Josephson current-phase relationships with unconventional superconductors

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The current (energy)-phase relationships for Josephson coupling involving unconventional superconductors are investigated. It is shown that in general the energy can have minima at phase differences of neither 0 nor π even for superconductors that do not break time-reversal symmetry in the bulk.

Recently Josephson interference experiments have played a very important role in studying whether the cuprates are d-wave (and in particular B_{1g} or $d_{x^2-y^2}$) superconductors.[1–4] In particular these experiments are based on the recognition[5–7] that 0 and π junctions can be formed between an s-wave and a d-wave superconductor[1,2] or between different grains of the d-wave superconductor itself.[3,4] By 0 and π junctions one means that, with the same convention for the phases of the superconducting order parameters, the π junctions have the current-phase relationship shifted from that of the 0 junctions by π; and in particular, while the 0 junctions have their energy minimum at phase difference $\chi = 0$, the π junctions have their energy minimum at $\chi = \pi$. That this is possible is due to the fact that, the order parameter of, e.g., B_{1g} symmetry changes its sign (or, more precisely, undergoes a phase change of π) when one moves from momenta closer to $\pm\hat{a}$ axis to those closer to the $\pm\hat{b}$ axis. In these publications the assumption that the current-phase relationships are sinusoidal is made either implicitly or explicitly.

Are 0 and π junctions the only possibilities, if one is only interested in superconductors without broken time-reversal symmetry? By the periodicity of the current in the phase difference χ with period 2π one has

$$I(\chi) = I(\chi + 2\pi) \ , \qquad (1)$$

while time-reversal symmetry implies

$$I(\chi) = -I(-\chi) \ . \qquad (2)$$

If one further assumes that I is sinusoidal in χ, using Eq. (1) one can write $I = I_c\sin(\chi - \alpha)$ for some constant α. Then Eq. (2) immediately implies that $\alpha = 0$ or π (mod 2π) are the only possibilities, the ones that were mentioned above. Correspondingly the energy must be minimum at either $\chi = 0$ or π. α deviating from these values is possible only under broken time-reversal symmetries.[5,8] Below I shall confine myself to cases where this symmetry is not broken.

It is, however, known[9,10] that a sinusoidal current-phase relationship is only a special case in Josephson tunneling, attainable only for, e.g., sufficiently high and wide potential barriers between the two superconductors (for convenience of referral later, I shall call this the tunnel-junction limit) or temperatures sufficiently close to T_c. What happens in general? A moment of reflection shows that Eqs. (1) and (2) impose very little restrictions. For example, while one knows that at $\chi = 0$ and π, $I = 0$ and hence are energy extrema, it is not necessary that either one will be a minimum.

In this paper I shall show that for the general Josephson coupling involving a superconducting order parameter with sign changes around the Fermi surface, that a χ_m junction with energy minima at $\chi = \chi_m$, neither 0 nor π is indeed allowed.[11,12] I shall first give a plausibility argument. Then I shall verify this by explicit microscopic calculations. Possible experimental consequences will then be discussed.

To see why $\chi_m \neq 0$ or π should be expected in general, consider a junction between an s-wave and a B_{1g} superconductor [order parameter $\Delta(\hat{k}) = \Delta_0^d(\hat{k}_x^2 - \hat{k}_y^2)$]. Generalization to the other order parameters is trivial and will not be presented. The B_{1g} order parameter consists of different parts on the Fermi surface where it differs in phase by π. I shall refer to them as part 1 (for $\hat{k}$ closer to $\pm\hat{a}$) and part 2 ($\hat{k}$ closer to $\pm\hat{b}$), respectively. For definiteness but without loss of generality I shall choose the phase of the s-wave superconductor to be zero and that of part 1 to be χ, which I shall also refer to as the overall phase of the B_{1g} order parameter. Imagine that the supercurrent through the junction between the two superconductors is the sum of two contributions from each portion of the Fermi surface, thus effectively we have two junctions in parallel. Since both superconductors are singlet each junction is qualitatively like one between two s-wave superconductors (see Ref. 13 and below). I shall take the simplest form for a nonsinusoidal current-phase relationship by adding a $\sin(2\chi)$ term to the usual $\sin\chi$ term. Thus I write the contribution to the Josephson current from part 1 of the Fermi surface as

$$I_1(\chi) = \gamma_1[\sin\chi - \beta_1\sin(2\chi)] \ . \qquad (3)$$

I shall for definiteness assume $\gamma_1, \beta_1 > 0$, i.e., that the form of I_1 has the form as in Fig. 1.[14] The contribution of part 2 is of the same form except that χ has to be shifted by π:

$$\begin{aligned} I_2(\chi) &= \gamma_2\{\sin(\chi + \pi) - \beta_2\sin[2(\chi + \pi)]\} \\ &= -\gamma_2[\sin\chi + \beta_2\sin(2\chi)] \ , \end{aligned} \qquad (4)$$

where I have also introduced new constants γ_2, β_2 since the magnitude of the critical current and the "skewness" are in general different. The total current through the junction is simply $I(\chi) = I_1(\chi) + I_2(\chi)$. Simple manipulation shows that $I = 0$ at either

$$\sin\chi = 0 , \tag{5}$$

i.e., $\chi = 0$ or π, or

$$\cos\chi = \frac{\gamma_1 - \gamma_2}{2(\beta_1\gamma_1 + \beta_2\gamma_2)} , \tag{6}$$

which indicates new possibilities for $I = 0$ and thus energy extrema if its right-hand side has magnitude less than 1. Expanding I near $\chi = 0$ one gets $I(\chi) \approx [\gamma_1 - \gamma_2 - 2(\beta_1\gamma_1 + \beta_2\gamma_2)]\chi + \cdots$. Thus $\chi = 0$ remains an energy minimum only if $[\gamma_1 - \gamma_2 - 2(\beta_1\gamma_1 + \beta_2\gamma_2)] > 0$. It becomes an energy relative maximum if the sign is reversed. One can show easily that $\chi = \pi$ remains an energy relative maximum if $[\gamma_1 - \gamma_2 + 2(\beta_1\gamma_1 + \beta_2\gamma_2)] > 0$. Notice that $[\gamma_1 - \gamma_2 - 2(\beta_1\gamma_1 + \beta_2\gamma_2)] < 0$ and $[\gamma_1 - \gamma_2 + 2(\beta_1\gamma_1 + \beta_2\gamma_2)] > 0$ implies that $|\frac{\gamma_1 - \gamma_2}{2(\beta_1\gamma_1 + \beta_2\gamma_2)}| < 1$ and thus new energy minima of Eq. (6) will be realized.

Thus new energy minima at $\chi_m \neq 0, \pi$ will always occur if $\beta_{1,2} \neq 0$ and γ_1 sufficiently close to γ_2, i.e., the basic current-phase relationship is skewed and the couplings to the parts of the order parameter with opposite signs are not too different.

Now I shall present a microscopic calculation showing that the above physics does indeed occur. I shall consider a pinhole between an isotropic s-wave superconductor and a B_{1g} superconductor, i.e., the two superconductors couple only via a small hole. This geometry is chosen for the simplicity of the calculation. Similar behavior is expected for a junction if the potential barrier between the superconductors is sufficiently low or thin.[10] I shall call the tunneling direction the $\hat{x}$ axis and study the energy-phase relationship as a function of θ, the angle of rotation about $\hat{z} = \hat{c}$ axis between the $\hat{x}$ axis and the crystalline $\hat{a}$ axis for the B_{1g} superconductor (i.e., $\hat{a}$ and $\hat{b}$ are in the x-y plane). I shall show that for θ sufficiently close to $\pi/4$, the junction has energy minima at $\chi = \chi_m$ with $\chi_m \neq 0, \pi$. The expression of the current, ignoring surface depairing, can be adopted directly from a previous calculation:[13]

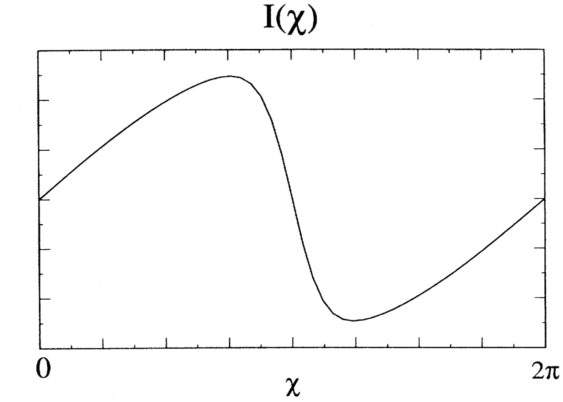

FIG. 1. A nonsinusoidal current-phase relationship.

$$I = 2S \int \frac{d\Omega}{4\pi} N(0)|v_{fx}|\pi T \sum_{\epsilon_n} |\Delta^L||\Delta^R(\hat{k})| \frac{\sin\chi(\hat{k})}{\epsilon_n^2 + \alpha^L\alpha^R + |\Delta^L||\Delta^R|\cos\chi(\hat{k})} . \tag{7}$$

The notations are as follows: $N(0)$ is the density of states for one spin, S the area, T the temperature, $v_{fx}(\hat{k})$ is the velocity of momentum $\hat{k}$ along the $\hat{x}$ direction. I shall assume that both the superconductors have cylindrical Fermi surfaces of identical radii with the open directions along $\hat{c} = \hat{z}$, hence $v_{fx} = v_f\cos\phi$, here ϕ is the azimuthal angle between $\hat{k}$ and $\hat{x}$. $|\Delta^{L,R}(\hat{k})|$ are the magnitudes of the gap for the superconductor on the left and right along $\hat{k}$. I shall assume that $|\Delta^L|$ is independent of ϕ and $|\Delta^R| = \Delta_o^d|\cos[2(\phi - \theta)]|$. ϵ_n are the Matsubara frequencies, $\alpha^{L,R} \equiv [\epsilon_n^2 + (\Delta^{L,R})^2]^{1/2}$, and $\chi(\hat{k})$ the phase difference of the order parameter between the two superconductors for momentum along $\hat{k}$. $\chi(\hat{k})$ is given by

$$\begin{aligned} \chi(\hat{k}) &= \chi \quad \text{if } \cos[2(\phi - \theta)] > 0 \\ &= \chi + \pi \quad \text{if } \cos[2(\phi - \theta)] < 0 \end{aligned} \tag{8}$$

corresponding to the two lobes of the B_{1g} order parameter on the Fermi surface. I shall call χ the overall phase difference between the two superconductors. One should notice that Eq. (7) has the necessary qualitative features used above in the discussion demonstrating the possibility of $\chi_m \neq 0, \pi$.

I shall discuss mostly only the energy-phase relationships. The current can be obtained easily by taking the derivative ($I = \frac{2e}{\hbar}\frac{\partial E}{\partial \chi}$). The (free) energy difference between the junction with phase difference χ and with phase difference 0 can be obtained from Eq. (7):

$$\begin{aligned} \Delta E(\chi,\theta) &\equiv E(\chi,\theta) - E(0,\theta) \\ &= \frac{h}{8e^2R} \int d\phi|\cos\phi|T \sum_{\epsilon_n} \ln\frac{\epsilon_n^2 + \alpha^L\alpha^R + \Delta^L\Delta^R(\phi)}{\epsilon_n^2 + \alpha^L\alpha^R + \Delta^L\Delta^R(\phi)\cos\chi} , \end{aligned} \tag{9}$$

where $\Delta^R(\phi) = \Delta_0^d\cos[2(\phi - \theta)]$. Here $1/R = 2N(0)e^2v_fS/\pi$ is the normal-state conductance through the junction. Note that besides the symmetries $\Delta E(\chi,\theta) = \Delta E(-\chi,\theta) = \Delta E(2\pi + \chi,\theta)$ [cf. Eqs. (1) and (2)] one has $\Delta E(\chi,\theta) = \Delta E(\chi,-\theta)$ due to reflection symmetry about the $\hat{x}$ axis and $\Delta E(\chi,\theta) = \Delta E(\chi + \pi,\theta + \frac{\pi}{2})$ since a rotation of $\frac{\pi}{2}$ of the B_{1g} order parameter is equivalent to a phase change of π. I shall discuss only $0 < \theta < \frac{\pi}{2}$, the other regions can be obtained using the symmetries discussed above.

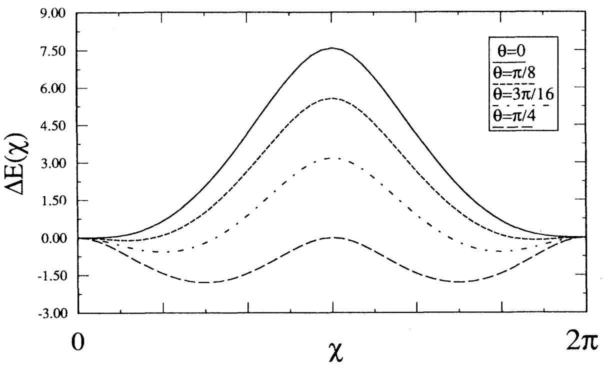

FIG. 2. ΔE of Eq. (9) as a function of χ between an s-wave and a B_{1g} superconductor rotated by θ as described in text. The gap maxima for the superconductors are chosen to be 17.6 K and $\sqrt{2} \times 176$ K. The temperature is at 5 K. Energy is in units of $\frac{h}{e^2 R} \times$ Kelvin.

$\Delta E(\chi, \theta)$ as a function of χ for various values of θ is plotted in Fig. 2. One sees that $\chi_m = 0$ for $\theta < \theta_c$ and $\chi_m = \pi$ for $\theta > \frac{\pi}{2} - \theta_c$ for some critical angle θ_c. However, for $\theta_c < \theta < \frac{\pi}{2} - \theta_c$ the energy indeed possesses minima at $\chi_m \neq 0, \pi$. Notice that for these values of θ's the current-phase relationships are very peculiar, with $I = 0$ at $0, \pi$ and $\chi_m, 2\pi - \chi_m$. The position χ_m for the minima as a function of θ for $\theta_c < \theta < \frac{\pi}{2} - \theta_c$ is practically a straight line.[15] The fit to a straight line is shown as the dashed line in Fig. 3.

Extension to tunneling between two unconventional superconductors is straightforward, and I shall only show some of the results. I shall first consider the case where the s-wave superconductor above is replaced by a B_{1g} superconductor with $\hat{a} = \hat{x}$ and $\hat{c} = \hat{z}$. In this case the symmetries in θ discussed above remain valid. I find that again the energy can have minima at $\chi_m \neq 0, \pi$. χ_m versus θ for $\theta_c < \theta < \frac{\pi}{2} - \theta_c$ are again indistinguishable from a straight line,[15] and is shown as the full line in Fig. 4. The dashed line shows the case where the left superconductor has $\hat{a}$ rotated by $\frac{\pi}{6}$ from the $\hat{x}$ axis (with $\hat{a}$ and $\hat{b}$ still in the x-y plane) and the right superconductor is

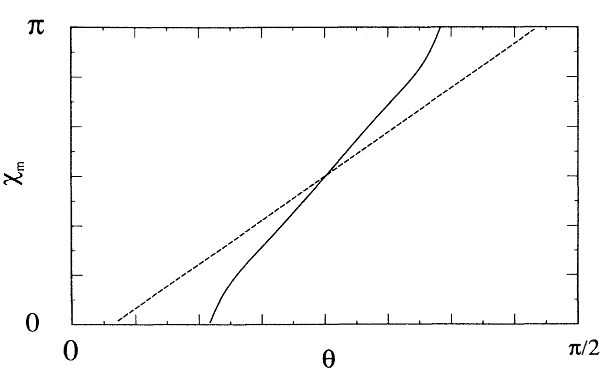

FIG. 3. χ_m versus θ for the s-d junction. Dashed line is the numerical result for unit transparency. The effect of finite barrier height and/or width is schematically shown as the full line. The parameters are as in Fig. 2.

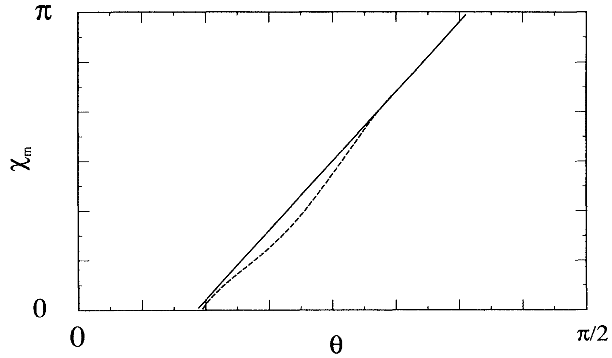

FIG. 4. χ_m versus θ for the d-d junctions as described in text. The parameters are as in Fig. 2.

rotated *further* by θ. This breaks the even symmetry of ΔE in θ. χ_m versus θ where $\chi_m \neq 0, \pi$ is plotted as the dashed line in Fig. 4. Thus for the same misorientation θ the value of χ_m can depend on the tunneling geometry, though the differences are small in this limit of unit transparency.

In the above the transmission coefficient through the pinhole was put at unity. In the presence of a barrier the relative contributions from quasiparticles with momenta further away from the junction normal will decrease due to the higher effective barrier height. Also the deviation from the sinusoidal current-phase relationship from each momenta will be less.[10] Thus the range of θ where $\chi_m \neq 0, \pi$ will decrease. I represent this behavior schematically as the full line in Fig. 3. Notice thus for given θ, the value of χ_m then in general depends on, e.g., the transmission coefficient through the junction. In the tunnel-junction limit the transition between $\chi_m = 0$ and π will be replaced by a jump at some critical value θ ($\pi/4$ in the case of Fig 3.)

In the rest of the paper I shall turn to some potential experimental consequences of these unconventional energies and/or current-phase relationships, assuming that at least one of the superconductors involved is indeed an unconventional superconductor. Consider the two-junction rings made between two Y-Ba-Cu-O grains as in Ref. 3. The two junctions, in principle, have the same misorientation angle θ. If these two junctions are identical (except possibly the area), then they have the same χ_m, and no spontaneous flux would be generated in the ring. However, if they do not have the same, say, transmission coefficients then in general their χ_m can be different, say $\chi_m^{a,b}$. (Here a and b do *not* refer to crystalline axes.) Then a finite flux can be spontaneously generated, which is given by $\frac{\Phi_o}{2\pi}(\chi_m^a - \chi_m^b)$ in the large inductance limit. However, if one produces many such rings, then since on the average the junctions are identical, this would produce a spread of the values of the measured fluxes about the ideal value of 0, with the width determined by the magnitude of θ and the variations in the barrier involved in the junctions.

Similarly consider the borders between two misoriented grains, as in the inclusions of Chaudhari and Lin[4] or Kirtley *et al.*[18] Although the misorientations are identical for the two interfaces originating from a corner, the values of χ_m for these two interfaces in general differ, either due to the geometric effects as discussed in Fig. 4, or the difference in the transmission coefficients of the interfaces. Then an argument as in Bulaevskii, Kuzii, and Sobyanin[16] or Millis[17] shows immediately that magnetic flux will be generated near the corner. In fact even for a planar interface different portions of the interface may have different transparency, perhaps due to the randomness of the strength or positions of defects that are present along the boundary. Thus in general χ_m can vary along the boundary, producing fluxes along it. These fluxes may have already been observed experimentally.[18–20]

Actually nonsinusoidal current-phase relations can have important influence on the types of superconducting quantum interference device (SQUID) experiments as in Wollman *et al.*[1] and Brawner and Ott.[2] For example if one investigates the *minima* of resistance of the SQUID *alone* then remarks similar to the ones above on the rings apply except that the concern is for the maxima in the current-phase relationships (rather than the energy minima χ_m). Thus even for SQUID made entirely of s-wave superconductors a shift is possible if the two junctions do not have the same current-phase relationship. (cf. Sec. IV of Ref. 8) It is clear that the flux through the SQUID needed to achieve the maximum current is actually $\frac{\Phi_o}{2\pi}(\tilde{\chi}^a - \tilde{\chi}^b)$ where $\tilde{\chi}^{a,b}$ are the values of χ such that the currents through the a, b junctions are maxima. In Wollman *et al.*[1] and Brawner and Ott[2] the resistances of the SQUID's as functions of the applied flux have been investigated. The fact that these dependences seem rather sinusoidal probably put an upper bound on the deviation of $I(\chi)$ in these two experiments from a sinusoidal relation.

In summary I have investigated the possible current and/or energy-phase relationships involving unconventional superconductors, and have shown that they possess interesting properties which are not present in the tunnel-junction limit.

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[11] Notice now since $I(\chi)$ is nonsinusoidal, the current-phase relationship of a χ_m junction is in general not given by that of a 0 junction shifted by χ_m.

[12] For tunneling along $\hat{z}$ between an s-wave and B_{1g} superconductors occupying $z \gtrless 0$, the result that one has a $\pi/2$ junction is actually implicit in Ref. 13.

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[14] This in fact corresponds to the situation in the microscopic calculations below. I shall not discuss the other cases due to the lack of space.

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[19] In the tunnel-junction limit the flux will not exist at a corner unless one of the interfaces is a 0 junction and the other a π junction, and in that case the flux generated will be $\frac{\Phi_o}{2}$, whereas there will be no fluxes along a planar interface, both contrary to the observations (Ref. 18).

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