent tunneling. However, qualitatively new results are obtained for c-axis break junction tunneling between two quasi-two-dimensional layered superconductors with sufficiently narrow c-axis band dispersions.[46] In either case, however, if we had included intralayer scattering in the bare Green's functions, Eq. (10), Γ would have appeared in the coefficients $a_0(T)$ and $b_0(T)$ in Eq. (18). But, since $\Gamma \approx T_c$ at T_c and decreases rapidly below T_c, the changes in a_0 and b_0 resulting from the presence of intralayer quasiparticle scattering are expected to be small and confined to the vicinity of T_c. As a consequence, the coherent contribution to the Josephson critical current is not related to the coherent quasiparticle current. The connection between I_n^{JC} and R_n is even more remote for d-wave superconductors because here the Josephson current arising from incoherent tunneling involves the parameter $\tau_{\perp 2}$, which can be very different from $\tau_{\perp 0}$ appearing in Eq. (40).

VI. BOUNDARY CONDITIONS

The influence of the twist grain boundary should be restricted to some limited number of adjoining layers so that on the extremal layers $n=\pm N$ of a large $(N \gg 1)$ but finite stack considered in the numerical calculations the order parameters should attain their bulk values X_∞ and Y_∞, which are characterized by their independence of the layer index n. If $T_{cA}^0 > T > T_{cB}^0$, Eq. (20), only the dominant order parameter, Eq. (26), is present. Because of our normalization we have the simple boundary condition

$$\begin{aligned} X_N &= X_{-N} = 1, \\ Y_N &= Y_{-N} = 0, \end{aligned} \tag{42}$$

for twist angles $\phi_0 \leqslant \pi/4$.

At sufficiently low temperatures the subdominant order parameter becomes nonvanishing. From Eq. (31a) it is obvious that for $\delta_{d,s} > 0$ the free energy is minimized if the phase difference between X_∞ and Y_∞ is $\pm\pi/2$, corresponding to a pair state with an anisotropic but nodeless energy gap. For $\delta_{d,s} < 0$ the phase difference is zero. Since the overall phase factor is arbitrary we can choose X_∞ real and Y_∞ real or imaginary, depending on the sign of $\delta_{d,s}$. For all the cases under discussion, X_∞ and Y_∞ can be determined from Eq. (28) with all interlayer coupling terms removed,

$$\begin{aligned} 0 &= 1 - X_\infty^2 - \gamma|Y_\infty|^2, \\ 0 &= \frac{t_B}{t_A} - \beta|Y_\infty|^2 - \gamma X_\infty^2, \end{aligned} \tag{43}$$

where

$$\begin{aligned} \gamma &= \epsilon_{d,s} - 2|\delta_{d,s}| \\ &= \tfrac{1}{2}\epsilon_{d,s} \quad \text{for weak coupling.} \end{aligned} \tag{44}$$

The weak-coupling expressions for the parameters are given in Eq. (29). The equations for X_∞^2 and $|Y_\infty|^2$ are easily solved with the results

$$\begin{aligned} |Y_\infty|^2 &= \frac{t_B - \gamma t_A}{-t_A(\gamma^2 - \beta)}, \\ X_\infty^2 &= 1 - \gamma|Y_\infty|^2. \end{aligned} \tag{45}$$

The transition temperature $T_{cB}^<$, below which Y_∞ becomes finite, follows from the condition $t_B - \gamma t_A = 0$, which gives

$$\frac{T_{cB}^<}{T_{cA}} = \frac{T_{cB}}{T_{cA}}\frac{1-\gamma}{1-\gamma\dfrac{T_{cB}}{T_{cA}}}. \tag{46}$$

As compared with the bulk transition temperature, $T_{cB}^<$ is reduced by the presence of the dominant order parameter.

For $\delta_{d,s}>0$ it would seem natural to use the boundary condition $X_{\pm N}=X_\infty$ and $Y_{\pm N}=i|Y_\infty|$, in agreement with the symmetry requirement, Eq. (33). When the Lawrence-Doniach equations for the dd case are solved with these boundary conditions, one finds a finite Josephson current across the sample that is unphysical. The source of this problem is that, with a complex d-wave order parameter locking onto the lattice, there exists a finite average phase difference across the twist grain boundary. The unphysical Josephson current can be made to vanish by compensating for this average phase difference. The correct boundary conditions are, therefore,

$$X_{\pm N}=X_\infty e^{\pm i\theta_\infty},\qquad Y_{\pm N}=i|Y_\infty|e^{\pm i\theta_\infty}, \tag{47}$$

where

$$\theta_\infty=-\frac{1}{2}\tan^{-1}\left(\frac{2\tan 2\phi_0 X_\infty|Y_\infty|}{X_\infty^2+|Y_\infty|^2}\right). \tag{48}$$

For $\phi_0=\pi/4$ one finds $\theta_\infty=-\pi/4$. The sign of the phase angle is such that $X''_{+N}<0$, in agreement with the discussion below Eq. (34). It is clear from Eq. (39) that no such problems arise for the ds case [Eq. (16)], so that we can take the phase $\theta_\infty=0$ for all twist angles ϕ_0.

The situation is even more complex in the dd case with $\delta_d>0$ for temperatures in the range $T_{cB}^{<}\leq T\leq T_{cB}$, where $Y_\infty=0$. It would appear that one possible solution would be to have both X_n and Y_n real for all n. However, since the dominant order parameter is suppressed near the twist grain boundary, it is less effective in suppressing the subdominant order parameter. We can thus expect to find a complex subdominant order parameter for small layer indices. A complex Y_n varying from layer to layer results in a finite Josephson current. This is compensated by a finite imaginary part X''_n. While $\lim_{n\to\infty}Y_n=0$, there is no reason for X''_∞ to vanish, because the phase of the dominant order parameter on either side of the twist grain boundary is arbitrary. Imposing $X''_{\pm N}=0$ has the consequence that X''_n varies linearly with n when Y_n is already negligible. This, again, results in an unphysical Josephson current, which has to be removed by a judicious choice of the phase for the dominant order parameter. For $\phi_0=\pi/4$ one can see from Eq. (38) that $I_1^J=0$ if we put $\theta_\infty=-\pi/4$. For arbitrary twist angles ϕ_0 there seems to be no analytic result for θ_∞.

VII. NUMERICAL RESULTS AND DISCUSSION

Across the twist grain boundary we expect a destructive proximity effect on the dominant order parameter. This is clearly seen in Fig. 2(a), which shows the suppression of the dominant $d_{x^2-y^2}$ order parameter for various temperatures well above the transition temperature to a two-component pair state. For the twist angle we have chosen the extremal value $\phi_0=45°$. We see that for high temperatures the suppression relative to the bulk value is very large and extends across many layers. As the temperature is reduced, the suppression of the order parameter on the layers forming the twist grain boundary becomes less severe and the number of layers affected becomes smaller. The latter effect simply reflects the temperature dependence of the coherence length.

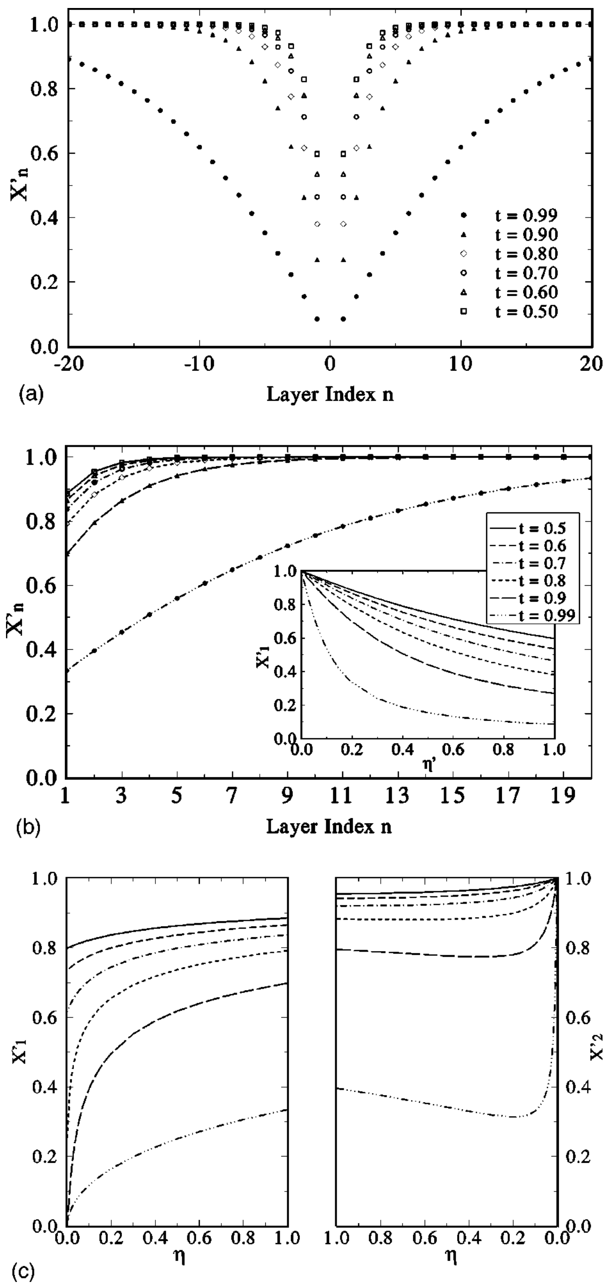

FIG. 2. (a) The real amplitude of the dominant order parameter $d_{x^2-y^2}$ [Eq. (15)], normalized to its bulk value [Eq. (26)], as a function of the layer index n for various reduced temperatures. The transition temperature for the subdominant order parameter has been taken as $T_{cB}=0.2T_{cA}$. Other parameters are $\epsilon_d=0.5$, $\delta_d=0.05$, and $\phi_0=45°$. For these parameters one obtains $T_{cB}^{<}=0.1304T_{cA}$ from Eq. (46). The Josephson coupling constants in Eq. (25a) are $\eta=\eta'=1$. (b) Same as (a), but for $\eta'=0.2$. The inset shows X'_1 as a function of η' for $\eta=1$ for the same set of reduced temperatures. (c) The real amplitude of the dominant order parameter $d_{x^2-y^2}$ [Eq. (15)], normalized to its bulk value [Eq. (26)], on layer 1 (left panel) and layer 2 (right panel) as a function of the bulk Josephson coupling constant η for $\eta'=0.2$, $\phi_0=45°$, and for the same set of reduced temperatures.

In these calculations we have chosen rather large values $\eta=\eta'=1$ for the coupling constants [Eq. (25)]. Such values would lead to a substantial T_c suppression, Eq. (22), unless the tunneling is predominantly coherent. As explained in Sec. V, these parameters cannot be estimated from the normal-state resistivity. Only measurements of the interplanar critical Josephson current could provide some information which, however, would still be rather ambiguous because of the uncertainty in the two-dimensional density of states. An independent measurement of the constant η', which describes coupling across the twist grain boundary, seems to be completely out of the question. However, it can be varied in some controlled way in the experimental sample preparation.

If anything, η' is likely to be smaller than η, so in Fig. 2(b) we show results similar to those in Fig. 2(a) but for $\eta=1$ and $\eta'=0.2$. The suppression of the order parameter is much reduced, as one would expect, since for $\eta'=0$ there would be no proximity effect. The inset shows the order parameter on layer 1 for $\eta=1$ as a function of η' for various temperatures. The number of layers affected remains largely the same, bearing in mind the overall reduction of the proximity effect. A different type of behavior can be expected only if we change the coupling constants η. In Fig. 2(c) we therefore show X' on layers 1 and 2 as functions of η for several temperatures. The left panel shows that if $\eta=0$, X_1' is vanishingly small at high temperatures because the intralayer condensation energy [Eq. (31a)] vanishes as $(1-t)^{3/2}$ while the coupling energy [Eq. (31c)] varies as $(1-t)^{1/2}$. Since we have chosen a fairly small value $\eta'=0.2$, the intralayer contribution soon becomes more important than the coupling term when the temperature is lowered. As one increases η, X_1' increases, because it is pulled up by the neighboring layer towards the bulk value $X_1'=1$. The left panel shows what happens on the second layer. If this is decoupled from the first layer, we simply find the bulk value. Turning on the coupling constant η allows the twist grain boundary to make itself felt on this more distant layer. The proximity effect on layer 2 at high temperatures is largest for $\eta\approx\eta'$.

Independent of the coupling constant η', the Josephson critical current across the twist grain boundary is, according to Eqs. (38) and (39), proportional to $\cos 2\phi_0$ and hence vanishes for $\phi_0=45°$ when only the order parameter $d_{x^2-y^2}$ is present. The proximity effect just discussed has the consequence that in addition to the junction between layers -1 and $+1$ several other junctions are driven normal at currents well below the bulk critical current. This means that the resistance should vary rapidly with the applied current, which would make it easier to identify a $d_{x^2-y^2}$ order parameter through the effect of a twist grain boundary. It is conceivable that the spatially varying suppression of the d-wave order parameter resulting from a lattice mismatch contributes significantly to the nonlinearity in the current response frequently observed in high-T_c materials. The proximity effect between d-wave states rotated relative to one another also affects the quasiparticle density of states that one might be able to study using scanning tunneling spectroscopy.

Probably the most interesting aspect of the present theory is the creation of a subdominant d-wave order parameter by the strain associated with the twist grain boundary, which would render the Josephson critical current finite even for a 45° twist. This process is, however, possible only if the pairing interaction, characterized by a bare transition temperature T_{cB}^0, is finite. On the other hand, if one assumes that the penetration depth measurements,[48] exhibiting linear-in-T behaviors at low T, are related to nodes in the superconducting order parameter, then one would need to have the actual T_{cB} very small, indeed.

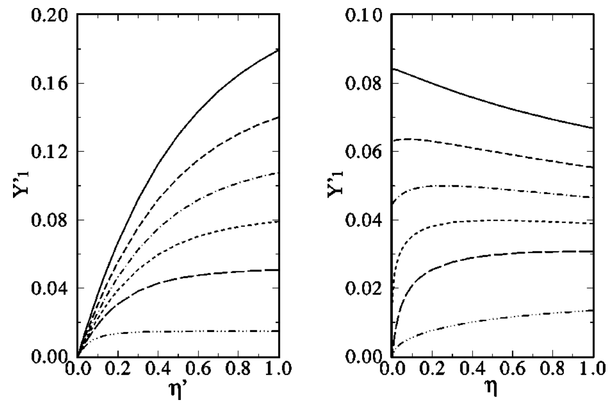

FIG. 3. The real amplitude of the subdominant order parameter d_{xy} [Eq. (15)], normalized to the bulk value [Eq. (26)] of the dominant order parameter, on layer 1 for $\phi_0=45°$ and the same set of temperatures considered in Fig. 2. The left panel shows Y_1' as a function of η' for $\eta=1$. The right panel shows Y_1' as function of η for $\eta'=0.2$.

We shall begin our discussion with choosing $T_{cB}/T_{cA}=0.2$, which is large enough to make the expected effects clearly visible but small enough to make the observation of a second superconducting transition in the bulk material unlikely. This value for T_{cB} is well below the temperatures T for which we can trust our Ginzburg-Landau approximation to give reliable results. We shall, therefore, only consider the regime $T>T_{cB}$ for which both order parameters are real. The results for the normalized dominant order parameter X_n' shown in Fig. 2 for $0.5T_{cA}\leqslant T\leqslant T_{cA}$ were, in fact, obtained for this finite value of T_{cB}. Reducing T_{cB} to zero has the effect of making the suppression of X_n' on layers close to the twist grain boundary even more pronounced. For $T_{cB}=0$, X_1' is found to be some 20% lower than the results shown in Fig. 2(a). According to Eq. (33) we expect the real part of the subdominant order parameter to be odd with respect to the layer index and this is indeed what we find. In Fig. 3 (left panel) we plot Y_1' as a function of the parameter η_d', Eq. (25a), which characterizes the strength of the coupling across the twist. To describe the coupling between pairs of layers on either side of the twist, we have chosen $\eta=1$. It is clear from Eq. (31c) that Y_1' must be zero for $\eta'=0$. The increase in Y_1' with increasing η' depends quite sensitively on temperature, because the cost in intralayer energy and interlayer coupling energy resulting from the generation of the subdominant order parameter is reduced as one approaches the transition temperature T_{cB}.

The right panel of Fig. 3 shows the η dependence of Y_1'. At the lowest temperature $0.5T_{cA}$, Y_1' (solid line) decreases as the coupling to more distant layers is increased because sufficiently far from the twist Y_n' must vanish. We find, in fact, that for the parameters used here Y_n' decreases very rapidly with layer index. For the higher temperatures, Y_1' initially increases with η. This is due to the fact that the

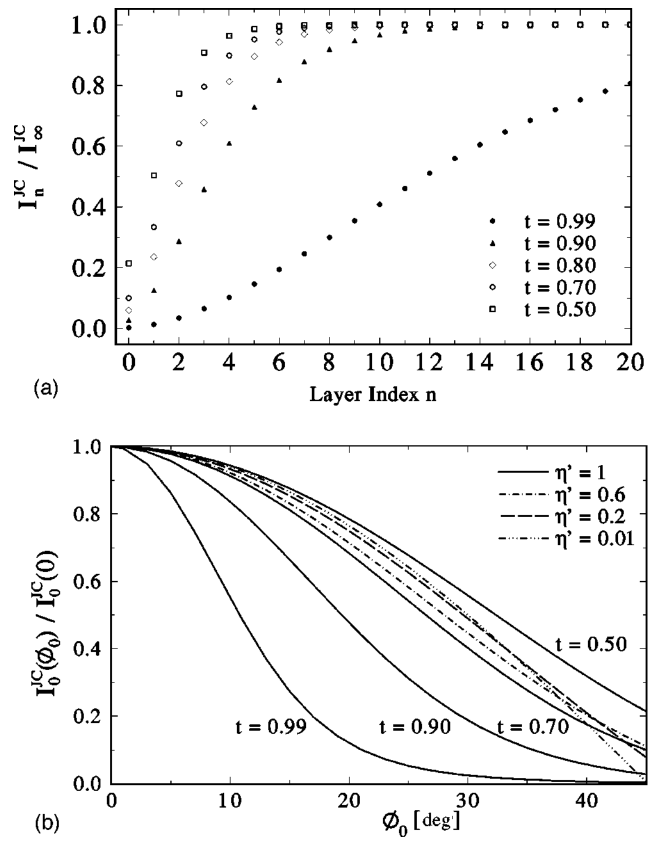

FIG. 4. (a) The Josephson critical current [Eq. (38)] with $\eta_d = \eta'_d$ between neighboring pairs of layers with $\phi_0 = 45°$, normalized by its value in the bulk. The layer index 0 designates the junction formed by the twist grain boundary between layers -1 and $+1$, and the layer index 1 designates the junction between layers 1 and 2, etc. Because I_n^{JC} is symmetric, we only show results for junctions on one side of the twist grain boundary. Parameters are the same as in Fig. 2(a). (b) The Josephson critical current [Eq. (38)] as function of the twist angle ϕ_0, normalized by its value at $\phi_0 = 0°$, for several reduced temperatures and $\eta' = 1$ (solid lines). The other parameters are the same as in Fig. 2(a). The various dashed lines show the changes in this angular dependence at $t = 0.7$ as η' is lowered.

finite value of Y'_1 arises from minimizing the free-energy contribution [Eq. (31c)], so that Y'_1 must scale with X'_1. For $T_{cB} \ll T_{cA}$ we have the analytic result, Eq. (27). Comparing with the left panel of Fig. 2(c), we see that such a relation between X'_1 and Y'_1 persists to much larger values of T_{cB}. It is for the same reason that the maximum of Y'_1 does not occur for the twist angle $\phi_0 = 45°$. At the highest temperature considered a broad maximum is found at around $\phi_0 = 12°$. As the temperature is lowered, this maximum shifts to larger twist angles and at $T = 0.5T_{cA}$ it is found near $\phi_0 = 37°$.

In Fig. 4(a) we show the Josephson critical current Eq. (38) between neighboring pairs of layers. The prefactor $4eN_{2D}(0)\eta_d$ in Eq. (38) has been omitted and the order-parameter amplitudes have been normalized, so that $\lim_{n\to\infty} I_n^{JC} = 1$ at all temperatures for which the subdominant order parameter vanishes in the bulk. Since $\phi_0 = 45°$, the finite value of I_0^{JC} is entirely due to the subdominant order parameter Y_1. For very low T_{cB} we can estimate Y_1 from Eq. (27). The normalized I_0^{JC} [Eq. (38)] reduces to $2X_1Y_1$ and thus depends linearly on the small parameter t_B^{-1}. Even for T_{cB}/T_{cA} as low as 0.001 we find $I_0^{JC} = 0.067$ for $\eta' = 1$ and temperatures low enough (e.g., $0.5T_{cA}$) such that X_1 is a sizable fraction ($X_1 = 0.524$ in this case) of its bulk value.

We see from Fig. 4(a) that, depending on the temperature, the Josephson critical current can be suppressed on a fair number of junctions. Unlike I_0^{JC}, I_n^{JC} for $n \geq 1$ is primarily determined by the dominant order parameter, which is seen from the inset of Fig. 2(b) to vary substantially with η'. The number of junctions with severely suppressed I^{JC} would thus be smaller for smaller η'. Remember that large values of η and η' are compatible only with coherent tunneling. From Fig. 2(c) we can infer that, at least at the lower end of our temperature scale, a variation of I_n^{JC}, $n \geq 1$, through the dependence of X'_n on η, is not very significant.

Figure 4(b) shows the dependence of I_0^{JC} on the twist angle ϕ_0 for several reduced temperatures and $\eta' = 1$ (solid lines). The other parameters are the same as in Fig. 2(a). Also shown is I_0^{JC} as a function of ϕ_0 for several values of η' at $t = 0.7$. The curve for $\eta' = 0.01$ is indistinguishable from $\cos 2\phi_0$, which is the dependence on twist angle expected at any temperature if only the dominant order parameter, unaffected by the proximity effect, were present.

So far we have not shown how the results depend on the parameters ϵ and δ that describe the strength of coupling between the dominant and the subdominant order parameter. The values used actually differ from the weak-coupling result [Eq. (29)]. We did change ϵ to 2/3 [Eq. (29b)] and varied δ between $+\epsilon/4$ and $-\epsilon/4$. Even changing the sign of δ, which would favor a real subdominant order parameter, has little effect on the results presented so far. The changes are at most a few percent and would be barely visible in these figures.

For the temperatures $T_{cA} > T > T_{cB}$ considered so far, the combination Eq. (16) of d- and s-wave order parameters only leads to the trivial solution $B_n = 0$ for all n and $I_0^{JC}(\phi_0 = 45°) = 0$. The proximity effect on A_n is the same as in the dd case discussed above with $T_{cB} = 0$.

The only other really relevant parameter, in addition to η and η', therefore is the strength of pairing in the subdominant channel, parametrized by T_{cB}. Results for the ds case with $T_{cB}/T_{cA} = 0.9$ are presented in Fig. 5, which shows the bulk solutions and the solutions on layer 1 together with I_0^{JC} as a function of temperature for the maximum twist angle $\phi_0 = 45°$. For this value of T_{cB} we obtain from Eq. (46) $T_{cB}^{<} = 0.8571T_{cA}$. At this temperature the bulk s-wave order parameter Y_∞ sets in with the usual square-root behavior while X_∞ drops with a discontinuity in slope.

As in the dd case with $T > T_{cB}$ it suffices to consider only two order-parameter amplitudes, X_n, which is chosen to be real, and Y_n, which is real or imaginary depending on the sign of δ_s in Eq. (31a). The phase is of no consequence here, since we consider the coupling between layers and the Josephson current only to lowest order in the order-parameter amplitudes. The difference between a time-reversal breaking state $d + is$ without nodes in the energy gap and a real combination $d + s$ with nodes can be expected to show up at low temperatures.

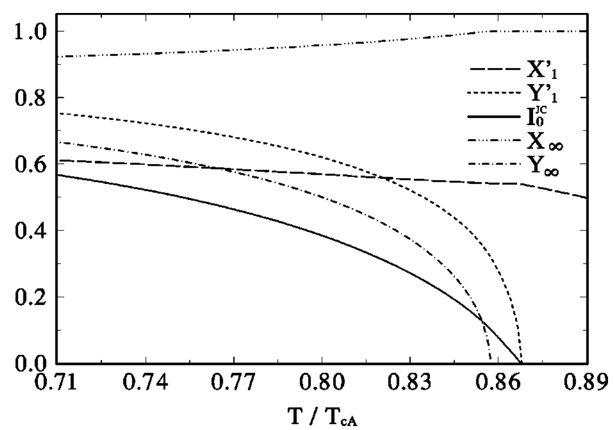

FIG. 5. Order-parameter components on layer 1 and in the bulk for the sd combination [Eq. (16)] as a function of temperature in the vicinity of the s-wave transition temperature. Also shown (solid line) is $I_0^{JC}(\phi_0)/I_0^{JC}(0)$, Eq. (39). The parameters are $T_{cB}/T_{cA}=0.9$, $\beta=1$, $\eta_d=\eta_d'=\eta_s=\eta_s'=0.2$, and $\phi_0=45°$.

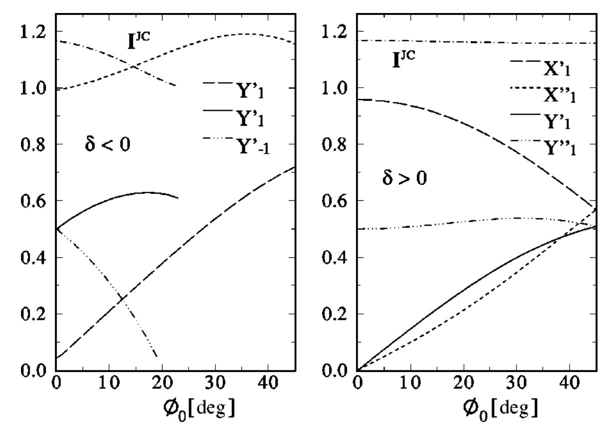

FIG. 6. The left panel shows the amplitude $Y'_{\pm 1}$ of the subdominant d-wave order parameter on layers 1 and -1 as a function of ϕ_0 for the case of a real dd superposition. The two solutions shown have different symmetries with respect to the layer index. In the right panel, the two d-wave order parameters differ in phase by $\pi/2$. The symmetry of these states is given in Eq. (33). $I^{JC}(\phi_0)$ is included in both panels. It is normalized to unity at $\phi_0=0$ when only a single order parameter is present. The parameters are $T_{cB}=0.9T_{cA}$, $T=0.8T_{cA}$, $\beta=1$, $\epsilon=1/3$, $\delta=\pm\epsilon/4$, and $\eta=\eta'=1$.

For the parameters chosen, X_1 at T_{cB} is reduced through the proximity effect to about half its bulk value. Equation (43) with X_∞ replaced by $X_1<X_\infty=1$ shows why the transition temperature for Y_1 is found to be higher than $T_{cB}^<$. An accurate estimate of this transition temperature is not possible because the coupling to outer layers also serves to suppress Y_1. It is only in this rather indirect way that the twist grain boundary has an effect on an isotropic subdominant s-wave order parameter. Note that, unlike X_∞, X_1 continues to grow with decreasing temperature, even after the onset of Y_1. This temperature variation of X_1 has been discussed extensively in connection with Fig. 2.

At $\phi_0=45°$ the Josephson current is carried solely by the s-wave component of the condensate so that, unlike the dd case considered above, I_0^{JC} is finite only below temperatures at which Y_1 is finite. At temperatures not very far below $T_{cB}^<$, Y_1 and X_1 are comparable in size. Since from our discussion of the tunneling matrix elements we would expect $\eta_s'\gg\eta_d'$, the Josephson current would flow primarily in the s channel at any twist angle so that I_0^{JC} would show little variation with ϕ_0 except very close to $T_{cB}^<$. This explanation for the absence of a strong variation of I_0^{JC} with twist angle implies, however, a substantial deviation in the nodal structure of the order parameter in the bulk material from that of the $d_{x^2-y^2}$ state.

Finally, we consider the case of two coexisting d-wave states, Eq. (15). As before, we choose $T_{cB}/T_{cA}=0.9$ and consider the temperature $T=0.8T_{cB}<T_{cB}^<=0.8571T_{cA}$. $T_{cB}^<$ is the same as for the ds case because we use the same parameter values for ϵ and δ. When δ_d in Eq. (31a) is negative, the phase difference between the $d_{x^2-y^2}$ and the d_{xy} state vanishes. As discussed above, in order to relieve the strain induced by the twist grain boundary the subdominant pair state should be antisymmetric [Eq. (33)] with respect to the layer index. Starting the iteration with a trial solution that has this symmetry, we obtain a convergent result for any twist angle. In the left panel of Fig. 6 we show the purely real solution $Y_1'=-Y_{-1}'$ for the subdominant state on layer 1 as a long dashed line and the Josephson critical current across the twist junction as a short dashed line. However, in the absence of the twist we expect that a solution with the symmetry $Y_1'=Y_{-1}'$ would minimize the free energy. Starting with a trial solution that has this symmetry we find convergence only up to twist angles $\phi_0\approx 25°$. For $\phi_0\neq 0$ the solution actually has no symmetry, as the two lines representing Y_1' (solid) and Y_{-1}' (dot-dot-dot-dashed) show. For equal coupling constants $\eta=\eta'$, the minimum Josephson critical current, shown as a dot-dashed line, does not occur at the twist junction but a few layers away from it, the distance depending on ϕ_0. In this case we compared the free energies to establish which is the correct solution. The result is that the most stable state is the one that has the largest *minimum* Josephson critical current. Thus, at the twist angle at which the short-dashed and the dot-dashed lines cross, the system undergoes a phase transition during which the order parameter changes its symmetry with respect to the layer index.

When $\delta_d>0$, as expected from weak-coupling theory, the phase difference between the two d-wave states is $\pi/2$. In order to avoid spurious Josephson currents we have to multiply the bulk solutions with a phase factor [Eq. (47)]. The phase angle θ in Eq. (48) is not quite the correct choice when the boundary conditions are imposed not at infinity but at some finite layer index N. For $N=80$, θ has to be modified by less than one degree to reduce the Josephson current to below the numerical error. The numerical solutions presented in the right panel in Fig. 6 have the symmetry expected according to Eq. (33) at all twist angles. At $\phi_0=0$, the amplitude of the dominant pair state is real, that of the subdominant state is purely imaginary. As ϕ_0 is increased, a real part Y' and an imaginary part X'' are created that serve to rotate the clover leaf of a d-wave state relative to the lattice to minimize the interlayer coupling energy.

In the intermediate-temperature regime $T_{cB}^<<T<T_{cB}$ the subdominant order parameter has a finite complex amplitude near the twist grain boundary. To cancel the Josephson cur-

rent that results from $Y''\neq 0$ the dominant state must acquire an imaginary part. While Y' and Y'' must go to zero far away from the twist since $Y_\infty = 0$, there is no reason for X'' to vanish in the bulk. When one imposes $X''=0$ as a boundary condition, one finds that X'' vanishes linearly at the outermost layer, whatever the number of layers considered may be. The result is again a spurious Josephson current. The correct solution is obtained by multiplying X_∞ with a suitable phase factor, Eq. (47). In this case we do not have an analytic formula to calculate the phase angle. The Josephson critical current for two such nearly degenerate d-wave states is very nearly independent of the twist angle at all temperatures.

VIII. CONCLUSIONS

If the in-plane order parameter of high-temperature superconductors has d-wave symmetry, the Josephson critical current from one conducting layer to the next is exactly zero[32,31] unless there is some coherent tunneling,[34,35] or else there is some momentum dependence to the incoherent tunneling amplitude[31–33,36] containing a component with d-wave symmetry. If either one or both of these preconditions is fulfilled, the Josephson critical current I_0^{JC} across a c-axis twist junction varies with twist angle ϕ_0 as $\cos 2\phi_0$ if the pair state with $d_{x^2-y^2}$ symmetry varies along the Fermi line as $\cos 2\phi$.

At intermediate twist angles, I_0^{JC} even falls below $\cos 2\phi_0$ because of the proximity effect, which suppresses the order parameter on layers close to the twist grain boundary. The size of this suppression, and the number of layers affected, depend on the strength of the Josephson coupling between the layers, which cannot be estimated directly from the normal-state resistance. The proximity effect depends via the coherence length strongly on temperature so that changes resulting from variations of the twist angle should be more easily detectable close to the transition temperature.

A nonvanishing Josephson critical current at twist angle $\phi_0 = 45°$ can result if a second pairing channel with d_{xy} or s symmetry exists. Even if the d_{xy} pairing is very weak, so that one would not expect to see a second superconducting transition, we find a finite order parameter with this symmetry on the layers forming the twist junction at all temperatures at which the dominant order parameter is nonvanishing. For weak d_{xy} pairing we would still expect to see a substantial variation of I_0^{JC} with the twist angle. This variation is stronger close to the transition temperature because, as the temperature is raised, $I_0^{JC}(\phi_0 = 45°)$ will drop much more rapidly than the bulk critical current. If the two d-wave states are nearly degenerate, the combined state is more or less free to rotate relative to the crystal axes and very little variation of $I_0^{JC}(\phi_0)$ would ensue. Such a state, however, would either have a finite energy gap everywhere on the Fermi surface or the nodal structure would disagree with the results of ARPES measurements.

The existence of an s-wave pairing channel has no effect on $I_0^{JC}(\phi_0 = 45°)$ at temperatures above the transition temperature T_{cs} at which this s-wave state would form in the absence of any other pairing. In a narrow temperature range $T_{cs}^{<} < T < T_{cs}$, where $T_{cs}^{<}$ is the temperature below which a two-component pair state is formed in the bulk, the s-wave component can form near the twist junction and thus render $I_0^{JC}(\phi_0 = 45°)$ finite. If the tunneling is predominantly incoherent, the Josephson coupling between s-wave states is expected to be much stronger than that between d-wave states, unless the quasiparticle momentum is very nearly conserved during the incoherent tunneling process. A small s-wave component, possibly too small to be detected by other means, could thus carry most of the Josephson current, in which case no dependence of I_0^{JC} on the twist angle would be expected. Unless the s and d components of the pair state coexist at all temperatures, possibly because the system does not have tetragonal symmetry, one would expect to see some dramatic change with temperature in $I_0^{JC}(\phi_0)$, even for $\phi_0 = 0$.

It is evident from Fig. 4(b) that if the dominant order parameter were the presumed $d_{x^2-y^2}$-wave order parameter, decreasing η' causes strong variations in the angular dependence of the normalized critical current, so that twist junctions with $\phi_0 = 45°$ would have a vanishing critical current for T values down to T_{cB}, the bare transition temperature of the subdominant order parameter. We remark that η', the Josephson coupling parameter across the twist junction, can be varied experimentally by chemically reacting the cleaved surfaces prior to forming the twist junction. In addition, since the actual critical current is proportional to η', weakening the twist junction decreases the critical current for all twist angles ϕ_0. Note that this would also be the case for a pure s-wave order parameter, except in that case there would be no dependence upon the twist angle ϕ_0. Decreasing η' substantially should provide evidence that effects of the twist boundary are indeed observed.

We thus encourage further experiments to be carried out near to T_c with zero applied magnetic field. These are predicted to give the maximum information regarding the symmetry of the superconducting order parameter and the nature of the tunneling process between layers. A preliminary set of such experiments is currently in progress.[16] Ideally, one should study groups of samples, each group having the twist junctions deliberately weakened with identical procedures. Furthermore, experiments should be carried out to determine whether the current paths are indeed homogeneous. This could be done by decreasing the area of the junction, and seeing if the critical current scales with the junction area. Also, the placement of the current and voltage leads should be varied.

ACKNOWLEDGMENTS

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APPENDIX

Here we list the full forms of $\Gamma_{\rm coh}$ and $\Gamma_{\rm inc}$ that appeared in Eq. (11). After integrating over ξ_0, we have

$$\begin{aligned}\Gamma_{\rm coh}(\omega,\Delta_n(\mathbf{k}'),\Delta_{n'}(\mathbf{k}'))=&\frac{\Delta_{n'}(\mathbf{k}')-\Delta_n(\mathbf{k}')}{D_n(\omega,\mathbf{k}')D_{n'}(\omega,\mathbf{k}')[D_{n'}(\omega,\mathbf{k}')+D_n(\omega,\mathbf{k}')]}\\&+\Delta_n(\mathbf{k}')\frac{2|\Delta_n(\mathbf{k}')|^2-\Delta_n(\mathbf{k}')\Delta^*_{n'}(\mathbf{k}')-\Delta^*_n(\mathbf{k}')\Delta_{n'}(\mathbf{k}')}{2D^3_n(\omega,\mathbf{k}')D_{n'}(\omega,\mathbf{k}')[D_n(\omega,\mathbf{k}')+D_{n'}(\omega,\mathbf{k}')]}\\&+\Delta_n(\mathbf{k}')\frac{2|\Delta_n(\mathbf{k}')|^2-\Delta_n(\mathbf{k}')\Delta^*_{n'}(\mathbf{k}')-\Delta^*_n(\mathbf{k}')\Delta_{n'}(\mathbf{k}')}{2D^2_n(\omega,\mathbf{k}')D_{n'}(\omega,\mathbf{k}')[D_n(\omega,\mathbf{k}')+D_{n'}(\omega,\mathbf{k}')]^2}\\&+\Delta_n(\mathbf{k}')\frac{|\Delta_{n'}(\mathbf{k}')|^2-|\Delta_n(\mathbf{k}')|^2}{D_n(\omega,\mathbf{k}')D_{n'}(\omega,\mathbf{k}')[D_n(\omega,\mathbf{k}')+D_{n'}(\omega,\mathbf{k}')]^3},\end{aligned}\tag{A1}$$

and

$$\Gamma_{\rm inc}(\omega,\Delta_n(\mathbf{k}'),\Delta_{n'}(\mathbf{k}''))=2\frac{\Delta_{n'}(\mathbf{k}'')-\Delta_n(\mathbf{k}')}{D_n(\omega,\mathbf{k}')D_{n'}(\omega,\mathbf{k}'')}+\Delta_n(\mathbf{k}')\frac{2|\Delta_n(\mathbf{k}')|^2-\Delta_n(\mathbf{k}')\Delta^*_{n'}(\mathbf{k}'')-\Delta^*_n(\mathbf{k}')\Delta_{n'}(\mathbf{k}'')}{D^3_n(\omega,\mathbf{k}')D_{n'}(\omega,\mathbf{k}'')},\tag{A2}$$

where $D_n(\omega,\mathbf{k})$ is given by Eq. (12). Expanding Eqs. (A1) and (A2) to linear order in the Δ_n, one obtains Eqs. (17a) and (17b), respectively. Note, that in the absence of the twist grain boundary there is no reason for the order parameter to vary from layer to layer. In the approximation that has led to Eq. (A1) we do not expect to see any effect of the coherent interlayer tunneling on the intralayer order parameter and, indeed, when $\Delta_n(\mathbf{k}')$ is independent of n, $\Gamma_{\rm coh}$ does vanish. Since the order parameters appearing in $\Gamma_{\rm inc}$ have different arguments, such a cancellation occurs only for isotropic s-wave states. For all other pair states, incoherent tunneling will suppress the transition temperatures in much the same way as random scattering events within the conducting planes.

Expanding the first term on the right-hand side of Eq. (11) to cubic order in the order parameters, and the interlayer tunneling terms to linear order in the order parameters, and letting $\Delta_{n1}=A_n$, $\Delta_{n2}=B_n$, respectively, we have

$$\begin{aligned}0=&A_n\ln(T/T^0_{cA})\langle\varphi^2_{n1}\rangle+b_0(T)[A^2_nA^*_n\langle\varphi^4_{n1}\rangle+(B^2_nA^*_n+2A_n|B_n|^2)\langle\varphi^2_{n1}\varphi^2_{n2}\rangle]+\sum_{\substack{n'\\\langle nn'\rangle}}\Big(|J|^2b_0(T)[A_n\langle\varphi^2_{n1}\rangle-A_{n'}\langle\varphi_{n1}\varphi_{n'1}\rangle\\&-B_{n'}\langle\varphi_{n1}\varphi_{n'2}\rangle]+\frac{a_0(T)}{2\tau_{\perp0}}[A_n\langle\varphi^2_{n1}\rangle-A_{n'}\langle\varphi_{n1}\rangle\langle\varphi_{n'1}\rangle-B_{n'}\langle\varphi_{n1}\rangle\langle\varphi_{n'2}\rangle]-\frac{a_0(T)}{2\tau_{\perp2}}\{A_{n'}[\langle\varphi_{n1}\cos2\phi_{\mathbf{k}}\rangle\langle\varphi_{n'1}\cos2\phi_{\mathbf{k}}\rangle\\&+\langle\varphi_{n1}\sin2\phi_{\mathbf{k}}\rangle\langle\varphi_{n'1}\sin2\phi_{\mathbf{k}}\rangle]+B_{n'}[\langle\varphi_{n1}\cos2\phi_{\mathbf{k}}\rangle\langle\varphi_{n'2}\cos2\phi_{\mathbf{k}}\rangle+\langle\varphi_{n1}\sin2\phi_{\mathbf{k}}\rangle\langle\varphi_{n'2}\sin2\phi_{\mathbf{k}}\rangle]\}\Big),\end{aligned}\tag{A3a}$$

$$\begin{aligned}0=&B_n\ln(T/T^0_{cB})\langle\varphi^2_{n2}\rangle+b_0(T)[B^2_nB^*_n\langle\varphi^4_{n2}\rangle+(A^2_nB^*_n+2B_n|A_n|^2)\langle\varphi^2_{n1}\varphi^2_{n2}\rangle]+\sum_{\substack{n'\\\langle nn'\rangle}}\Big(|J|^2b_0(T)[B_n\langle\varphi^2_{n2}\rangle-B_{n'}\langle\varphi_{n2}\varphi_{n'2}\rangle\\&-A_{n'}\langle\varphi_{n2}\varphi_{n'1}\rangle]+\frac{a_0(T)}{2\tau_{\perp0}}[B_n\langle\varphi^2_{n2}\rangle-B_{n'}\langle\varphi_{n2}\rangle\langle\varphi_{n'2}\rangle-A_{n'}\langle\varphi_{n2}\rangle\langle\varphi_{n'1}\rangle]-\frac{a_0(T)}{2\tau_{\perp2}}\{B_{n'}[\langle\varphi_{n2}\cos2\phi_{\mathbf{k}}\rangle\langle\varphi_{n'2}\cos2\phi_{\mathbf{k}}\rangle\\&+\langle\varphi_{n2}\sin2\phi_{\mathbf{k}}\rangle\langle\varphi_{n'2}\sin2\phi_{\mathbf{k}}\rangle]+A_{n'}[\langle\varphi_{n2}\cos2\phi_{\mathbf{k}}\rangle\langle\varphi_{n'1}\cos2\phi_{\mathbf{k}}\rangle+\langle\varphi_{n2}\sin2\phi_{\mathbf{k}}\rangle\langle\varphi_{n'1}\sin2\phi_{\mathbf{k}}\rangle]\}\Big).\end{aligned}\tag{A3b}$$

Two additional equations are obtained by complex conjugation. In Eqs. (A3), $\langle\cdots\rangle\equiv\int_0^{2\pi}(d\phi_{\mathbf{k}}/2\pi)\cdots$ is an angular average over the Fermi surface. Because of the orthonormality of the basis functions,

$$\langle\varphi^2_{ni}\rangle=1\tag{A4}$$

for all n,i. We note that the terms proportional to $1/\tau_{\perp0}$ in each of the above equations contain averages over *single* gap functions. Thus, symmetry forces these to vanish for the d-wave states, but not for the s-wave state. For an s-wave superconductor, these incoherent terms just add to the respective coherent interlayer coupling terms, albeit with a different T dependence, which is of no importance near to the maximum T_c. For a d-wave superconductor, since the incoherent interlayer coupling terms vanish, they do not cancel the intralayer incoherent tunneling terms which arise from self-energy corrections. This lack of cancellation breaks the

d-wave pairs, reducing the ''bare'' transition temperature. As usual, the bare transition temperature for s-wave superconductivity is not reduced by this incoherent interlayer tunneling. In addition, we note that the terms containing the integrals $\langle\varphi_{n1}\rangle\langle\varphi_{n'2}\rangle$ always vanish, since we assume at most only one s-wave order parameter on each layer. Also, coherent tunneling terms containing the integrals $\langle\varphi_{n1}\varphi_{n'2}\rangle$ vanish except for the case of two d-wave order parameters across the twist boundary (e.g., $d_{x^2-y^2}$ for $n=1$ and d_{xy} for $n=-1$, with $\phi_0\neq 0$).

On the other hand, the last terms in each of Eq. (A3) vanish for s-wave superconductivity, but not for d-wave superconductivity. For d-wave superconductivity, these terms have the effects of raising T_c (albeit by a value less than the reduction in T_c due to the $1/\tau_{\perp 0}$ terms), and of adding to the Josephson tunneling.

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