Restoration of $hc/2e$ Magnetic Flux Periodicity in a Hollow $d$-Wave Superconducting Cylinder

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The magnetic flux dependence of order parameter and supercurrent is studied in a hollow $d$-wave superconducting cylinder. It is shown that the existence of line nodal quasiparticles in a pure $d_{x^2-y^2}$ pairing state gives rise to an $hc/e$ periodicity in the order parameter and a first-order quantum phase transition for a large system size. We demonstrate that the flux periodicity in the supercurrent is sensitive to the detailed electronic band structure and electron filling factor. In particular, we find that, in cooperation with the increase of the cylinder circumference, the $hc/2e$ periodicity can be restored significantly in the supercurrent by avoiding the particle-hole symmetry point. A similar study of a $d_{x^2-y^2}+id_{xy}$ pairing state verifies the peculiarity of unconventional superconductors with nodal structure.

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A fundamental property of all known superconductors is the formation of Cooper pairs in the superconducting state. A far-reaching implication of this fact is the quantization of magnetic flux in units of $hc/2e$ in multiply connected superconducting geometries. The $hc/2e$ flux quantization has been used as a proof of electron pairing nature of both conventional and high-temperature superconductors in the superconducting state. Other related phenomena include the quantum oscillation in the transition temperature and magnetic vortices each carrying an $hc/2e$ flux quantum.

Quantum mechanically, there is no fundamental reason why the minimal flux periodicity must be $hc/2e$ in a superconductor. The gauge invariance can only guarantee a fundamental period of $\Phi_0 = hc/e$. Only when all Cooper pairs move in the same group velocity, can a substantial $\Phi_0/2$ periodicity be obtained. The $\Phi_0$-periodicity has been in mesoscopic conventional superconducting rings due to the level discreteness and Landau depairing effect. More surprisingly, recent studies have shown a severe breaking of $hc/2e$-periodicity in a $d$-wave superconducting loop, as a result of the Cooper-pair angular momentum selection for the existence of Doppler-shifted zero-energy states.

In this Letter, by a systematic study of the supercurrent in a hollow $d$-wave superconducting cylinder, we show an $hc/e$ magnetic periodicity in the $d$-wave order parameter and demonstrate that the flux periodicity in the supercurrent is sensitive to the detailed electronic band structure and electron filling factor. In particular, we find that the breaking of $hc/2e$ periodicity in the case of $d$-wave pairing is closely related to the particle-hole symmetry in the normal state band structure, which gives rise to the van Hove singularity. When the particle-hole symmetry point is avoided, the $hc/2e$ periodicity can be restored almost completely in the supercurrent.

To be specific, we consider a hollow $d$-wave superconducting cylinder, as schematically shown in Fig. 1.

Experimentally, the cylinder can be formed by a high-temperature superconductor film with its normal perpendicular to the CuO$_2$ plane. A magnetic flux $\Phi$ threads the cylinder parallel to its axis, and also to the crystal $b$-axis of the CuO$_2$ plane. Due to the weak interlayer coupling, the problem can be reduced to one on an essentially two-dimensional system. We define the $x$- and $y$-axis to be perpendicular and parallel to the flux direction, respectively. This set up can also avoid the nucleation of Abrikosov vortices, which will complicate the analysis. By choosing a gauge, where the vector potential does not appear explicitly in the Hamiltonian, the Bogoliubov-de Gennes (BdG) equations can be written as

$$\sum_j \left( \mathcal{H}_{ij} \Delta_{ij} - \Delta^*_{ij} \mathcal{H}^*_{ij} \right) \left( \begin{array}{c} u^j_n \\ v^j_n \end{array} \right) = E_n \left( \begin{array}{c} u^j_n \\ v^j_n \end{array} \right), \quad (1)$$

subject to the flux-modified boundary condition

$$\left( \begin{array}{c} u^j_{n+iN_x} \\ v^j_{n+iN_x} \end{array} \right) = \left( \begin{array}{cc} e^{i2\pi \Phi/\Phi_0} & 0 \\ 0 & e^{-i2\pi \Phi/\Phi_0} \end{array} \right) \left( \begin{array}{c} u^j_n \\ v^j_n \end{array} \right), \quad (2)$$

Here $(u^j_n, v^j_n)$ are the eigenfunctions corresponding to eigenvalues $E_n$. The single particle Hamiltonian $\mathcal{H}_{ij} = -t_{ij} - \mu \delta_{ij}$ with $t_{ij}$ and $\mu$ being the hopping integral and chemical potential. We consider the nearest neighbor, $t$, and next-nearest neighbor, $t'$, hopping integral.
The bond order parameter for \( d \)-wave pairing is determined self-consistently as 
\[
\Delta_{ij} = (V_{x^2-y^2}/2) \sum_{n} [u_{i}^{n}v_{j}^{n*} + u_{j}^{n}v_{i}^{n*}] \tanh(E_{n}/2k_{B}T) \]
with \( V_{x^2-y^2} \) being the pairing strength in the \( d_{x^2-y^2} \) channel. Notice that the quasiparticle excitation energy is measured with respect to the Fermi energy.

If the electron wave vector is \( \mathbf{k} = (k_{x}, k_{y}) \) and that for the collective drift motion (superfluid motion) of the paired electrons is \( \mathbf{q} = (q_{x}, q_{y}) \), the initial \( \mathbf{k} \) and \( -\mathbf{k} \) pairing is adjusted to pair the states \( \mathbf{k} + \mathbf{q} \) and \( -\mathbf{k} + \mathbf{q} \). The solution to the BdG equations is then found as:
\[
\begin{pmatrix}
u_{i} \\
\end{pmatrix} = \begin{pmatrix}
\tau_{x} & 0 \\
0 & \tau_{x}
\end{pmatrix} \begin{pmatrix}
u_{i} \\
\end{pmatrix},
\]
where
\[
\begin{pmatrix}
u_{i} \\
\end{pmatrix} = \begin{pmatrix}
u_{k,q} \\
\end{pmatrix}
\]
and
\[
\begin{pmatrix}
u_{i} \\
\end{pmatrix} = \begin{pmatrix}
u_{k,q} \\
\end{pmatrix}
\]
respectively. A factor of 2 has been included to account for spin degeneracy.

In the numerical calculations, we take \( k_{B}t = 1 \). Throughout the work, the energy is measured in units of \( t \) unless specified otherwise. The temperature is fixed at \( T = 0.01 \) and the \( d \)-wave channel pairing interaction is chosen to be \( V_{x^2-y^2} = 4 \). Both the hopping parameter \( t' \) and the electron filling \( n_{e} \) will be changed. For a given \( n_{e} \), the chemical potential should be adjusted and, therefore, will be a function of \( \Phi/\Phi_{0} \).

In Fig. 2 we show the flux dependence of the persistent current in a normal state metallic cylinder, where there is no existence of superconducting order parameter. These results are known from the study of persistent current in normal state mesoscopic rings \cite{19} in the presence of an Aharonov-Bohm flux \cite{20}. The main point is that the persistent current in a normal state ring has a periodicity of \( \Phi_{0} \). We present them here to demonstrate that our theoretical formulae designed for the superconducting state can reduce to describe the normal state, and to provide a starting point for our discussion on the case of \( d \)-wave superconducting state below.

FIG. 2: (Color online) Flux dependence of the persistent current for a normal state metallic cylinder of size \( N_{L} = 40^{2} \) (solid line) and \( N_{L} = 80^{2} \) (dashed line), with \( n_{e} = 1.0 \) and \( t' = 0 \). The current is measured in units of \( I_{0} = e^{t} \). The other parameter values are defined in the main text.

\[
I = \frac{4te}{N_{L}} \sum_{k} [f(E_{k,q}^{(+)})|\nu_{k,q}^{(0)}|^2 + f(E_{k,q}^{(-)})|\nu_{k,q}^{(0)}|^2] \times \sin(k_{x} + q_{x}),
\]
respectively. A factor of 2 has been included to account for the spin degeneracy.

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phase transition when the flux across $\Phi/\Phi_0 = (2n - 1)/4$ with $n$ an integer, by exhibiting a discontinuous jump. The jump amplitude also decreases with increased system size, indicating the first order quantum phase transition will be changed into a second order one in the thermodynamic limit. The $\Phi_0$ periodicity in the pairing order parameter renders that the supercurrent does not develop fully the $\Phi_0/2$ periodicity, in a mathematically rigorous sense, regardless of the system size and electron filling. The reason lies in the fact that for a pure $d_{x^2-y^2}$-wave superconductor, low energy quasiparticle states can be populated by the Doppler shift rapidly along the nodal direction, for which the orientation dependent coherence length is divergent. As a hallmark of superconducting state, one can see clearly that flux-induced current has a different sign from that of the normal state in the region approximately from $\Phi/\Phi_0 = n - 1/4$ to $\Phi/\Phi_0 = n + 1/4$ (compare Fig. 3(b1-b2) with Fig. 2). At the half filling, the particle hole symmetry holds, which makes a large level spacing at the Fermi energy when the circumference of the cylinder is small. Therefore, the supercurrent exhibits an activation-like behavior for the magnetic flux close to $\Phi/\Phi_0 = n$, and is very different from that at $\Phi/\Phi_0 = n/2$. It explains why the $\Phi_0$ periodicity of supercurrent is pronounced in this specific case. Furthermore, it is not difficult to anticipate that, as a canonical mesoscopic effect, the breaking of $\hbar c/2e$ periodicity will be even more stronger for a smaller zero-field $d$-wave pair potential, and therefore a larger momentum averaged superconducting length $\xi = (\hbar v_k / \pi \Delta_k)_{FS}$, where $v_k$ is the quasiparticle velocity. We notice that, in the region $\Phi/\Phi_0 \in [n - 1/4, n + 1/4]$, the flux dependence of the supercurrent in a $d$-wave superconducting cylinder is different from that in a square $d$-wave superconducting loop, where a zig-zag feature was obtained. We argue that in the geometry considered in Ref. 15, the elastic scattering from hard-wall boundaries of a mesoscale system populates a significant number of the lower energy states, which plays an important role in the flux-dependent current. Naturally, the increase of the cylinder circumference is one way to reduce the activation behavior, and therefore reducing the $\Phi/\Phi_0$ component in the Fourier spectrum of supercurrent. Alternatively, when the electronic filling factor is tuned away from half filling, the particle hole symmetry is broken and the Fermi surface becomes more isotropic. The activation-like behavior in the supercurrent is replaced by a more linear-like behavior, similar to the behavior exhibiting at $\Phi/\Phi_0 = n/2$. In addition, the current peaks at $\Phi/\Phi_0 = (2n - 1)/4$ becomes more symmetrized about $I = 0$ axis, tending to restore the more of $\Phi_0/2$ periodicity in supercurrent. Figure 4 shows the flux dependence of the $d$-wave order parameter and persistent current for various electron filling and system size but with $t' = -0.2$. When a finite nearest-neighbor hopping integral is introduced, the particle hole symmetry is broken at the onset for the hole doped (i.e., $n_e < 1$) system, where the chemical potential is not zero. In this case, the level repulsion at the Fermi energy is weakened for flux close to $\Phi/\Phi_0 = n$ even for a small cylinder circumference, and the activation behavior in the current does not show up. Consequently, the $\Phi_0$ component in the current spectrum is dramatically decreased, which makes the total current looks to have $\Phi_0/2$ periodicity completely. We note that when the zero-field averaged superconducting coherence is not so small in comparison to the cylinder circumference, the restoration is always incomplete, due to the mesoscopic effect.

To understand better the magnetic flux periodicity in unconventional superconductors, we turn to consider a...
which is much smaller than the cylinder circumference. This is the characteristic of all superconductors with nodal quasiparticles. In the present case, the magnetic flux periodicity only happens to a cylinder formed by unconventional superconductors with nodal structure. In particular, one case see that the evolution of two components of order parameter is continuous when \( \Phi/\Phi_0 \) crosses \((2n - 1)/4\), indicating that the flux-induced first order quantum phase transition is unique to a cylinder formed by unconventional superconductors with nodal quasiparticles. In the present case, the magnetic \( hc/e \) periodicity in the current is complete. The \( hc/e \) periodicity is set in as long as the cylinder circumference is much larger than the superconducting coherence length. We point out (but do not show) that the peculiar \( hc/e \) magnetic flux periodicity only happens to unconventional superconductors with nodal structure.

FIG. 5: (Color online) Flux dependence of the \( d \)-wave order parameter (a1-a2) and persistent current (b1-b2) for a \( d_{x^2-y^2} + id_{xy} \)-wave superconducting cylinder of size \( N_L = 40^2 \) (a1-b1) and \( N_L = 80^2 \) (a2-b2), with \( n_c = 1.0 \). In (a1-a2), the relative amplitude of the respective \( d_{x^2-y^2} \) (solid line) and \( d_{xy} \) (dashed line) components are plotted. Here \( t' = 0 \) and the other parameter values are defined in the main text.

\( d_{x^2-y^2} + id_{xy} \) pairing state by taking the pairing strength in the \( id_{xy} \) channel as \( V_{xy} = 3.0 \). Now the quasiparticle excitations are gapfull. In Fig. 5, we show the flux dependence of the \( d \)-wave order parameter and supercurrent in a hollow \( d_{x^2-y^2} + id_{xy} \)-wave superconducting cylinder. Noticeably, even in the presence of the particle-hole symmetry and for the same system size as the case of a pure \( d_{x^2-y^2} \) pairing state, both the \( d_{x^2-y^2} \) and \( d_{xy} \) components of order parameter have the periodicity of \( \Phi_0/2 = hc/2e \). In particular, one case see that the evolution of two components of order parameter is continuous when \( \Phi/\Phi_0 \) crosses \((2n - 1)/4\), indicating that the flux-induced first order quantum phase transition is unique to a cylinder formed by unconventional superconductors with nodal quasiparticles. In the present case, the magnetic \( hc/2e \) periodicity in the current is complete. The \( hc/2e \) periodicity is set in as long as the cylinder circumference is much larger than the superconducting coherence length. We point out (but do not show) that the flux dependence of order parameter and supercurrent in a hollow \( s \)-wave superconducting cylinder exhibit similar behavior to the case of \( d_{x^2-y^2} + id_{xy} \) pairing state.

One remark is in order: Our calculations have shown that the magnitude of the order parameter can be enhanced in the presence of magnetic flux throughout the whole period of \( \Phi_0 \) (see e.g., Fig. 3(a2) and Fig. 5(a1)-(a2)). This is the characteristic of all superconductors (including \( s \)-wave case) with short coherence length, which is much smaller than the cylinder circumference. We have calculated the case of a pure \( d_{x^2-y^2} \)-wave superconductor and a conventional \( s \)-wave superconductor both with a pairing interaction equal to 1, and found the flux dependence of the order parameter similar to that shown in Fig. 2 in Ref. 11 or Fig. 6 in Ref. 12, which again is a mesoscopic effect.

In conclusion, we have studied the flux dependence of order parameter and supercurrent in a hollow \( d \)-wave superconducting cylinder. For a pure \( d_{x^2-y^2} \)-wave pairing state, we find a \( hc/e \) periodicity of order parameter due to the existence of nodal quasiparticle states, and an associated quantum phase transition. When the particle hole symmetry holds in the normal state band structure, there is a noticeable component of \( hc/e \) in the supercurrent spectrum when the cylinder circumference in the mesoscopic regime. However, in addition to the increase of system size, this component can be suppressed more effectively by avoiding the particle hole symmetry point through the tuning of electron filling and band structure. By studying the case of a \( d_{x^2-y^2} + id_{xy} \) pairing state, where the quasiparticle excitations are gapfull, we verify that the peculiar \( hc/e \) magnetic flux periodicity only happens to unconventional superconductors with nodal structure.

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