

Interface roughness and proximity effect on a c -axis Josephson junction between s -wave and d -wave superconductors

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(Received 18 December 2000; revised manuscript received 6 July 2001; published 4 April 2002)

The scanning superconducting quantum interference device microscope on tri-crystal high-temperature superconductor (HTSC) samples unambiguously identifies the d -wave pairing symmetry as a predominant component. This fact was also seen clearly from the current phase relation (CPR) for an in-plane junction between HTSC's, where both π periodicity and 2π periodicity are observed, depending on the relative crystal orientation. However, for c -axis junctions between HTSC's and conventional superconductor, ac Josephson effect shows that the main Shapiro steps occur at $V = nhf/2e$ (n is integer) and thus a significant s -wave component is indicated. To understand the experimental measurements, we have studied interface roughness and proximity effect on CPR of such junctions. The order parameter profiles and current phase relation are computed self-consistently using the quasiclassical theory and rough interface model. Our results suggest that the existence of a minor surface s -wave component stemming from a repulsive s -channel pairing potential in the d -wave superconductor is able to give a coherent picture.

DOI: 10.1103/PhysRevB.65.144527

PACS number(s): 74.20.Mn, 74.50.+r

I. INTRODUCTION

The symmetry of order parameter in high- T_C superconducting oxides has always been a focal point ever since its discovery 14 years ago.^{1,2} The determination of the order parameter symmetry not only helps us to pin down the essential ingredients in the high- T_C superconducting mechanism, but also offers guidance on the ongoing search for even higher- T_C superconductors. After many years of experimental and theoretical studies, great progresses have been made in our understanding on the normal as well as superconducting properties. A predominant d -wave pairing symmetry is now well established through the scanning superconducting quantum interference device (SQUID) microscope in the phase sensitive tricrystals³⁻⁶ and the Fraunhofer diffraction pattern of corner junctions between s -wave and high- T_C superconductors.^{7,8} Further experimental evidence was given by Il'ichev *et al.*⁹⁻¹¹ through direct measurement of current phase relation (CPR) of in-plane junctions between two high- T_C superconductors. Being consistent with the predominant d -wave pairing symmetry, both π periodicity and 2π periodicity were observed, depending on the relative crystal orientation. For c -axis Josephson junctions involving both conventional superconductor (Pb) and high- T_C superconductors,¹²⁻¹⁴ the microwave investigation, however, shows that Shapiro steps take place only at multiples of $V = hf/2e$. These results were widely cited as an indication that a sizeable s -wave component would exist in high- T_C superconductors, but they disagree with the tricrystal measurements since nodes in the order parameter are clearly shown at [110] directions³⁻⁶ in the tetragonal compounds. At the same time, physical properties of Josephson junction involving high- T_C superconductors have also been studied theoretically by many groups.⁶ It was indicated that

the current phase relation takes approximately the $\sin 2\phi$ pattern if a Josephson junction is made between s -wave and d -wave superconductors along the c -axis.¹⁵⁻¹⁷ Such a current-phase relation was shown to hold also for the in-plane junction between two d -wave superconductors rotated with each other by 45° .¹⁸⁻²⁰ Note that the result for the c -axis Josephson junction by Tanaka¹⁵ is seriously questioned by Arnold and Klemm²¹ who used a tight binding Hamiltonian to address the same issue.

Unlike the scanning SQUID microscope which directly probes the half-integer magnetic flux and thus the phase difference between the a and b axis, the CPR and microwave measurements in Josephson junctions depend very much on the electronic structures in the *neighborhood* of the junction region. It is well known that for conventional isotropic superconductors, a surface does not play a significant role. But the situation changes for anisotropic superconductors where the surface pair breaking effect can be dramatic. Recently, several proposals have been made concerning the Josephson effect in junctions involving high- T_C superconductors. Kuboki and Sigrist,²² and Sigrist²³ investigated the surface Cooper pairing state using the Ginzburg-Landau theory. They found that an s -wave component arises if local time-reversal symmetry is broken near interface due to the angular structure of d -wave pairing, but the effect vanishes when the relative a axis's angle approaches 45° . On the other hand, a similar Ginzburg-Landau formalism by Ren, Xu, and Ting^{24,25} showed that a small s -wave component near a surface is always locked in phase with d -wave component to form a real combination. Since the broken time-reversal symmetry states takes place only when the phase of order parameter changes sign on the quasiparticle trajectory,^{26,27} it may happen solely for the in-plane junction and not for the c -axis junction. However, the broken time-reversal symmetry

state was not observed up to now in the scanning SQUID microscope in tricrystal samples.⁶ To understand the usual Shapiro steps $V = nhf/2e$ in c -axis Josephson junctions, it was proposed that the deformation of the Fermi surface in the Pb was a possible cause,²⁸ but the effect is extremely small. Also recently, it was assumed that the surface scattering not only suppresses the d -wave order parameters near the interface, but also transforms the d -wave pairing state into s -wave pairing state.^{29,30}

Since the current phase relation of the Josephson junction plays an important role in identifying the pairing symmetry of high- T_C superconductors, the impact of interface scattering on the order parameter as well as on its symmetry has to be further elucidated. As the d -wave superconductor has an anisotropic pairing state, the order parameter is vulnerable to the presence of surface, defects, etc., and self-consistent evaluation of the order parameter is highly desired. In this paper, taking into account the interface roughness and proximity effect self-consistently, we study the current phase relation of c -axis Josephson junction between s and d -wave superconductors. The c -axis junction is chosen because (i) the phase of d -wave order parameter does not change sign for the incident and reflected quasiparticle trajectories near interface, thus such configuration avoids the possible broken time-reversal symmetry states; (ii) there exists a controversy concerning the validity of tunneling expression by Tanaka and Kashiwaya,^{15–17,21} which calls for more studies using different methods. Note that faceting has a pronounced effect on in-plane junctions because of the interference phenomena among grains with different facets, but such an effect does not occur for the c -axis junction since grains with different facets in a - b plane contribute coherently.

To deal with the Josephson effect in high- T_C superconductors, most theoretical methods are based either on the phenomenological Ginzburg-Landau theory or on the Fermi liquid theory of superconductivity. In principle, high- T_C superconductors are strongly correlated electronic systems, and they behave as a Fermi liquid only in the overdoped region; physics is so complicated and yet to be understood clearly in the underdoped region where different orderings compete with each other. We will concentrate on the region where high- T_C superconductors can be treated as Fermi liquid. A very useful formulation of Fermi liquid theory of superconductivity is based on the quasiclassical transport theory,^{31,32} which describes slowly varying phenomena in space and time with the requirements that the order parameter Δ is much smaller than the Fermi energy E_F and the coherence length $\xi_0 = \hbar v_F / 2\pi k_B T_C$ is much larger than the inverse Fermi wavelength k_F^{-1} .^{33,34} For high- T_C superconductors, $E_F \sim 0.2$ eV (Refs. 21,35) and $\Delta \sim 0.02$ eV, $\Delta/E_F \sim 0.1$, and $1/(\xi_0 k_F) \sim 0.1$; they are still reasonably small although large in comparison with those of conventional superconductors. Since the quasiclassical theory is expanded in terms of these small parameters, the conclusion drawn from these calculations should be qualitatively correct though it may be quantitatively in error by 10%.

Our detailed study shows that interface scattering does not change the π periodicity of the current phase relation and the impact of interface roughness is to reduce the critical tunnel-

ing current. Therefore, rough scattering at an interface is unable to explain the experimental observation.²⁹ On the other hand, we notice that symmetries of s - and d -wave Cooper pairings are orthogonal to each other and thus there would be zero critical current between such junctions without taking into consideration of the proximity effect. The proximity effect induces an s -wave component in the quasiclassical propagator,³⁰ but the corresponding s -wave order parameter is still missing because of the absence of s -channel pairing potential. Thus, the proximity effect itself yields only the π periodicity. Only when a repulsive s -channel pairing potential is taken into account in the d -wave superconductor,^{24,25} an exponentially decaying s -wave component can prevail in the d -wave superconductor near the interface. This enables us to explain the experimental properties of the Josephson junction between the s - and d -wave superconductors along the c axis. Our self-consistent calculation shows that 5% of the s -wave component at the *interface* is necessary to change the current phase relation from π periodicity to 2π periodicity.

In the following, we will first discuss the importance of proximity effect in the Josephson junction between superconductors with different pairing symmetries. Then we show that the scattering alone does not bring about the 2π periodicity in the current phase relation, but only reduces the critical current. Finally, we show that the 2π periodicity is recovered if a small surface s -wave component resulting from a repulsive s -channel pairing potential is taken into account.

II. QUASICLASSICAL METHOD

In this paper, we present a self-consistent calculation of the Josephson effect for a c -axis junction consisting of d -wave superconductor, insulating layer, and s -wave superconductor. In the quasiclassical theory, the superconducting state is described by the 2×2 Matsubara propagator $g^M(\hat{k}, \vec{R}; \epsilon_n)$ in particle-hole space, which satisfies the transportlike equation³⁴

$$[i\epsilon_n \hat{\tau}_3 - \hat{\Delta}, \hat{g}^M(\hat{k}, \vec{R}; \epsilon_n)]_- + i\hbar v_F \hat{k} \cdot \vec{\nabla}_{\vec{R}} \hat{g}^M(\hat{k}, \vec{R}; \epsilon_n) = 0 \quad (1a)$$

and normalization condition

$$[\hat{g}^M(\hat{k}, \vec{R}; \epsilon_n)]^2 = -(\pi\hbar)^2. \quad (1b)$$

\hat{k} and $\epsilon_n = \pi k_B T(2n+1)$ denote the trajectory and the Matsubara frequency of the propagator. $\hat{\Delta}$ is the superconducting order parameter and $\hat{\tau}_3$ is the third Pauli matrix in particle-hole space. In the bulk superconductor, Eq. (1) forms a closed set together with the self-consistent equation for the order parameter

$$\begin{aligned} \hat{\Delta}_{12}(\hat{k}, \vec{R}) = & \frac{k_B T}{\hbar} \sum_n' \int \frac{d\Omega_{\hat{k}'}}{4\pi} f(\hat{k}) f(\hat{k}') \hat{g}_{12}^M(\hat{k}', \vec{R}, \epsilon_n) \\ & \times \left[\ln(T/T_C) + \sum_n' \frac{1}{2n+1} \right]^{-1}. \end{aligned} \quad (2)$$

Here, a prime means a cut off on the frequency summation and the function $f(\hat{k})$ denote the orbital wave function of the Cooper pair. The superconducting current can be calculated from

$$\vec{j} = \frac{k_B T}{R_0 e \hbar} \sum_n' \int \frac{d\Omega_{\hat{k}}}{4\pi} \hat{k} \text{Re} g^M(\hat{k}, \vec{R}, \epsilon_n), \quad (3)$$

where e is the electron charge and $R_0 = [2N(E_F)e^2 v_F]^{-1}$ is the Sharvin resistance.³⁶ The rough interface can be simulated by the model devised by Ovchinnikov³² and Culetto *et al.*³⁷ which reads

$$[\hat{g}^M(\hat{k}, \xi; \epsilon_n), \langle \hat{g}^M \rangle(\xi, \epsilon_n)]_- + \frac{2\pi i}{\rho} \hbar k_{\perp} \frac{d}{d\xi} \hat{g}^M(\hat{k}, \xi; \epsilon_n) = 0 \quad (4a)$$

with

$$\langle \hat{g}^M \rangle(\xi, \epsilon_n) = \int \frac{d\Omega_{\hat{k}}}{4\pi} \hat{g}^M(\hat{k}, \xi; \epsilon_n) \quad (4b)$$

denoting the impurity self-energy and k_{\perp} is the projection of trajectory perpendicular to the interface. ρ is the roughness parameter of the interface and is related to the conventional diffusivity parameter p (Ref. 38) through the relation $p = 1 - 4 \int_0^{\pi/2} d\theta \cos \theta \sin^3 \theta \exp(-\rho/\cos \theta)$, with $p(\rho=0) = 0$ standing for the transparent interface and $p(\rho=\infty) = 1$ for the fully diffuse interface. $\xi = \pm 1/2$ corresponds to $\vec{R} = \vec{R}_{\text{surf}} \pm 0^+$, where \vec{R}_{surf} is the coordinate of interface layer.

To describe a planar c -axis junction between s -wave and d -wave superconductors situated, respectively, on the right and left sides, the Cartesian coordinate is chosen such that the xy plane is within the interface of the junction and $z = c$ axis is normal to the interface. Since the qualitative feature of the current phase relation depends mainly on the pair-

ing symmetries of the two superconductors, spherical Fermi surfaces for both s - and d -wave superconductors are assumed. To calculate the current phase relation, the phase difference between right and left bulk superconductors are fixed and the order parameters in the bulk are given by

$$\hat{\Delta}_{12}(\hat{k}, z) = \begin{cases} \Delta_s(T) f_s(\hat{k}) \exp(i\phi/2), & z \gg 0, \\ \Delta_d(T) f_d(\hat{k}) \exp(-i\phi/2), & z \ll 0, \end{cases} \quad (5)$$

$f_s(\hat{k}) = 1$ and $f_d(\hat{k}) = (\sqrt{15}/2)(\hat{k}_a^2 - \hat{k}_b^2)$ correspond to the conventional s -wave and $d_{x^2-y^2}$ -wave pairing states, respectively.

III. RESULTS AND DISCUSSIONS

It is well-known from tunneling Hamiltonian calculation that if two superconductors forming the Josephson junction are in orthogonal pairing states, the superconducting tunneling current vanishes if the tunneling matrix is assumed as a constant. To investigate how the high order terms arises as a result of proximity effect, we first consider the simplest case where an s -wave superconductor is placed directly on top of a d -wave superconductor along the c axis and assume that the order parameters are not perturbed. In this case, the problem can be studied analytically. The quasiclassical equation generally has three types of solutions: the constant solution which represents also the bulk physical solution; the exponentially decreasing and exponentially increasing solutions. However, only the constant and exponentially decreasing solutions towards bulk can appear near an interface, thus the physical solution in the vicinity of an interface is a combination of these two. After matching the left and right physical solutions at the interface and using the short notations $E_{ns} = \sqrt{\epsilon_n^2 + [\Delta_s f_s(\hat{k})]^2}$ and $E_{nd} = \sqrt{\epsilon_n^2 + [\Delta_d f_d(\hat{k})]^2}$, the diagonal propagator at the interface reads

$$g^M(\hat{k}, 0, \epsilon_n) = \frac{i\pi \Delta_d f_d(\hat{k})}{E_{ns} E_{nd}} \times \frac{\{\epsilon_n(E_{nd} - E_{ns})(\epsilon_n - k_{\perp} E_{ns}) e^{i\phi} + \Delta_s f_s(\hat{k}) [\Delta_s f_s(\hat{k}) E_{nd} e^{i\phi} - \Delta_d f_d(\hat{k}) E_{ns}]\}}{[\Delta_s f_s(\hat{k})(\epsilon_n + k_{\perp} E_{nd}) - \Delta_d f_d(\hat{k})(\epsilon_n - k_{\perp} E_{ns}) e^{i\phi}]} \quad (6)$$

and the corresponding current is given by

$$J = \frac{k_B T}{R_0 e \hbar} \sum_n \int \frac{d\Omega_{\hat{k}}}{4\pi} k_{\perp} g^M(\hat{k}, 0, \epsilon_n). \quad (7)$$

To carry out the numerical integration over momentum space, one needs also the information on transition temperatures for both superconductors. As the characteristic feature of current phase relation is determined mainly by the symmetrical properties of pairing states, we take the same T_C for both superconductors to facilitate numerical computation. The temperature dependent order parameter for s -wave superconductor is well described by the interpolation formula³⁹ $\Delta_s(T) = \delta_{sc} k_B T_C \tanh[(\pi/\delta_{sc}) \sqrt{\frac{2}{3}} \times \Delta C/C_N \times (T_C/T - 1)]$,

where the weak coupling values $\delta_{sc} = 1.76$ and $\Delta C/C_N = 1.43$ are used. The temperature dependent order parameter for the d -wave superconductor in bulk can be calculated from Eqs. (1) and (2). At $T = 0$ K, $\Delta_d(0) = e^{16/15}/\sqrt{15} \delta_{sc} k_B T_C$. It is found that $\Delta_d(T)/\Delta_d(0)$ differs only slightly from the ordinary BCS curve $\Delta_s(T)/\Delta_s(0)$ which was also found by Arnold and Klemm.²¹ So the temperature dependent d -wave order parameter is approximated by $\Delta_d(T) = e^{16/15}/\sqrt{15} \Delta_s(T)$. The resulting current phase relation is plotted in Fig. 1 for different reduced temperature T/T_C , in which the π periodicity in CPR at higher temperatures agrees with that obtained using multiple tunneling method.¹⁵⁻¹⁷ However, we see an overall phase change of π in CPR between $T/T_C = 0.1$ and $T/T_C = 0.2$. Physically, the intrinsic phase shift can take either $\pi/2$ or $-\pi/2$ if the low

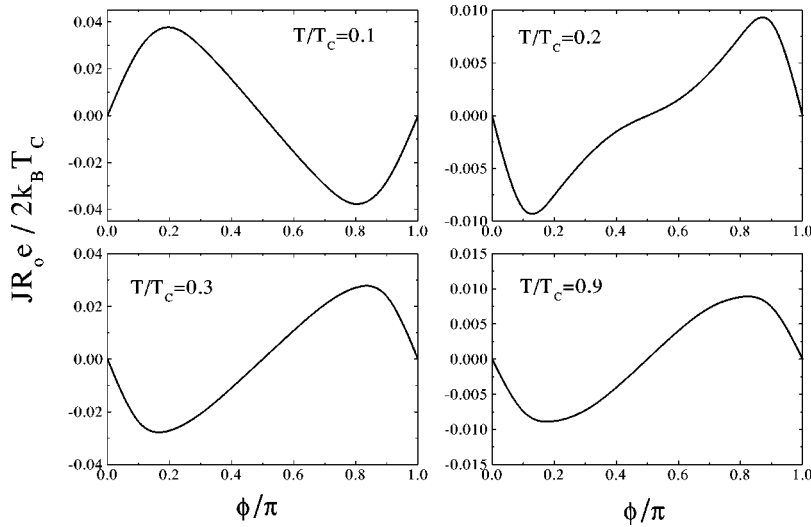


FIG. 1. The CPR of an unperturbed c -axis junction between s -wave and d -wave superconductors. (a) $T/T_c=0.1$, (b) $T/T_c=0.2$, (c) $T/T_c=0.3$, (d) $T/T_c=0.9$.

order Josephson current is absent,²³ which indicates that the intrinsic phase may change from one to another at certain temperature, leading to the π -phase change in the CPR. A similar effect was also found by Kashiwaya and Tanaka¹⁷ for in-plane junctions between two d -wave superconductors if the relative orientation is close to $\pi/4$. For the general mirror symmetrical in-plane junction, Barash *et al.*⁴⁰ showed that the sign change in J_C results from the competition between the midgap states at low temperature and the gap edge and continuum states near critical temperature. Such phenomenon has been in fact observed for the in-plane junction by Ili'chev,⁴¹ but it has not been tried for the c -axis junction due to very low critical current. The critical tunneling current $J_C(T)$ as a function of temperature is also analyzed and illustrated in Fig. 2. The large J_C at low temperature is caused by the midgap states,⁴⁰ and it crosses zero and picks up the π phase around $T/T_c \approx 0.2$. Note that the overall phase shift of π depends on the transition temperatures of the two superconductors; no π -phase shift appears when the transition temperatures are very different.

Although the distinct π periodicity in current phase relation was reported by Ilichev *et al.*^{9–11} for the in-plane junc-

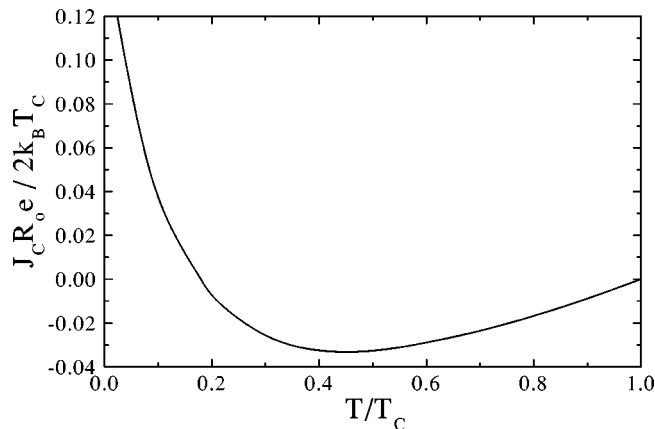


FIG. 2. The critical tunneling current as a function of temperature for an unperturbed c -axis junction between s - and d -wave superconductors.

tion, the ac Josephson effect shows that the main Shapiro steps occur at $V = nhf/2e$ for the c -axis junction.^{12–14} This suggests that an s -wave component in the d -wave superconductor is involved in such tunneling process, otherwise the main Shapiro steps should appear at $V = nhf/4e$. Note that the existence of s -wave component does not affect the conclusion for the in-plane junction, but does have significant impact on the c -axis junction. Previous studies concentrated on the bulk s -wave component^{16,17} or the surface s -wave component resulting from time-reversal symmetry breaking.^{22,23,26,27} However, for the tetragonal high- T_c superconductor $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+x}$, the bulk s -wave component is very unlikely since the scanning SQUID microscope clearly identifies the nodes at (110) directions.^{3,6} The time-reversal symmetry breaking states is unlikely to appear in c -axis junctions too since quasiparticle does not encounter a phase change near an interface.⁶ Thus, it was speculated that interface scattering might induce a s -wave component from a d -wave pairing state if a rough realistic interface is considered.²⁹ To analyze the interface scattering quantitatively, we adopt the well established rough interface model as described before^{32,37} and solve the above quasiclassical

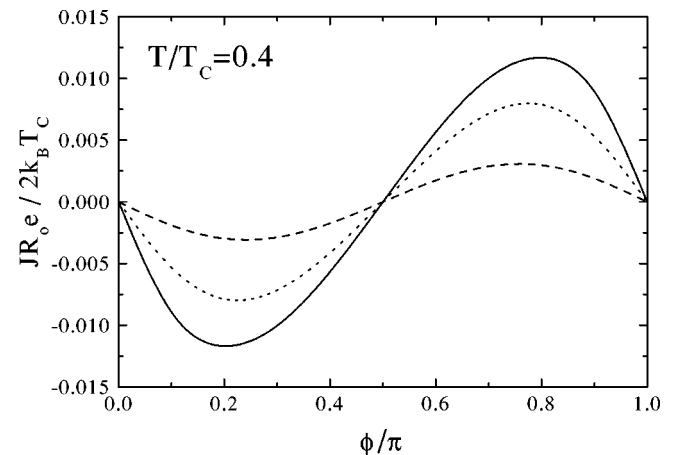


FIG. 3. The CPR of a c -axis junction between s - and d -wave superconductors at $T=0.4T_c$. The solid line, dotted line, and dashed line correspond to $\rho=0$, $\rho=0.27$, $\rho=1.27$, respectively.

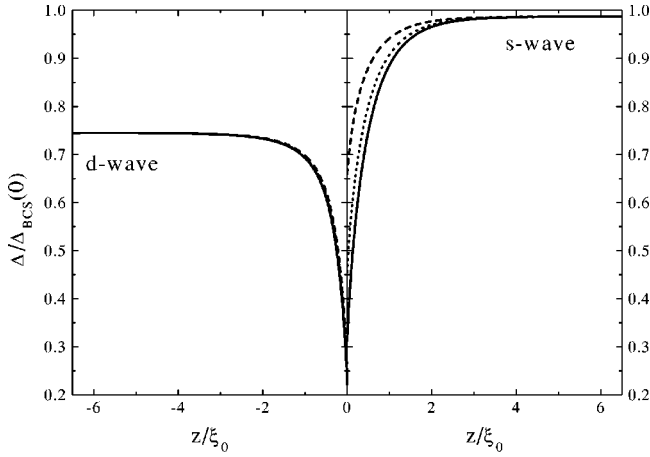


FIG. 4. The order parameter profile in a c -axis junction between s - and d -wave superconductors at $T=0.4T_C$ and $\phi=0$. The solid line, dotted line and dashed line correspond to $\rho=0$, $\rho=0.27$, $\rho=1.27$, respectively.

equation numerically. The self-consistent order parameters and current are obtained through iteration scheme until convergence. For numerical calculation below, we set temperature $T/T_C=0.4$. Both the transparent ($\rho=0$) and rough interfaces ($\rho=0.27, 1.27$) are considered and their corresponding current phase relations are shown in Fig. 3. To our surprise, rough interface does not change the π periodicity expected from an intuitive physical picture, but mainly reduces the critical tunneling current.⁴² The reason is that the surface scattering mainly affects the propagator, the s -wave component of the order parameter is still missing because of the absence of s -channel pairing potential. Thus, we conclude that rough scattering is not enough to account for the experimental observation. In Fig. 4 we present the self-consistently calculated order parameters in the vicinity of interface in the absence of phase difference. It is noted that both s - and d -wave order parameters are greatly depleted near the interface due to the proximity effect, but the inter-

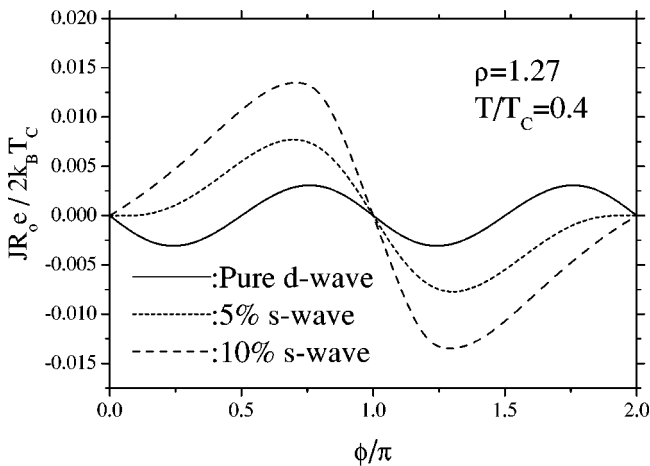


FIG. 5. The CPR of a c -axis junction between s - and d -wave superconductors at $T=0.4T_C$ and $\rho=1.27$. The solid line, dotted line, and dashed line correspond to the surface s -wave component 0, 5, and 10 % of the d -wave component, respectively.

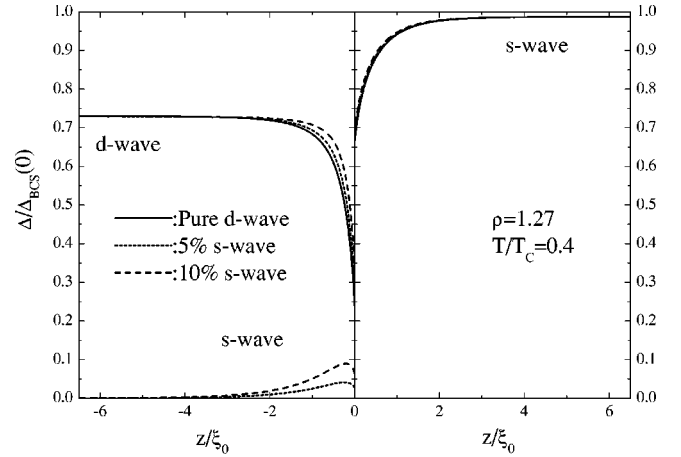


FIG. 6. The order parameter profile in a c -axis junction between s - and d -wave superconductors at $T=0.4T_C$, $\rho=1.27$, and $\phi=0$. The solid line, dotted line, and dashed line correspond to the surface s -wave component 0, 5, and 10 % of the d -wave component, respectively.

face roughness prevents Cooper pairs from leaking to the opposite side and the impact is most profound for s -wave superconductors.

Up to now, the proximity effect is taken into account on the level of quasiclassical propagator, while the feedback of the proximity effect is not considered since a pure d -channel pairing potential is assumed. As was pointed out earlier,⁴³ a repulsive s -channel pairing potential can exist in a d -wave superconductor since it does not give rise to a bulk s -wave component. However, the proximity effect results in an exponentially decaying s -wave component near an interface. According to the analyses in Refs. 24, 25, the surface or interface energy favors phase locking between s - and d -wave order parameters. This s -wave component in a d -wave superconductor does not affect the thermodynamical properties as it vanishes rapidly towards bulk, but it does change the behavior of Josephson junction involving such superconductors. By taking the repulsive s -channel pairing potential into account, we have calculated the order parameters and tunneling current self-consistently. In Fig. 5, the current phase relation is shown for a fixed surface roughness parameter $\rho=1.27$ but with different s -wave components in a d -wave superconductor near an interface. These results demonstrate the great sensitivity of the current phase relation on the proximity-induced interface s -wave component. When the s -wave component increases, the CPR approaches rapidly to the 2π -periodicity pattern, which then corresponds to the Shapiro steps at $V=n\hbar f/2e$ observed experimentally. In fact, 5% of the s -wave component at the interface is enough to change the overall behavior. The corresponding order parameters at $\phi=0$ are plotted in Fig. 6, where one finds that there is a tiny element of s -wave component near the interface on a d -wave superconductor. But its role in changing the π periodicity to the 2π periodicity is decisive.

IV. CONCLUSION

We have studied in this paper the impact of interface roughness and proximity effect on the current phase relation of c -axis junction between s -wave and d -wave superconduct-

ors. Our results show that the interface roughness is not sufficient to change the current phase relation from π periodicity to that of 2π periodicity, but the proximity induced s -wave component near interface does play that role and causes the CPR to be consistent with the Shapino steps observed experimentally. Note that the abovementioned interface s -wave component does not affect the phase sensitive tricrystal measurement as well as the CPR for in-plane junction since it is very small in comparison with the d -wave component.

ACKNOWLEDGMENTS

The work was supported by the Croucher Foundation, the RGC of Hong Kong under Grant No. HKU7092/01P, and the “973 Program” of Ministry of Science and Technology of China under Grant Nos. 199806 and 1999064602. W.Z. acknowledges partial support by the NSFC under Grants Nos. 19767202, 10021001, and 0025419, and Z.D.W. also thanks the Texas Center for Superconductivity at the University of Houston for partial support.

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