Frustration in $d$-wave Superconducting Circuits: $\pi$-Ring Behaviour

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A closed superconducting circuit containing an odd number of $\pi$-junctions, a $\pi$-ring, has a finite current in the ground state. We explicitly construct such rings for $d$-wave superconductors and demonstrate the existence of spontaneous currents by direct self-consistent solutions to the Bogoliubov de Gennes equations. We show that the current has a topological origin due to the frustration of the $d$-wave order parameter, which is only partially explained by the Sigrist-Rice tunneling formula.

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It has very recently become clear that the flux quanta in a superconducting ring are in general of the form $\Phi = (n + \gamma)\Phi_o$, where $\Phi_o = \hbar/2e$, rather than simply $\Phi = n\Phi_o$ as stated in the textbooks. The constant $\gamma$ is analogous to the Maslov index in Bohr-Sommerfeld quantization for single particle dynamics. The prediction [3] and subsequent experimental observation [4] of half-integer flux quantization ($\gamma = \frac{1}{2}$) has been one of the most dramatic developments in the field of superconductivity in recent years. This discovery is profound for several reasons. The experiments provided clear and direct confirmation of the existence of $d$-wave superconductivity in these materials. Previously, Wollman et al. [8] had observed a closely related effect: split Fraunhofer interference peaks in corner SQUIDs. However, the tricrystal ring experiments [9] were the first to measure non-integral flux quantization directly. But the implications of non-integral flux quantization go beyond simply confirming the pairing state symmetry, and have not been fully explored. The theoretical possibility of rings with flux quanta other than $\gamma = 1/2$ or $\gamma = 0$ has been discussed recently [5,6] and this has not yet been observed.

Rings with half-integer flux quantization also have some unique properties, including an exactly two-fold degenerate ground state. This opens up new possibilities for novel superconducting devices, which may find applications in quantum computing [9–11] or elsewhere. The topology of half-integer quantization has been discussed recently by Volovik [12].

The original prediction of the half-integer flux quantization in $d$-wave superconducting rings was by Sigrist and Rice [2], following earlier work for the $p$-wave case [1]. They considered a ring containing a single grain boundary junction, and assumed that the junction current was of the form

$$I = I_o \cos(2\theta_1) \cos(2\theta_2) \sin(\varphi)$$

for $d_{x^2-y^2}$ pairing, where $\varphi$ is the order parameter phase difference across the grain boundary junction, and $\theta_1$ and $\theta_2$ are the misalignment angles between the grain boundary normal and the crystal axes on either side of the junction. Provided that these angles are such that the junction is a $\pi$-junction (i.e. the pre-factor of $\sin(\varphi)$ is negative in Eq. [1]) and the ring inductance is large enough then the ring will exhibit a spontaneous current in the ground state.

However, Eq. [1] probably does not apply. The grain boundary junctions have a complicated microstructure and measured critical currents are approximately exponential in the misalignment angles [13]. Also the current-phase relationship of the junctions is not simply given by $\sin(\varphi)$ [14]. Furthermore the concept of a single $\pi$-junction is not well defined since gauge transformations make $\varphi$ ill defined for a single junction [15]. Gauge invariant definitions can only be made for closed rings, and so one should talk about $\pi$-rings rather than $\pi$-junctions.

In this letter we show that the existence of $\pi$-rings stems directly from the frustration of the $d$-wave order parameter in certain ring topologies. The frustration can only be resolved by a spontaneous ground state supercurrent. Our calculations are the first to show this phenomenon at a microscopic quantum mechanical level. We show that for a frustrated $d$-wave ring there is a metastable energy maximum with zero current which has a zero energy state (ZES) at the Fermi level. In the ground state the ZES is removed, but at the cost of a spontaneous circulating current. In contrast non-frustrated $d$-wave rings have no ground state current. Our numerical results for grain boundary junctions also differ considerably from the Sigrist-Rice model Eq. [1]: the current is not proportional to $\sin(\varphi)$, and the angle dependence is not given by $\cos(2\theta_1) \cos(2\theta_2)$.

First let us review the symmetry principles underlying the Josephson characteristics of grain boundary junctions in $d_{x^2-y^2}$ superconductors. Assuming time reversal symmetry, the current can be expanded [15]

$$I(\theta_1, \theta_2, \varphi) = \sum_n I_n(\theta_1, \theta_2) \sin(n\varphi).$$

For tetragonal lattice symmetry the functions $I_n(\theta_1, \theta_2)$ are obviously periodic in $\theta_1$ and $\theta_2$ with period $\pi$. Rotation of one crystal by $\pi/2$ changes the sign of the $d$-wave order parameter, and so we have a symmetry $\theta_1 \rightarrow \theta_1 + \pi/2$, $\varphi \rightarrow \varphi + \pi$. The implications of this symmetry are different for current harmonics with $n$ even or odd.
The odd \( n \) harmonics have sign changes at certain angles, but the even \( n \) harmonics need not. The existence of \( \pi \)-junctions is therefore not guaranteed by symmetry alone. Our earlier calculations \([10]\) and experiments of Il’ichev \et al. \[13\] show that the \( n > 1 \) harmonics cannot be ignored. These higher harmonics give a \( 4e/\hbar \) Josephson coupling at angles where the \( 2e/\hbar \) coupling vanishes \[17\].

In the weak coupling Josephson regime where only the \( n = 1 \) current component is significant the critical current \( I_c = I_1(\theta_1, \theta_2) \) and this can be expanded as a Fourier series \[18\]

\[
I_c = C \cos 2\theta_1 \cos 2\theta_2 + S \sin 2\theta_1 \sin 2\theta_2 + \ldots \quad (5)
\]

The Sigrist-Rice form, Eq. \(5\), is merely the first expansion term. If the other terms are significant then one cannot predict whether a given junction orientation has \( \pi \)-junction or normal junction behaviour merely from the sign of \( \cos 2\theta_1 \cos 2\theta_2 \). Also, in contrast to Eq. \(1\), the current does not vanish for the case \( \theta_1 = \theta_2 = \pi/4 \), corresponding to a twin boundary in a slightly orthorhombic crystal.

In our calculations we directly compute the current in \( d \)-wave superconducting circuits by solving the Hartree-Fock Gorkov or Bogoliubov-de Gennes (BdG) equations \[19\]. We use a tight binding lattice with nearest neighbor hopping, \( t \), and retarded attractive interaction \( U_{ij} = -3.5t \) with a frequency cutoff \( E_c = 3.0t \). We used a temperature of \( T = 0.01t \) and a chemical potential of \( \mu = 0 \). The calculation \[13\] is self-consistent in the non-local order-parameter, \( \Delta_{ij} = U_{ij} c_i^\dagger c_j \), and in the hopping, \( t_{ij} = t + U_{ij} n_{ij} \), where \( n_{ij} = \sum_\sigma c_{i\sigma} c_{j\sigma}^\dagger \). Currents are computed for each nearest neighbor bond \[14\], \( I_{ij} \), and self-consistency ensures that current conservation is obeyed at each site.
increases until it reaches their mean value of \(-60^\circ\) (a straight line) at self-consistency. Thus, for this system the ground state has no ground-state circulating current, and is therefore not a \(\pi\)-ring.

The conclusion that this first geometry is not a \(\pi\)-ring is not surprising. In our earlier work \([16]\) we calculated the supercurrent-phase characteristic \(I(\theta_1, \theta_2, \varphi)\) for a grain boundary junction between two bulk superconductors for this geometry. Choosing a gauge so that zero phase difference corresponds to the \(d\)-wave orientation indicated in Fig. 3 leads to a positive current with a positive phase difference, \(\varphi\), as expected for a normal junction \([10]\). The sign of the \(d\)-wave order parameter can be chosen consistently around the circuit as indicated, implying the ring geometry of Fig. 3 has no intrinsic frustration.

Now contrast this with the ring geometry shown in Fig. 3, where again edges \(A\) and \(B\) are joined. In this geometry the topology clearly indicates that the \(d\)-wave order parameter is frustrated \([13]\). Suppose we define the gauge so that zero phase difference across the junction corresponds to that indicated in Fig. 3. Then one can see that one must introduce a sign change at the point where the \(A\) and \(B\) edges are joined to make a close ring. Alternatively in a different gauge convention one could impose no sign change at the \(A-B\) interface, but then necessarily there must be a sign change elsewhere in the loop. This intrinsic frustration is a new feature of the system Fig. 3, and is quite different from Fig. 3 where there was no similar frustration. Topologically Fig. 3 is a globally non-orientable surface, equivalent to the Möbius strip (one cannot continuously assign a unique orientation (gauge) at each point), while Fig. 3 is globally orientable and topologically equivalent to the surface of an ordinary cylinder. See Ref. \([12]\) for further implications of this topology.

The dramatic effect of this topological difference is apparent in the evolution to self-consistency, as seen in Fig. 4. Starting the evolution to self-consistency with \(\Delta_{ij} = 0\) for all sites on the left hand side of the boundary and a bulk \(d\)-wave state with an arbitrary phase of \(30^\circ\) on the right, we obtain the order parameter phase shown in Fig. 4. The phase becomes increasingly linear, corresponding to a uniform and non-zero supercurrent throughout the ring. The system has therefore a spontaneous ground state current and is therefore a \(\pi\)-ring. Note that the discontinuity in phase at the join of the \(A\) and \(B\) edges is purely due to the sign convention chosen in Fig. 3, and does not correspond to any physical discontinuity in the \(\Delta_{ij}\). Also the slight non-linearity in the phase gradient at \(x = 0\) is consistent with the increased cross-section width of the strip at this point. Fig. 4 is a direct microscopic example of a \(\pi\)-ring due to topological frustration in \(d\)-wave superconductors. In order to understand the microscopic origin of this spontaneous current it is helpful to first consider a single \(\theta_1 = \theta_2 = 45^\circ\) junction between two bulk superconductors. This would be a \(\{110\}\) twin boundary for two slightly orthorhombic superconductors. The geometry is identical to Fig. 3 except that the edges \(A\) and \(B\) are not joined, but rather connect to infinite bulk superconductor on either side of the junction. Now there is translational symmetry parallel to the interface, and every site is symmetrically equivalent to one of those indicated in black on Fig. 3. In this case we can use the numerical methods of Ref. \([16]\) to determine the characteristics of this junction. We choose to define zero phase difference \(\varphi\) as indicated in Fig. 3. In this case the non-local order parameter \(\Delta_{ij}\) clearly has a perfect bulk \(d\)-wave shape at every site, including the sites at the center of the boundary. Calculating the local density of states for this does indeed yield an ideal bulk \(d\)-wave density of states.

Suppose now that we apply a phase difference \(\varphi\) across the interface. Rotating the order parameter on the right hand side of the interface by \(90^\circ\) corresponds to a phase difference of \(\varphi = 180^\circ\). In this case the local density of states is shown in Fig. 3(a). There is a strong zero energy state (ZES), or resonance, at the center of the gap. This ZES is essentially of the same origin as the one described by Belzig, Bruder and Sigrist \([21]\).
The final self-consistent answer yields a $d$-wave order parameter but with a small extended-s component at this phase difference. The pairing state at the junction is locally $s + d$ and not $s + id$. We have also calculated the supercurrent-phase characteristic of this $[110]$ twin boundary junction. We apply a phase difference $\varphi$ between the two bulk superconductors and calculating self-consistently the order parameter $\Delta_{ij}$, charge $n_{ij}$ and current $I_{ij}$ on each bond in the region of the junction. Fig. 5(b) shows that the current versus phase profile is an almost linear saw-tooth function with sharp discontinuities at $\pm \pi$. It is qualitatively the same as for the other boundaries previously reported [10]. The shape is indicative of a strong coupling junction [22], and we attribute the sharp discontinuity to the existence of the ZES at $\varphi = \pi$. Obviously the fact that the curve is not simply a sine wave indicates that the higher harmonics are relevant in Eq. 2, consistent with the experiments of Il'ichev et al. [13]. Also note that in this junction geometry the Sigrist-Rice formula Eq. 1 predicts no supercurrent flow at all, but the non-zero current is due to the sin $2\theta_1 \sin 2\theta_2$ or higher order terms in the expansion Eq. 3.

The state $\varphi = \pi$ in Fig. 5(a) with the ZES is the energy maximum for the junction, as can be seen by integrating the current, $\int Id\varphi$, of Fig 5(b). It corresponds to a phase slip of $\pi$ in the order parameter across the junction. Such states are also possible in the ring geometry. Fig. 5(c) shows a self-consistent order parameter phase for the same ring geometry of Fig. 4. This was obtained by starting the self-consistent calculation with a bulk $d$-wave order parameter and with the phase arrangement shown in Fig. 3 Thus, the calculation begins with a phase-slip at the A-B boundary. At this point the magnitude of the $d$-wave order parameter $|\Delta_d|$ is heavily suppressed, as shown in Fig. 5(d). This is because locally there are sites where the $\Delta_{ij}$ to the four neighboring sites are $(+,-,-,+) \text{ rather than } (+,+,-,-)$ counting clockwise. We interpret this phase slip solution for the ring as the meta-stable energy maximum state which separates the two equivalent energy minima corresponding to positive or negative circulating current.

In summary we identify ring geometries in $d$-wave superconductors as either frustrated or not. Frustrated rings have a circulating current in the ground state for but no ZES. The only available states without current flow have a phase slip, but with the onset of a non-split ZES (i.e. no time reversal symmetry breaking). We also calculated the current versus phase profile and demonstrated that the Sigrist Rice formula is not a valid approximation. Finally, we suggest that experiments designed to measure the differential conductance in these rings are an important next step in understanding the role of the ZES.

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