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Sign reversal of the order parameter in s wave superconductors

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Abstract

We show that in a superconductor where two or more bands cross the Fermi level it is possible, in the framework of the conventional (s wave) BCS theory, that the sign of the superconducting gap is different on the different sheets of the Fermi surface. At least one of two conditions has to be satisfied: (1) The interband pairing interaction is weaker than the Coulomb pseudopotential, while the intraband one is stronger, or (2) there is strong interband scattering by magnetic impurities. In the case of $\text{YBa}_2\text{Cu}_3\text{O}_7$ we shall argue that the first condition is possibly satisfied, and the second one very likely satisfied. In many aspects such a sign-reversal s wave superconductor is similar to a d wave superconductor, and thus demands revising recent experiments aimed to distinguish between the s and d wave superconductivity in this compound.

Recently, a number of experiments probing the relative phase of the order parameter Δ on different parts of the Fermi surface in the superconducting $\text{YBa}_2\text{Cu}_3\text{O}_7$ have been reported [1–8]. Some of them [2,5,7] seem to indicate the conventional pairing state with Δ having the same sign over the whole Fermi surface, while others suggest that Δ changes in sign, as consistent, e.g., with d pairing. The question of the symmetry of the superconducting state, and thus of the interpretation of these experiments, is of crucial importance for distinguishing between the conventional mechanism for superconductivity and more exotic mechanisms, or among the unconventional theories themselves.

It is generally believed that the s pairing is inconsistent with sign reversal of Δ . This is not true. A simple counterexample is the case of two concentric Fermi spheres, which have gaps (order parameters) of oppo-

site signs. Such a state has pure s symmetry. The two-dimensional analog is the case of two coaxial Fermi cylinders. A Josephson contact between two such superconductors, or with a conventional superconductor, may show an unusual behavior, sometimes similar to the d pairing case.

In this paper we shall show under which conditions the situation similar to the examples above, which we shall call the interband sign reversal of the gap (ISRG), can be realized, and we will also argue that these conditions are not at all exotic but are likely to be realized in $\text{YBa}_2\text{Cu}_3\text{O}_7$. We shall also discuss briefly how ISRG can make itself manifest in Josephson tunneling, and we shall make a link to the existing experiments.

The extension of the BCS theory for two or more superconducting bands was first worked out by Suhl et al. [9] and independently by Moskalenko [10], and later elaborated on by many. It was realized [11] that the fact that several bands cross the Fermi level is not

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sufficient to have considerable many-band effects in superconductivity. Only when the bands in question have a very different physical origin, can a substantial effect appear.

This is the case in many high- T_c cuprates. In particular, $\text{YBa}_2\text{Cu}_3\text{O}_7$ is known to have four sheets of the Fermi surface, all four having a different physical origin [12]: One is formed by the chain $p\text{d}\sigma$ (seen by positron annihilation), another is an apical-oxygen band (seen in de Haas–van Alphen experiments), and the last two are bonding and antibonding combinations of the two $p\text{d}\sigma$ plane bands (seen by angular-resolved photoemission). Based on the richness of the band structure of $\text{YBa}_2\text{Cu}_3\text{O}_7$, several groups pointed out that at least the two-band [13,14], or probably the whole four-band [15,16], picture should be used to describe superconductivity in this system. Various experiments have been interpreted as indicating two or more different superconducting gaps.

We shall now remind the basic equations of the multiband BCS theory [9,11]: The hamiltonian has the following form:

$$H = \sum_{i,k\alpha} \epsilon_{i,k} c_{i,k\alpha}^* c_{i,k\alpha} - \sum_{ij, k'k''\alpha\beta} \frac{g_{ij}}{2} c_{i,k'\alpha}^* c_{j,k''\alpha} c_{i,-k\beta} c_{j,-k'\beta},$$

where $\epsilon_{i,k}$ is the kinetic energy in the i th band, $c_{i,k\alpha}^*$ and $c_{i,k\alpha}$ are the corresponding creation and annihilation operators, and g_{ij} is the averaged pairing potential.

The order parameter Δ on the i th sheet of the Fermi surface is given by the equation

$$\Delta_i = \sum_j A_{ij} \Delta_j \int_0^{\omega_D} dE \frac{\tanh(\sqrt{E^2 + \Delta_j^2}/2k_B T)}{\sqrt{E^2 + \Delta_j^2}}, \quad (1)$$

if the cut-off frequency ω_D is assumed to be the same for all sheets. T_c is defined in the usual way by the effective coupling constant, $\log(2\gamma^* \omega_D / \pi T_c) = 1/\lambda_{\text{eff}}$, $\gamma^* \approx 1.78$. The effective coupling constant λ_{eff} in this case is simply the maximal eigenvalue λ_{max} of the matrix $A_{ij} = g_{ij} N_j$, where N_j is the density of states at the Fermi level (per spin) in the j th band. A_{ij} plays the role of the coupling constant λ in the one-band BCS theory. Note that the conventional (isotropic) λ is also defined in terms of A_{ij} : $\lambda = \sum_{ij} A_{ij} N_i / N = \sum_i \lambda_i N_i / N$, where the mass renormalization for the i th band is $\lambda_i = \sum_j A_{ij}$, and $N = \sum_i N_i$. Obviously $\lambda_{\text{eff}} \geq \lambda$, which

means that due to a larger variational freedom T_c in the multiband theory is always larger than in the one-band theory. The two are equal in the isotropic case, i.e. when g_{ij} does not depend on i, j . An instructive example of the opposite case is the two-band model with $A_{11} = A_{22} = \Lambda > 0$, $A_{12} = A_{21} = -\Lambda$. Then $\lambda = 0$, while $\lambda_{\text{eff}} = 2\Lambda$. Note that the last value is the same as when $A_{12} = A_{21} = \Lambda$. The physical reason is that although there is no solution of Eq. (1) with $\Delta_1 > 0$, $\Delta_2 > 0$, there is an obvious solution with $\Delta_1 = -\Delta_2 \neq 0$. Near T_c , the solution of Eq. (1) is $\Delta_2/\Delta_1 = (\lambda_{\text{eff}} - A_{11})/A_{12}$, demonstrating directly that the sign reversal of the order parameter, Δ_2/Δ_1 , takes place when nondiagonal matrix elements A_{12} and A_{21} are negative. The fact that conventional BCS theory (Eq. (1)) allows for the ISRG solution, has never, to our knowledge, been mentioned in the extensive literature existing on multiband superconductivity [17]. One can easily check that Eq. (1) may have a superconducting solution even for all $g_{ij} < 0$, i.e., when no attractive interaction is present in the system. The condition for that is $|g_{12}| > (|g_1| N_1^2 + |g_2| N_2^2) / 2N_1 N_2$. This is similar to the well-known fact that in a system with repulsion superconductivity with higher angular momenta (p, d) is possible, because of the sign reversal of the order parameter. The main difference is that in the example above the symmetry of the superconducting state is the same as of the normal state. Below we shall demonstrate that even a fully attractive interaction $g_{ij} \geq 0$ can lead to the sign reversal if

- (1) interband pairing interaction is weaker than Coulomb pseudopotential,
- (2) there is strong interband scattering by magnetic impurities.

If g 's are electron–phonon pairing potentials, then Eq. (1) should be corrected for a Coulomb repulsion, which can be readily done [11] by substituting $g_{ij} \rightarrow g_{ij} - U_{ij}^* \approx g_{ij} - U^*$, where the effective Coulomb repulsion U^* is logarithmically renormalized in the same way as in one-band superconductivity theory (U^* is assumed to be independent on i, j). A direct consequence of that is that if the interband electron–phonon coupling is weak, the situation with a negative gap, $g_{ij} - U^* < 0$, can easily be realized because of the interband repulsion. We illustrate that by numerical calculations presented in Fig. 1. In these calculations the following parameters have been used: $g_{12} = g_{22} = 0$,

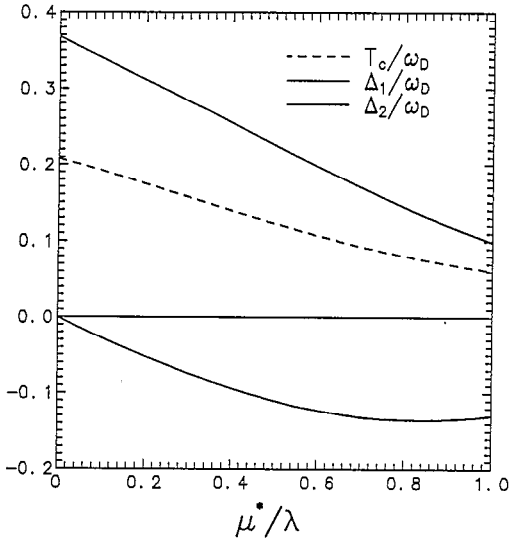


Fig. 1. Critical temperature and superconducting gaps in a system with induced superconductivity in the second band, as a function of Coulomb pseudopotential.

$N_1 = 4N_2$, and $g_{11} = N_1^{-1}$ so that to have $\lambda = 1$. This choice of parameters corresponds to the plane and chain bands in $\text{YBa}_2\text{Cu}_3\text{O}_7$, as discussed below in Section 5. Several facts draw attention: First, in this model T_c decreases with the increase of $\mu^* = U^*N$ substantially slower than in a one-band case when $T_c \rightarrow 0$ when $\mu^* \rightarrow \lambda$. Second, the order parameter induced in the second band (“chains”) is always negative; its absolute value reaches a maximum when $|\Delta_1| = |\Delta_2|$, i.e., at $U^* = g_{pp}N_p/2(N_p - N_c)$.

equations for the renormalized frequency ω_n and order parameter $\tilde{\Delta}_n$ (n is the Matsubara index), which completely define the superconductive properties of the system (see, e.g. Ref. [19]):

$$\begin{aligned} \hbar\tilde{\omega}_{i,n} &= \hbar\omega_n + \sum_{j,m} \frac{\hbar^2\tilde{\omega}_{j,m}}{2Q_{j,m}} (\gamma_{ij} + \gamma_{ij}^s), \\ \tilde{\Delta}_{i,n} &= \Delta_i + \sum_{j,m} \frac{\hbar^2\tilde{\Delta}_{j,m}}{2Q_{j,m}} (\gamma_{ij} - \gamma_{ij}^s), \\ \Delta_i &= \pi T \sum_{j,n} A_{ij}\tilde{\Delta}_{j,n}/Q_{j,n}. \end{aligned} \quad (2)$$

Here $\omega_n = (2n+1)\pi T$, $Q_{i,n} = \sqrt{\tilde{\omega}_{i,n}^2 + \tilde{\Delta}_{i,n}^2}$, γ_{ij} is the scattering rate from band i into band j due to nonmagnetic impurities, and γ_{ij}^s is the same for magnetic impu-

rities. Near T_c Eqs. (2) can be solved analytically [20]. For two bands, in the linear in γ , γ_s approximation, the solution reduces again to Eqs. (1), with the effective coupling matrix Λ :

$$\begin{aligned} \Lambda_{\text{eff}} &= \Lambda - \frac{\pi}{8T_{c0}} \Lambda \\ &\times \begin{pmatrix} 2\gamma_{11}^s + \gamma_{12}^s + \gamma_{12} & \gamma_{12}^s - \gamma_{12} \\ \gamma_{21}^s - \gamma_{21} & 2\gamma_{22}^s + \gamma + \gamma_{21} \end{pmatrix} \cdot \Lambda. \end{aligned}$$

When all Λ 's are equal, the standard Abrikosov–Gor'kov result is recovered: $\delta\lambda \approx -\pi\lambda^2(\gamma_{11}^s + \gamma_{12}^s + \gamma_{21}^s + \gamma_{22}^s)/8T_{c0}$. The main point of the AG theory [18] is that γ^s enters the equations for ω and Δ with opposite signs. That is why the magnetic impurities appear to be pair breakers, and the nonmagnetic ones not. The above solution shows that in the multiband case of Eqs. (2) this argument works only for the intraband nonmagnetic scattering (γ_{ii} drop out), while all other scattering rates are, in principle, pair breaking.

An interesting special case is $\Lambda_{12}, \Lambda_{21} \ll \Lambda_{11}, \Lambda_{22}$. Then in the effective Λ matrix nondiagonal elements $\Lambda_{ij}^{\text{eff}} (i \neq j) = \Lambda_{ij} + \pi\Lambda_{ii}\Lambda_{jj}(\gamma_{ij} - \gamma_{ij}^s)/8T_{c0}$ can become negative, if γ_{ij}^s is sufficiently large. As discussed above, this situation will lead to ISRG. In order to demonstrate this effect quantitatively, we solved the Eqs. (2) in the Eliashberg approximation numerically, using the following parameters: $\Lambda_{11} = 1$, $\Lambda_{22} = 0.5$, $\Lambda_{12} = 0.025$, $\Lambda_{21} = 0.1$. This choice is again inspired by the situation in $\text{YBa}_2\text{Cu}_3\text{O}_7$: The ratio of the densities of states in the bonding and antibonding bands in $\text{YBa}_2\text{Cu}_3\text{O}_7$

this value (see discussion below). Correspondingly, we used $\gamma_{21} = 4\gamma_{12}$, $\gamma_{21}^s = 4\gamma_{12}^s$. The results for the low-temperature regime, $T \ll T_c$, are shown in Fig. 2. In accord with the condition derived above, when the difference $\gamma_{12}^s - \gamma_{12}$ becomes larger than some critical value (in this case, $0.042\pi T_c$), the second gap changes sign. In other words, when the attractive interband coupling is relatively weak and the magnetic interband scattering is strong the system will choose to have two gaps of opposite signs, losing in pairing energy, but avoiding the pair breaking due to interband scattering.

Let us consider now two cases relevant for $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$, and their applications for the Josephson effect.

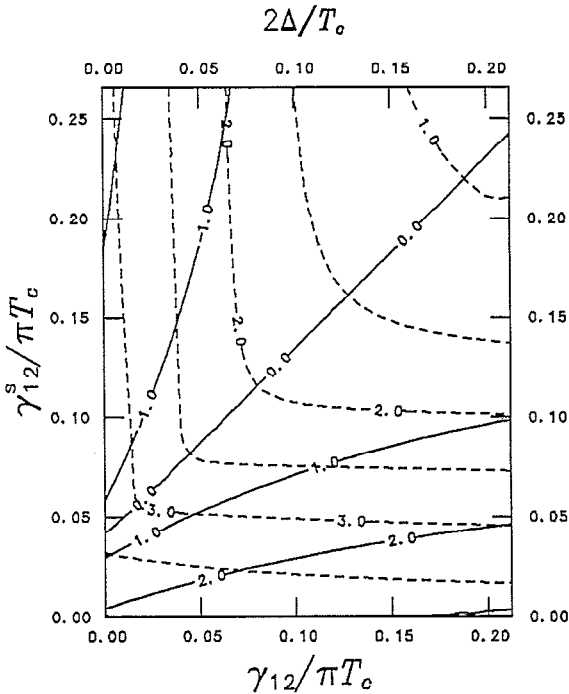


Fig. 2. Superconducting gaps at $T \ll T_c$ in a two-band system with interband scattering on magnetic and non-magnetic impurities. Solid lines show Δ_2/T_c , dashed lines Δ_1/T_c . Note the straight line corresponding to $\Delta_2=0$.

(1) It is believed by many (e.g., Ref. [13]) that the chain electrons would not be superconducting, or only weakly superconducting, if not for the ‘‘proximity effect’’ from the planes. In our language, this means that $\lambda_c - \mu_c^* = (g_{cc} - U^*)N_c \approx 0$, where c stands for chains. Then the sign of the gap, induced in the chains, will be determined by the sign of $g_{pc} - U^*$; in the quite likely case of $g_{cc} < U^*$, ISRG between the chain and the plane bands takes place.

(2) One can also look for the ISRG between the bonding (b) and antibonding (a) combinations of the two plane bands. According to the calculations [21] and experiment [22], it is the a band which has Van Hove singularities near the Fermi level. In the calculations the singularities are bifurcated, which makes the density of states in the antibonding band 2.5 times larger than in the bonding band, and is extremely sensitive to the warping of the CuO_2 planes, thus resulting in strong electron–phonon interaction. Experimentally, the singularities are even closer to the Fermi level than in the calculations, and are extended towards the Γ point. If, as is often claimed, this singularity plays a

crucial role in superconductivity, then the a band is the superconducting one, and the superconductivity in the b band is induced. Consequently, one has the situation similar to the above-described ‘‘p–c’’ scheme.

(3) Furthermore, the ISRG due to magnetic impurities may also be relevant for $\text{YBa}_2\text{Cu}_3\text{O}_7$. Let us assume that the main magnetic scatterers are antiferromagnetic (AF) spin fluctuations on the plane Cu sites. For the moment we assume these fluctuations to be static (see, however, the discussion below). Inelastic neutron-scattering studies [23] show that the AF correlations between the planes survive even in the fully oxygenated samples, where the intraplanar correlations are virtually non-existent (correlation length $\xi/a = 0.84 \pm 0.04$). This is in direct contradiction with the popular assessment that the intraplane AF correlations are more important than those between the planes. To understand the consequences of this fact we shall again consider the bonding and the antibonding band. The former is even with respect to the $z \rightarrow -z$ reflection, and the latter is odd. The standard hamiltonian for the magnetic scattering is

$$H_{ij}^s = - \sum_R \sum_{\alpha\beta} \langle i\alpha | J(\mathbf{r}-\mathbf{R}) S_R \sigma | j\beta \rangle,$$

where S_R is the spin of the impurity at point \mathbf{R} , and α, β are spin indices. In case of two antiferromagnetically correlated impurities in the two planes, $\langle i\alpha |$ and $\langle j\beta |$ must be of different parity to render a non-zero H_{ij}^s . This means that only τ_{ab}^s is non-zero.

In the previous paragraph we considered static impurities. In this context ‘‘static’’ means that the characteristic frequency of the AF fluctuations $\hbar\omega_{AF} \leq \pi T_c = 25$ meV. It is not clear yet how large ω_{AF} is in $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$. Detailed calculations will have to include the proper frequency dependence of the magnetic susceptibility in the same way as it is done with the phonons in the Eliashberg theory. It is obvious, however, that the qualitative conclusions will not change.

Let us discuss the consequences for the Josephson effect separately for each of the above cases. Rather than trying to explain the contradictory experimental results reported so far [1–8], we shall indicate some qualitative predictions of our model.

The supercurrent density through a grain boundary in a two-band superconductor can be written as

$J_s = \sum_{ij} J_c^{ij} \sin \phi^{ij}$, where J_c^{ij} is the Josephson critical current density corresponding to tunneling between the bands i and j , and ϕ^{ij} is the gauge-invariant phase difference of the order parameters Δ_i and Δ_j . In the simplest case of the Ginzburg–Landau regime [24]

$$J_c^{ij} = \pi \Delta_i \Delta_j / 4eR_{ij} k_B T,$$

where $R_{ij} = (\hbar/e^2)(p_F/2\pi\hbar)^2/\langle D \rangle$ is the tunneling resistance per unit area, $\langle D \rangle$ is the angle-averaged transparency of the barrier and $p_F = \min(p_{Fi}, p_{Fj})$. Following Geshkenbein and Larkin [25], we obtain immediately that if the order parameters have different signs, $\text{sign}(\Delta_i) = -\text{sign}(\Delta_j)$, then in the stationary case ($J_s = 0$) a finite phase difference appears, $\phi_{ij} = \pi$. This is similar to the “ π contact” considered by Bulaevskii et al. [26], but in our case it is due to the sign reversal of the order parameter in different bands.

Generally, the total critical current, J_c^{tot} , depends on the orientation of the boundary relative to the crystallographic axes because of the angular dependence of R_{ij} . It can become negative for certain directions when the contribution due to interband tunneling prevails. The condition is $J_c^{12} + J_c^{21} > J_c^{11} + J_c^{22}$ for the HTS/HTS junction and $J_c^{12} > J_c^{11}$ for the HTS/LTS one. To some extent this effect is similar to that considered by Sigrist and Rice [27] for the d pairing, but some of our predictions differ qualitatively, as discussed below.

(a) Let us first consider the c–p scenario. For a HTS/LTS junction the tunnel resistance $R_{12}(\theta)$ depends strongly on the angle θ relative to the b -axis, namely $R_{12}(\theta)$ has a sharp minimum at $\theta=0$ due to the strong angle dependence of a barrier transparency $\langle D \rangle$ for a tunneling process. Moreover, according to band-structure calculations [21] the kinetic energy of carriers along the chains is larger than that in the plains, thus leading to larger $\langle D \rangle$ values. As a result, $J_c^{\text{tot}}(\theta) < 0$ for small θ , whereas for all other angles $J_c^{\text{tot}}(\theta) > 0$. Therefore an intrinsic π phase shift will occur in this case between tunneling along the a and along b directions. Then a DC SQUID with junctions on the a and b faces of a crystal, will show a $\Phi_0/2$ shift of a field dependence $I_c(H)$. This effect was observed in Refs. [1,3,4] and attributed to the $d_{x^2-y^2}$ pairing state. Another consequence is a shift of a Fraunhofer pattern for a single junction formed on the corner of a crystal, because J_c changes sign along the junction, as was discussed in Refs. [1 and 4] for d pairing. Evidently, the same effect will take place in the case considered.

We should also mention that the nonzero Josephson current, observed for c -axis tunneling in Pb/insulator/ $Y_{1-x}\text{Pr}_x\text{Ba}_2\text{Cu}_3\text{O}_7$ tunnel junctions in Ref. [5] is contradictory to the $d_{x^2-y^2}$ symmetry. Indeed, a nonzero Josephson current was predicted theoretically for c -axis contact between s wave and d wave superconductors in Ref. [28], but only in the second order in the boundary transparency $\langle D \rangle$, therefore this model cannot explain the rather large values of the $I_c R_n$ products of the order of 1 meV observed in Ref. [5]. On the other hand, this observation is consistent with the suggested c–p scenario. The reason is that, contrary to the case of $d_{x^2-y^2}$ symmetry, the average order parameter in the ab plane is nonzero.

Interesting consequences appear for HTS/HTS (grain-boundary) junctions. As follows from the above arguments, if $\theta=0$ in *only one* of the grains, then the grain boundary is a π contact, otherwise it is a conventional one. Consider a closed contour crossing N grain boundaries. The flux-quantization condition in zero external field reads $n\Phi_0 = LI_s^{ij} + \sum_{m=1,N} (\Phi_0/2\pi) \phi_{ij}^{(m)}$, where L is the self-inductance of a ring and $\phi_{ij}^{(m)}$ is a phase difference across the m th junction. Then it follows immediately, that if a contour crosses an *odd number* of $\theta=0$ junctions, a spontaneous magnetization of a ring with half-integer flux quantum will occur, and when it crosses an even number of $\theta=0$ junctions the flux quantum will be integer.

Spontaneous magnetization with half-integer flux quantum in a three-junction ring and with integer flux quantum in a two-junction ring was demonstrated recently for $\text{YBa}_2\text{Cu}_3\text{O}_7$ in Ref. [6]. In this experiment all grain boundaries were of $\theta=0$ type. Thus, the results [6] are in agreement both with our proposal and with the d wave scenario discussed by Sigrist and Rice. To distinguish between these two explanations measurements for different grain orientations are necessary. At the same time, the absence of an angular dependence of J_c observed in Ref. [2] for a number of different grain-boundary orientations in YBCO does not contradict our scheme. Indeed, in Ref. [2] all six grain boundaries have had $\theta \neq 0$ which results in $J_c^{\text{tot}}(\theta) \approx J_c^{11}(\theta) \approx \text{const}$.

Another interesting phenomenon observed first in Bi based HTS [29] and more recently in YBCO [8] is the paramagnetic Meissner effect (“Wohlfleben effect”). The explanation was proposed in Refs. [27,29,30] in terms of intrinsic π junctions between

weakly coupled superconducting grains, giving rise to spontaneous orbital currents in arbitrary directions. An external magnetic field will align those spontaneous current loops and can produce a net positive magnetization. Therefore, the existence of π junctions between at least some of the superconducting grains is a key point for the Wohleben effect. As discussed above, such intrinsic π junctions may exist in the considered two-band superconductor with interband gap-sign reversal, thus leading to the possibility of the Wohleben effect.

(b) For our second scenario a sign of the total critical current in an HTS/LTS and an HTS/HTS junction in any given direction depends crucially on the relation between the current components J_c^{12} and J_c^{11} , i.e. on the corresponding tunnel resistances. From symmetry considerations, there exists no fundamental reason for a sign change of $J_c^{12} - J_c^{11}$ versus θ in the ab plane. As a result, the intrinsic phase shift between the two bands cannot be detected by Josephson experiments, similar to the c-p scenario discussed above. In all junction geometries such an ISRG superconductor will behave like a conventional s wave one.

However, a possibility of the Wohleben effect still exists: Each given contour would include an even number of π contacts, which in an ideal case would compensate one another. But in reality the tunnel resistances of these contacts, depending of the local state of each grain boundary, will be different, so that the compensation would become incomplete.

We note, that this scenario may be relevant not only to YBCO but also to all double-plane materials, like Bi based compounds.

The main goals of the current paper were to demonstrate the possibility of the existence of an s wave superconductor with the sign reversal of the gap, to point out some factors which favor such a state in $\text{YBa}_2\text{Cu}_3\text{O}_7$, and to emphasize that some experiments interpreted as unambiguous evidence for the d wave pairing can, in fact, be explained by the suggested ISRG s pairing.

In addition to that, we would like to outline some implication of our analysis to a model of spin-fluctuation induced superconductivity (Ref. [31] and references therein). In this model, AF fluctuations are dynamic, and serve as the intermediate bosons to give superconductivity. Only one plane is considered, and,

much in the same spirit as in our analysis, the order parameters $\Delta(k)$ and $\Delta(k+Q)$, where Q is the AF vector ($\pi/a, \pi/b$), are of the opposite signs, which in the case of the $\text{YBa}_2\text{Cu}_3\text{O}_7$ Fermi surface leads to the $x^2 - y^2$ symmetry for $\Delta(k)$. Apparently, if one considers two AF coupled planes, and two bands, a and b, then only in the a-b channel does a non-zero pairing potential appear. This is similar to the observation [32] that in YBCO the *gerade* (with respect to $z \rightarrow -z$) phonons contribute to the intraband (a-a and b-b) coupling only, and the *ungerade* phonons to the interband coupling only. Even without solving the corresponding equations, one can immediately predict the results: Since in a bilayer there is no problem having gaps of the same sign on a given sheet of the Fermi surface, an s wave solution must exist, with Δ_a and Δ_b having opposite signs. Direct numerical calculations show indeed that the Montoux-Pines model for a bilayer has a stronger instability in the s channel with ISRG than in the d-channel [33]. Another interesting point is that the intraband phonon pairing and the interband spin-fluctuation pairing can coexist and even help each other.

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