Restoration of the Magnetic hc/e-Periodicity in Unconventional Superconductors

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(Received 23 November 2007; published 9 May 2008)

We consider the energy of the filled quasiparticle's Fermi sea of a macroscopic superconducting ring threaded by an $hc/2e$ vortex, when the material of the ring is of an unconventional pairing symmetry. The energy relative to the one for the hc/e vortex configuration is finite, positive, and inversely proportional to the ring's inner radius. We argue that the existence of this energy in unconventional superconductors removes the commonly assumed degeneracy between the odd and the even vortices, with the loss of the concomitant $hc/2e$-periodicity in an external magnetic field as a consequence. This macroscopic quantum effect should be observable in nanosized unconventional superconductors with a small phase stiffness, such as deeply underdoped YBCO with $T_c < 5$ K.

DOI: 10.1103/PhysRevLett.100.187006 PACS numbers: 74.25.Jb, 74.25.Qt, 74.72.−h

A fundamental property of all known superconductors is that their electrons form Cooper pairs. A direct manifestation of this phenomenon is the quantization of magnetic flux in units of $hc/2e$ in multiply connected geometries [1]. Such flux quantization may be considered as an effective spectroscopy of the charge of the carriers, and is often used as a proof of paired nature of the superconducting state. A closely related phenomenon is the periodicity of various properties of multiply connected superconductors in the external magnetic field with the period that corresponds to the half flux quantum [2].

In this Letter we argue that this periodicity is in principle *not exact* in superconductors with unconventional pairing symmetry that support quasiparticle excitations at *arbitrarily low* energies. Our argument is qualitative and fundamental in nature, and based on a calculation of the difference in ground state energies of nodal quasiparticles of an unconventional superconductor in a presence of a single ($hc/2e$) and a double (hc/e) vortex in an annular geometry. An estimate of this energy difference indicates that the deviations from the familiar $hc/2e$-periodicity may become directly observable in recently fabricated deeply underdoped cuprates. This manifestation of macroscopic quantum coherence is a fundamental effect and raises the possibility of manipulation of spin currents (carried by quasiparticles) by controlled motion of magnetic fluxes (using, for example, a Hall bar) with applications to spintronics and other areas of applied science.

The energy in question stems from the essential difference in the interactions between the quasiparticles and hc/e and $hc/2e$ vortices. Apart from the semiclassical Doppler shift of the quasiparticle energies common to both single and double vortices, the statistical, purely *quantum* Aharonov-Bohm (AB) phase of an hc/e vortex can be exactly gauged away whereas the one of an $hc/2e$ vortex cannot. The ensuing topological frustration is felt by the quasiparticles arbitrary far from the center of the vortex via the AB gauge field [3], which encodes the sign change in the quasiparticle's wave function as it is adiabatically dragged around the vortex. Vortices, their fluctuations, and the concomitant AB and Doppler effects on quasiparticles in d-wave superconductors have been a subject of much research in the past [4–12]. Here we consider the filled Fermi sea of nodal quasiparticles in an annular geometry (Fig. 1), and determine the excess in energy due to the AB gauge field of the $hc/2e$ vortex. We find a positive contribution to the condensation energy that derives predominantly from the quasiparticles near the nodes and is inversely proportional to the hole radius R. For parameters relevant to cuprates the excess energy is ~0.2 K for a thick ring whose inner radius is about a *micrometer*. Consequences for the quantization of magnetic flux in underdoped cuprates are briefly discussed.

Let us assume a magnetic flux localized in the annulus made of an unconventional superconductor. At low energies, the dynamics of quasiparticle excitations near a single node in the field of a vortex in the superconducting order parameter carrying a half flux quantum $hc/2e$ may be described by the Hamiltonian

$$\hat{H} = v_F(p_x + a_x)\sigma_1 + v_\Delta(p_y + a_y)\sigma_2 - m\sigma_3, \tag{1}$$

where v_F and v_Δ are characteristic velocities of the quasiparticle excitations in the two directions around a nodal point, σ_i are the Pauli matrices. $\mathbf{a}(\mathbf{r}) = (x\mathbf{e}_y - y\mathbf{e}_x)/(2r^2)$

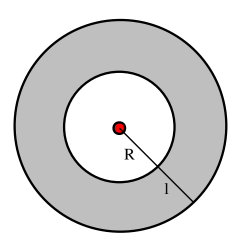

FIG. 1 (color online). Annular system with the vortex in the nodal superconductor (gray region).

is the AB vector potential resulting from the Franz-Tešanović [3] (FT) gauge transformation in the presence of the $hc/2e$ vortex in the order parameter. In (1) we have included a gap m at the nodes for generality and set $\hbar = c = 1$. We have also neglected the Doppler shift of quasiparticles, based on the following argument: the Doppler effect enters Hamiltonian (1) as another gauge field $\mathbf{v}(\mathbf{r})$ generated by the FT transformation. It always appears in the combination $\mathbf{v}(\mathbf{r}) - (e/c)\mathbf{A}(\mathbf{r})$, where $\mathbf{A}(\mathbf{r})$ is the electromagnetic vector potential. When the hole radius R (Fig. 1) grows to become comparable to the magnetic field penetration depth λ, $\mathbf{A}(\mathbf{r})$ will *screen* out $\mathbf{v}(\mathbf{r})$, leaving the topological frustration encoded by $\mathbf{a}(\mathbf{r})$ as the sole long range effect. Thus, in practical situations, we expect the Doppler shift to be a secondary effect in rings of macroscopic size.

We consider first the simpler case of isotropic velocities, $v_F = v_\Delta$. Setting the velocity to unity the eigenstates of the above Hamiltonian are found to be

$$\Psi_{q,k,l}(r,\phi) = \sqrt{\frac{k}{4\pi|E|}} \times \begin{pmatrix} \sqrt{q(E-m)}J_{l-1/2}(kr)e^{i(l-1)\phi} \\ iq\sqrt{q(E+m)}J_{l+1/2}(kr)e^{il\phi} \end{pmatrix} \tag{2}$$

for $l > 0$, and

$$\Psi_{q,k,l}(r,\phi) = \sqrt{\frac{k}{4\pi|E|}} \times \begin{pmatrix} \sqrt{q(E-m)}J_{-l+1/2}(kr)e^{i(l-1)\phi} \\ -iq\sqrt{q(E+m)}J_{-l-1/2}(kr)e^{il\phi} \end{pmatrix} \tag{3}$$

for $l \leq 0$. Here the quantum number $q = \pm 1$ distinguishes particlelike and holelike states, $l \in Z$ is angular momentum, $k > 0$ is radial wave vector, and energy is $E_{q,k} = q\sqrt{k^2 + m^2}$. $J_l(x)$ are Bessel functions of the first kind. To find the above eigenstates it is necessary to regularize the gauge potential. Namely, the requirement of the square-integrability unambiguously determines all the eigenstates of the Hamiltonian (1), except ones with zero angular momentum. There are two $l = 0$ states diverging as $1/\sqrt{r}$ at the origin, but keeping both of them leads to an overcomplete basis in the Hilbert space. On the other hand, requirement of nondivergence of the states at the origin is too restrictive, since it leads to an incomplete eigenbasis. Only linear combinations of the two states specified by a single parameter are allowed [13] but in order to select a single eigenstate from all allowed states, the gauge potential has to be regularized. Here, we considered the vortex as a cylinder of a finite radius R in which the AB flux is uniformly distributed. By matching the solutions inside and outside the cylinder, and taking the limit $R \to 0$, we found that the eigenstate in the zero angular momentum channel has the form given by (3), with the lower component diverging at the origin. This is in agreement with the result of an alternative regularization [11,13].

Let us now calculate the local density of states (LDOS) for gapless nodal quasiparticles, $m = 0$, defined as

$$\rho(\epsilon,\mathbf{r}) = \sum_{q,l}\int dk|\Psi_{q,l,k}|^2\delta(\epsilon - E_{q,k}). \tag{4}$$

Using the eigenstates given by Eqs. (2) and (3), we reproduce the LDOS of Ref. [10] in the form

$$\rho(\epsilon,\mathbf{r}) = \frac{\cos(2|\epsilon|r)}{2\pi^2 r} + \frac{|\epsilon|}{\pi}\sum_{l=0}^{\infty} J_{l+1/2}^2(|\epsilon|r). \tag{5}$$

The expression for the LDOS can further be simplified using the little known Mitrinović identity [14]

$$\sum_{l=1}^{\infty}[J_{p+l}(x)]^2 = p\int_0^x \frac{dt}{t}[J_p(t)]^2 - \frac{1}{2}[J_p(x)]^2. \tag{6}$$

For $p = 1/2$, this yields the form of the LDOS which is more convenient for the later calculations

$$\rho(\epsilon,\mathbf{r}) = \frac{1}{\pi^2}\left[\frac{\cos(2|\epsilon|r)}{2r} + |\epsilon|\mathrm{Si}(2|\epsilon|r)\right], \tag{7}$$

where the standard sine-integral function is defined as $\mathrm{Si}(x) \equiv \int_0^x dt \sin t/t$. In the vicinity of the vortex, in the region $r \ll 1/|\epsilon|$, the LDOS diverges as $1/r$. This behavior of the LDOS originates from the states in the zero angular momentum channel that diverge as $1/\sqrt{r}$, when $r \to 0$. On the other hand, far from the vortex, $\rho(\epsilon,\mathbf{r}) \to \rho_0(\epsilon,\mathbf{r}) = |\epsilon|/2\pi$, as in the vortex-free system. Of course, the LDOS in the system with the vortex carrying an integer number of the flux quanta, nhc/e, $n \in Z$, is the same as in the free system. Namely, the vector potential corresponding to nhc/e vortex is $2n\mathbf{a}(\mathbf{r})$, and in that case the eigenstates of (1) have the form

$$\Psi_{q,k,l}(r,\phi) = \sqrt{\frac{k}{4\pi|E|}} \times \begin{pmatrix} \sqrt{q(E-m)}J_{|l-1+n|}(kr)e^{i(l-1)\phi} \\ iq\sqrt{q(E+m)}J_{|l+n|}(kr)e^{il\phi} \end{pmatrix}. \tag{8}$$

The LDOS for gapless nodal quasiparticles $\rho_0(\epsilon,\mathbf{r})$ is then uniform and independent of the integer n, as required by gauge invariance.

Starting with the compact form of the LDOS, we may compute the energy cost of having an $hc/2e$ vortex by integrating the Eq. (7) over the energy and the area of the ring in Fig. 1. This procedure should be accurate for a ring of a macroscopic size, when the effects of the boundaries and of the discreetness of the spectrum become negligible. The DOS for the ring is then

$$\rho(\epsilon) = \int d^2\mathbf{r}\rho(\epsilon,\mathbf{r}) = I(R+l,\epsilon) - I(R,\epsilon), \tag{9}$$

where

$$I(R,\epsilon) \equiv \frac{\epsilon R^2}{\pi}\left[\mathrm{Si}(2\epsilon R) + \frac{\cos(2\epsilon R)}{2\epsilon R} + \frac{\sin(2\epsilon R)}{(2\epsilon R)^2}\right]. \quad (10)$$

$R + l$ and R are the radii of the outer and the inner annulus, respectively. The total energy of the system then becomes

$$\mathcal{E} = -\int_0^\Lambda d\epsilon\epsilon\rho(\epsilon) = \tilde{\mathcal{E}}(R+l) - \tilde{\mathcal{E}}(R), \quad (11)$$

with

$$\tilde{\mathcal{E}}(R) = -\frac{\Lambda^3 R^2}{3\pi}\left[\mathrm{Si}(2R\Lambda) + \frac{\cos(2R\Lambda)}{2R\Lambda} + \frac{\sin(2R\Lambda)}{(2R\Lambda)^2} + \frac{1-\cos(2R\Lambda)}{4R^3\Lambda^3}\right]. \quad (12)$$

Here, Λ is a high-energy cutoff, and the minus sign in Eq. (11) takes into account that only holelike states are occupied in the ground state. Using the asymptotic form of the sine-integral function for large values of its argument, we find the energy cost of an $hc/2e$ vortex in the annulus of a macroscopic size $R \gg 1/\Lambda$ to be

$$\mathcal{E}_v \equiv \mathcal{E} - \mathcal{E}_0 = \frac{l}{12\pi R(R+l)}\left(1 + \mathcal{O}\left(\frac{1}{\Lambda R}\right)\right), \quad (13)$$

where the total energy for the hc/e vortex (or the vortex-free system) is $\mathcal{E}_0 = \Lambda^3[R^2 - (R+l)^2]/6$. When the thickness of the annulus is much larger than its inner radius, $l \gg R$, the extra energy cost due to the presence of an $hc/2e$ vortex in the order parameter, to the leading order in $1/\Lambda R$ and R/l, is simply

$$\mathcal{E}_v = \frac{\hbar v_F}{12\pi R}, \quad (14)$$

where we have also restored Planck's constant and the Fermi velocity $v_F = v_\Delta$ previously set to one. The energy cost for having an $hc/2e$ vortex in the system therefore is *positive*, and in the macroscopic limit, for a thick annulus, inversely proportional to its inner radius. Notice that the leading term in $\mathcal{E}_v$ is independent of the high-energy cutoff Λ, in accord with our assumption that the effect is due to the low-energy quasiparticles near the nodes. The long-wavelength, linearized, description we postulated in Eq. (1) is thus internally consistent for an annulus of a macroscopic size. The result in Eqs. (13) and (14) also reflects the fact that the presence of the vortex affects the LDOS in its (macroscopic) vicinity the most.

We can now turn to the general and a physically more relevant case when the two characteristic velocities of the nodal quasiparticles, v_F and v_Δ, are different. By rescaling the coordinates, $x' = x/v_F$, $y' = y/v_\Delta$, and choosing a gauge such that the vector potential has the same form as below Eq. (1) in the new coordinates (x', y'), Hamiltonian (1) may be transformed to a form with isotropic velocities [4,10,11]. The rescaled momenta are now $k_x' = v_F k_x$, $k_y' = v_\Delta k_y$, and the dispersion assumes an isotropic form, $E_{q,k'} = qk'$, with $k' \equiv \sqrt{k_x'^2 + k_y'^2}$. The LDOS then becomes $\rho(\epsilon, \mathbf{r}')/2\pi$, with the extra factor of 2π arising from the elliptic shape of the Brillouin zone in the new coordinates, shown in Fig. 2.

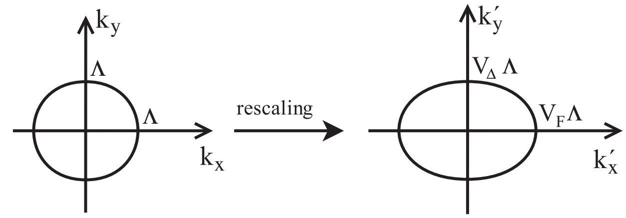

FIG. 2. Shape of the Brillouin zone before and after rescaling of the momenta.

The total energy of the anisotropic vortex-free system in the annular geometry is then $\mathcal{E}_0 = G(R+l) - G(R)$, where

$$G(R) \equiv -\int_{r\le R} d^2\mathbf{r}\int_{\Sigma(\Lambda)} d^2\mathbf{k}'\rho_0(k'). \quad (15)$$

$\Sigma(\Lambda)$ is the Brillouin zone in Fig. 2, and $\rho_0(k') = k'/(2\pi)^2$ is the LDOS of the vortex-free system. The integration yields the total energy of the flux-free system

$$\mathcal{E}_0 = -\frac{\Lambda^3}{12}\frac{v_\Delta^2}{v_F}[(R+l)^2 - R^2]\left[{}_2F_1\left(\frac{1}{2},\frac{3}{2};1;1-\frac{v_\Delta^2}{v_F^2}\right) + {}_2F_1\left(\frac{3}{2},\frac{1}{2};1;1-\frac{v_\Delta^2}{v_F^2}\right)\right], \; v_F \ge v_\Delta, \quad (16)$$

and ${}_2F_1(a,b;c;x)$ is the hypergeometric function. If $v_\Delta > v_F$, the two velocities should be exchanged. In the presence of an $hc/2e$ vortex the total energy of the system is thus

$$\mathcal{E} = \mathcal{G}(R+l) - \mathcal{G}(R), \quad (17)$$

where

$$\mathcal{G}(R) = -\int_{\Omega(R)} d^2\mathbf{r}'\int_{\Sigma(\Lambda)} d^2\mathbf{k}'k'\rho(k',\mathbf{r}'). \quad (18)$$

$\Omega(R)$ is the ellipse $v_F^2 x'^2 + v_\Delta^2 y'^2 \le R^2$. To the leading order in $1/(\Lambda R)$, one then finds $\mathcal{E} = \mathcal{E}_0 + \mathcal{E}_v$, where $\mathcal{E}_0$ is the energy of the flux-free system given by Eq. (16), and the contribution to the total energy arising solely from the presence of the AB vector potential when $v_F \ge v_\Delta$ is

$$\mathcal{E}_v = \frac{\hbar l v_F}{12\pi R(R+l)}\,{}_2F_1\left(\frac{1}{2},-\frac{1}{2};1;1-\frac{v_\Delta^2}{v_F^2}\right). \quad (19)$$

In the isotropic case, $v_F = v_\Delta = 1$, we obtain the result (13), since ${}_2F_1(1/2,-1/2;1;0) = 1$. In the opposite limit of a large velocity anisotropy, the energy cost is determined by a larger of the two velocities, because the function ${}_2F_1(1/2,-1/2;1;x)$ is monotonic and bounded on the interval $[0, 1]$, $2/\pi = {}_2F_1(1/2,-1/2;1;1) < {}_2F_1(1/2,-1/2;1;x) < {}_2F_1(1/2,-1/2;1;0) = 1$.

The result in Eq. (19) pertains to the energy of filled quasiparticle Fermi sea. However, we can straightforwardly import it into the fully *self-consistent* computation of the *total* superconducting condensation energy:

$$E_{\rm tot}(\Delta, hc/2e) = E_{qp}(\Delta, hc/2e) + \frac{|\Delta|^2}{g}, \qquad (20)$$

where $E_{qp}(\Delta, hc/2e)$ is the energy of the Fermi see with an $hc/2e$ vortex and gap parameter Δ and g is the effective coupling constant. We have assumed that Δ is essentially uniform since any nonuniformity enters only on the microscopic scale $\ll R$ or l. By adding and subtracting $E_{qp}(\Delta, 0)$ we obtain

$$E_{\rm tot}(\Delta, hc/2e) = \mathcal{E}_v + E_{\rm tot}(\Delta, 0), \qquad (21)$$

where $\mathcal{E}_v$ is given by Eq. (19). By minimizing $E_{\rm tot}(\Delta, hc/2e)$ with respect to Δ we obtain the total condensation energy in the presence of the $hc/2e$ vortex. This gives $\Delta = \Delta_0 + \delta\Delta$, where Δ_0 is the value that minimizes $E_{\rm tot}(\Delta, 0)$, and $\delta\Delta \propto \mathcal{E}_v$. For macroscopic $R, l \gg 1/\Lambda$, $\mathcal{E}_v$ is arbitrarily smaller than $E_{\rm tot}(\Delta, 0)$ and $\delta\Delta \ll \Delta_0$. This implies that, to the leading order, the presence of an $hc/2e$ vortex increases the condensation energy by precisely $\mathcal{E}_v$ (19), with $\Delta = \Delta_0$; the leading correction is $\sim(\delta\Delta)^2/\Delta_0^2$.

For a finite s-wave gap $mR \ll 1$ the calculation is similar but considerably more cumbersome. We find that the excess energy in Eq. (14) decreases with the gap m, and is essentially zero already for $mR \approx 1$, which, crudely, would correspond to an inner radius of a micrometer in an aluminum ring. This is in accord with our interpretation of the effect as being due to the nodal quasiparticles, and with the high accuracy of the observed $hc/2e$-periodicity in standard low-T_c superconductors.

We can estimate the above energy cost of the $hc/2e$ vortex from the values of the Fermi velocity and the velocity anisotropy in $YBa_2Cu_3O_{7-\delta}$ (YBCO) and $Bi_2Sr_2CaCu_2O_{8+\delta}$ (BSCCO) obtained by ARPES [15] and the thermal conductivity measurements [16]. ARPES yields a value of the Fermi velocity $v_F \sim 3 \times 10^5$ m/s, which appears to be universal in cuprates. The velocity anisotropy is $v_F/v_\Delta \sim 14$ in YBCO, while in BSCCO $v_F/v_\Delta \sim 19$, yielding the total energy penalty of having an $hc/2e$ vortex, $\mathcal{E}_v^{\rm tot} = N\mathcal{E}_v \sim 0.2$ K, for an annulus with the inner radius $R = 1$ μm, and $N = 4$ as the number of nodes in a d-wave superconductor.

The finite energy cost of an $hc/2e$ vortex will affect the quantization of the magnetic flux when it becomes comparable to the second relevant energy scale in the problem, namely, the superfluid density, $\rho(T)$. By lifting the parabolas centered at the $hc/2e$ flux in the textbook energy vs magnetic flux plot [1] by $\mathcal{E}_v$ it is easy to see that the width of the hc/e relative to the one of the $hc/2e$ plateau becomes longer by an amount proportional to $\delta = \mathcal{E}_v/\rho(T)$. This is typically a small number: in optimally doped YBCO, for example, $\delta \approx 10^{-4}$. Recently, however, single crystals [17] and thin films [18] of severely underdoped YBCO have been studied with the unprecedented low $\rho(0) \sim 1$ K, when expressed in energy units [19]. This extremely underdoped regime where the phase stiffness can be rendered arbitrary small with underdoping offers the best chance for an observation of the asymmetry between even- and odd-flux vortices predicted in this Letter.

The asymmetry between hc/e and $hc/2e$ vortices in unconventional superconductor has also been recently found in the numerical solution of the Bogoliubov–de Gennes equations for a mesoscopic superconducting loop [20] (see also [21]). The results and conclusions of this work seem broadly consistent with ours.

The authors are grateful to D. Bonn, M. Franz, J. Kirtley, K. Moller, and O. Vafek, for useful discussions, and the Aspen Center for Physics where this work was initiated. V. J. and I. F. H. acknowledge the support from the NSERC of Canada, and Z. T. from NSF Grant No. DMR-0531159.

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