

Superconducting order parameter in bilayer cuprates: Occurrence of π phase shifts in corner junctions

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We study the order-parameter symmetry in bilayer cuprates such as Y-Ba-Cu-O, where interesting π phase shifts have been observed in Josephson junctions. Taking models that represent the measured spin-fluctuation spectra of this cuprate, as well as more general models of Coulomb-correlation effects, we classify the allowed symmetries and determine their associated physical properties. π phase shifts are shown to be a consequence of repulsive interactions, independent of whether a magnetic mechanism is operative. While it is known to occur in d states, this behavior can also be associated with (orthorhombic) s symmetry when the two subband gaps have opposite phase. Implications for the magnitude of T_c are discussed.

The observation in Y-Ba-Cu-O of unusual Josephson-junction behavior¹⁻⁴ is one of the most important experimental results to emerge from the cuprate literature in recent years. Here in a Josephson superconducting quantum interference device (SQUID) experiment the two junctions are configured so that their normals lie along the a and b axes of the CuO_2 plane. This measurement has been widely interpreted as support for a d symmetry of the order parameter, as well as for a magnetic mechanism for superconductivity. In this paper we show that both of these inferences may be inappropriate. For notational precision, throughout this paper we use the terms s (or d) symmetry to correspond to states which have the same (or opposite) sign under a $\pi/2$ rotation. Thus the d states under consideration are not necessarily of the specific $d_{x^2-y^2}$ form.

The gap equation for bilayer systems has been studied earlier in the context of a magnetic mechanism for superconductivity.^{5,6} There it was observed that the d -symmetric state of the single-layer problem is transformed to a pair of in-phase d states on each of the two subbands, and that these compete with a pair of out-of-phase s states. Here we take the problem to a greater level of generality, establishing that this situation persists for a wide class of repulsive interactions, which are unrelated to the antiferromagnetic spin-fluctuation picture. Alternate classes of the order-parameter symmetry are also generated. These correspond to in-phase s states and out-of-phase d states. We establish how the relative stability of the two competing states is affected by changes in band structure, orthorhombicity, and hole filling.

It should not be surprising that d states have an origin beyond the antiferromagnetic spin exchange models. In a one-layer cuprate, the lattice symmetry requires that all gap states are either even (s) or odd (d) under a $\pi/2$ rotation. In bilayer systems, these one-layer states generalize naturally to a pair of even or odd, in-phase or out-of-phase states, associated with each of the two subbands. Thus, as one of two allowed states, d symmetry should be widespread, and independent of the microscopic details of the model.

In the presence of both intra- and interlayer interactions (V_{\parallel} and V_{\perp}), the weak-coupling BCS gap equation becomes

a set of coupled equations for the gaps on each of the subbands. It is simpler to write the gap equations in terms of the two subband gaps Δ_+ , Δ_- rather than the intralayer (Δ_{\parallel}) and interlayer (Δ_{\perp}) components. These are related via the unitary transformation which diagonalizes the Hamiltonian. In this model t_{\perp} is the matrix element for hopping between layers; t and t' refer to the first- and second-nearest-neighbor in-plane hopping which may contain orthorhombic effects. On-site Coulomb effects U are assumed to enter via a renormalization of the band-structure parameters as shown by Si *et al.*⁷

Following the usual procedure,⁸ the gap equations become

$$\Delta_+ + \Delta_- = - \sum_{\mathbf{q}'} \frac{V_{\parallel} \Delta_+}{2E_+} \tanh\left(\frac{E_+}{2T}\right) - \sum_{\mathbf{q}'} \frac{V_{\parallel} \Delta_-}{2E_-} \tanh\left(\frac{E_-}{2T}\right), \quad (1a)$$

$$\Delta_+ - \Delta_- = - \sum_{\mathbf{q}'} \frac{V_{\perp} \Delta_+}{2E_+} \tanh\left(\frac{E_+}{2T}\right) + \sum_{\mathbf{q}'} \frac{V_{\perp} \Delta_-}{2E_-} \tanh\left(\frac{E_-}{2T}\right), \quad (1b)$$

where the superconducting quasiparticle energies are $E_{\pm} = \sqrt{\epsilon_{\pm}^2 + \Delta_{\pm}^2}$, where

$$\epsilon_{\pm} = -2t[\cos(q_x a) + \cos(q_y b)] + 4t' \cos(q_x a) \cos(q_y b) \pm t_{\perp}. \quad (2)$$

It follows that each of the two subband gaps can be written in terms of the parallel and perpendicular components as

$$\Delta_{\parallel} = (\Delta_+ + \Delta_-)/2, \quad \Delta_{\perp} = (\Delta_+ - \Delta_-)/2. \quad (3)$$

In the case of a magnetic pairing mechanism, the two interactions are related to components of the dynamical spin susceptibility. This susceptibility has been calculated for the bilayer cuprate Y-Ba-Cu-O,^{7,9} in the strong U limit. For realistic Fermi surface shapes, and moderate in-plane and out-of-plane exchange interactions, the results are in reasonable agreement with neutron experiments.¹⁰ Because the in-plane magnetism is not independent of interplane effects any proper treatment of spin-fluctuation-induced superconductivity should incorporate both components. A reasonable ap-

proximation of both the theoretical results⁹ and the experimental neutron data¹⁰ is to take

$$V_{\parallel} = g_{\parallel}^2 \chi_{\parallel}(\mathbf{q} - \mathbf{q}'), \quad (4a)$$

$$V_{\perp} = g_{\perp}^2 \chi_{\perp}(\mathbf{q} - \mathbf{q}') = -g_{\perp}^2 \chi_{\parallel}(\mathbf{q} - \mathbf{q}'), \quad (4b)$$

with

$$\chi_{\parallel}(k_x, k_y) = \frac{1}{[1 + J_o(\cos k_x a + \cos k_y b)]^2} \quad (4c)$$

and $J_o \approx 0.3$. Here we have absorbed overall coefficients into the coupling constant prefactors g_{\parallel} and g_{\perp} . This model is similar to that used in Ref. 5, except that we have assumed an arbitrary relation between the magnitudes of two superconducting coupling constants, which are taken to be the same in Ref. 5. Moreover, we fit the dynamical susceptibility to neutron, rather than NMR data.¹¹

It may be noted from Eq. (4c) (as well as experimental neutron data¹⁰) that the antiferromagnetic fluctuations show up as a weak peak around $(\pi/a, \pi/a)$ with short coherence lengths, suggesting that the system is far from any real instability; thus high T_c is difficult to explain.¹¹ Consequently we explore more general mechanisms by extending Eqs. (4a) and (4b) to the case where the overall signs are unconstrained and the $\mathbf{q} - \mathbf{q}'$ peaks occur at arbitrary wave vector. Furthermore, we vary the width of the peak structure by changing J_o and therefore incorporate the limit of rather structureless interactions. The model is viewed as a general representation of pairing mechanisms of the electronic and phononic variety. Since the former usually derives from a generalized susceptibility, and the latter from a phonon propagator, there are no sign changes as a function of momentum transfer. This poses important constraints on the allowed superconducting states. We define

$$V_{\parallel, \perp} = \frac{\lambda_A, \lambda_B}{\{1 - J_o[\cos(k_x \pm Q_x) + \cos(k_y \pm Q_y)]\}^2}, \quad (5)$$

where all signs are summed over. We divide our numerical analysis into four distinct cases in which either the interlayer or the intralayer interaction dominates and in which the respective interaction is repulsive ($\lambda > 0$) or attractive ($\lambda < 0$). These results are summarized in Figs. 1 and 2 for the case of characteristic wave vectors $\mathbf{q} - \mathbf{q}'$ along $(\pi/a, \pi/a)$ and along $(\pi/a, \pi/2a)$. The latter wave-vector choice is made for illustrative purposes only, to show the generality of our results. Plotted in these figures are the form of the gap functions in the two regimes. The figures on the left (right) in each box correspond to intralayer (interlayer) dominated behavior. Our conclusions from both Figs. 1 and 2 may be succinctly summarized. We find that d -symmetry is associated with repulsive and s symmetry with attractive interactions. In-phase gap behavior occurs when the intralayer interaction is the larger; out-of-phase behavior arises in the opposite case. This phase dependence can be deduced from Eqs. (3). In the case of dominant interlayer effects, $|\Delta_{\perp}| > |\Delta_{\parallel}|$. This will occur when Δ_+ and Δ_- have opposite signs.

To establish the universality of these results, we have varied the Fermi surface shape (via the ratio of t'/t), the posi-

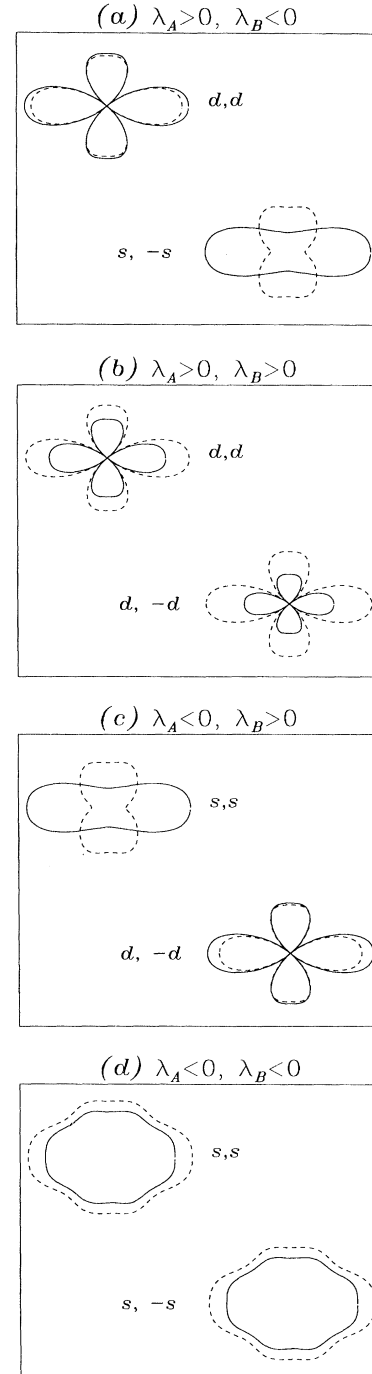


FIG. 1. Superconducting gap for interactions peaked at $\mathbf{q} - \mathbf{q}' = (\pi, \pi)$, for the case of attractive and repulsive intralayer (λ_A) and interlayer (λ_B) interactions. Figures on left (right) are for intra- (inter-) layer dominated regimes. Solid and dashed lines represent Δ^+ and Δ^- , respectively.

tion of the Fermi energy or hole filling, and the width J_o of the peak structure. These variations introduce only quantitative but not qualitative changes in the physical picture shown in the two figures.

It is important to note from Figs. 1(a)–(c) and 2(a) and (b)

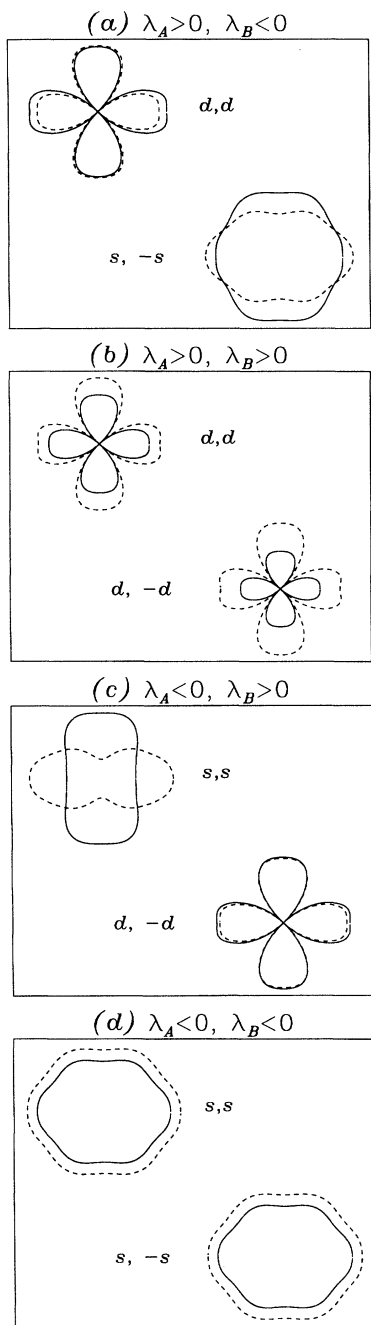


FIG. 2. Superconducting gap for interactions peaked at $\mathbf{q}-\mathbf{q}'=(\pi, \pi/2)$.

that the out-of-phase s - and d -wave states will exhibit π phase shifts in a corner SQUID experiment.¹⁻⁴ This corresponds to a change in sign of the “sum” order parameter Δ_{\parallel} of Eqs. (3) upon varying from 0 to $\pi/2$. While not a general feature of all solutions, its presence requires (a modest amount of) orthorhombicity. The observation of π phase shifts in bilayer cuprates is thus not as strong a constraint on the order-parameter symmetry as in one-layer materials. All orthorhombic states which exhibit these π phase shifts will

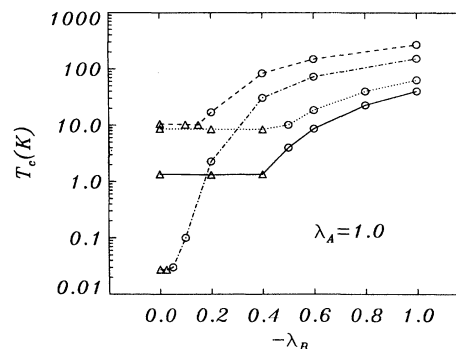


FIG. 3. Effect of interlayer correlation on the superconducting transition temperature T_c . (Δ) indicate the (d,d) states and (\circ) represent the $(s,-s)$ states. We consider different shapes of Fermi surface and Fermi energies—orthorhombic lattice with next-nearest-neighbor hopping, $E_F=-0.2$ (dotted line), $E_F=-0.1$ (solid line); and tetragonal lattice with $t'=0$, $E_F=-0.6$ (dot-dashed line), $E_F=-0.4$ (dashed line).

also show finite c -axis tunneling in untwinned crystals.¹² However, twinning effects (if they average fully over the a and b axes), will lead to a cancellation of Josephson coupling, whenever the corner SQUID experiment has the observed π phase shift.

It should be stressed that the out-of-phase s states have the additional advantage as a candidate gap symmetry, over d states (in or out of phase), of being relatively insensitive to impurity effects. Another advantage of the $s,-s$ state should be noted: this state can be compatible with neutron experiments,¹⁰ which show no nodal signature. In contrast to experiment, because nodes are not present, at least in the clean limit, power laws in thermodynamical properties¹³ are not expected.

We have searched for nodal behavior in these s -wave states with some care, since there is recent photoemission evidence¹⁴ to suggest that they may exist in bilayer Bi-Sr-Cu-O. Several observations are important to note in this context. (1) As the interlayer hopping t_{\perp} becomes small the magnitudes of the two gaps become equal and they are less able to respond to orthorhombicity by producing gap anisotropy. Consequently Bi-Sr-Cu-O 2212, which is believed to have a very small t_{\perp} , would be unlikely to exhibit nodal s -wave behavior. (2) The eight-node s state which has been conjectured as a candidate for Bi-Sr-Cu-O (Ref. 14) appears quite generally as a metastable state whose solution has a lower T_c than the nodeless s -wave or (four-node) d -wave symmetric gap. Within the manifold of metastable states, the more nodes, the lower is the T_c . (3) We have studied solutions to a separable pairing potential model in which the susceptibility of Eq. (4c) is replaced by a product of cosine terms: $\cos(q_x a)\cos(q'_x a) + \cos(q_y b)\cos(q'_y b)$, since it was speculated¹⁵ that this potential would give rise to an eight-node s state. We find that d -wave states arise naturally in this model as well, and they are always more stable than s -wave states.

In Fig. 3 is plotted the dependence of the transition temperature on the interplane coupling constant T_c for the magnetic pairing model of Fig. 1(a), for two different Fermi surface shapes⁷ corresponding to Y-Ba-Cu-O (with two-hole

concentrations as well) and La-Sr-Cu-O ($t'=0$). Here, because we use a weak-coupling approximation, the absolute values of T_c are not meaningful. However, the relative changes with different parametrizations are expected to be accurately captured. The circles correspond to the out-of-phase s states and triangles to in-phase d states. As expected, for sufficiently small interplane coupling the d -wave state is the more stable; however, depending on the band structure and Fermi surface shape, this state may be readily destabilized to a pair of s states by the introduction of a very small interplane interaction. This reflects the general result that (nodeless) s -wave states are able to take better advantage of the superconducting interaction than can d -wave states, which require a cancellation of positive and negative terms to satisfy the gap equation. Note that in the La-Sr-Cu-O model the T_c 's are generally higher as a consequence of the better Fermi surface nesting along the direction of the wave vector (π, π) . For each parameter set, the various curves tend to coalesce at higher λ_B , where the (s -like) states are found to be more isotropic. This is a consequence of the fact that these isotropic states are not able to utilize the Van Hove singularity effect, which is relatively more important for $d_{x^2-y^2}$ states.

In summary, by solving the gap equation for bilayer models with repulsive interactions, we find that $d_{x^2-y^2}$ states arise quite generally and are not uniquely associated with wave-vector structure along the antiferromagnetic direction. Moreover, we have established that π phase shift behavior,

which is often cited as the strongest evidence for d -wave pairing, can also be associated with (orthorhombic) s symmetry when the two subband gaps have opposite phase. This state has some advantages over d states in large part because of the relatively small sensitivity of T_c to nonmagnetic impurities. An important conclusion from our analysis is that there are always competing states in bilayer systems, and that the order-parameter symmetry would be expected to vary from cuprate to cuprate as well as within a given cuprate class at different hole concentrations. One can conclude that the Josephson-junction data, in particular, provide strong evidence for superconductivity mediated by some form of repulsive interaction. On the other hand, these collected observations (in bilayer cuprates) weaken the often cited support for theories of spin-fluctuation-mediated superconductivity.

Note added in proof. Recently, we received unpublished work from K. Kuboki and P. A. Lee, in which an RVB description of bilayer superconductivity was used to infer a spontaneous breaking of tetragonal symmetry. This s, d mixing will not occur in the present model, as a result of the free energy form which contains a quadratic, rather than quartic, mixing of the in- and out-of-plane gaps.

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