hc/e Periodicity in loops of nodal superconductors

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A B S T R A C T

A superconducting state in a multiply connected geometry is characterized by the center of mass momentum $\mathbf{q}$ of a Cooper pair $\mathbf{q} = 0$ in the ground state of the standard BCS theory without magnetic field. Here we consider superconducting loops threaded by a magnetic flux. In these systems the ground state has a pair momentum $\mathbf{q}$ equal to the number of superconducting flux quanta $hc/2e$ threading the loop. For unconventional superconductors, the ground state is different for even and odd numbers of flux quanta and, consequently, their physical properties are hc/e rather than $hc/2e$ periodic.

1. Introduction

The BCS theory of superconductivity [1], as originally formulated, describes pairing of electrons with opposite momenta $\mathbf{k}$ and $-\mathbf{k}$. In the presence of magnetic fields, pairing of electrons with a finite center of mass (COM) momentum $\mathbf{q}$ may be energetically favorable. A simple example is a superconducting (SC) loop threaded by a magnetic flux Φ, where the ground state has a pair angular momentum $\mathbf{q}$ depending on Φ, leading to a flux periodic variation of physical quantities with the flux [2,3]. These systems have been studied decades ago for conventional superconductors [4–7] and are well understood. But more complex is the situation for unconventional superconductors with gap nodes, as shown by new and surprising results concerning their flux periodicity [8–11].

Another well known example of finite momentum pairing is the SC state described by Fulde and Ferrell [12] and by Larkin and Ovchinnikov [13] (FFLO), which occurs in high magnetic fields. This state depends explicitly on the breaking of time-inversion symmetry, although there is no net current flowing. Recently, a close relative of the FFLO state, but without magnetic field, was introduced, the so called "pair density wave" (PDW) state [14–16]. This state is characterized by an order parameter (OP) $\Delta(\mathbf{R}) = \Delta_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{R}} + \Delta_{-\mathbf{q}} e^{-i\mathbf{q}\cdot\mathbf{R}}$ in real space, where $\mathbf{R}$ is the COM coordinate and $\mathbf{q}$ the COM momentum of an electron pair. It preserves time-inversion symmetry, but it is spatially inhomogeneous and shows a striped charge pattern with wave vector $2\mathbf{q}$. This special characteristics made it a favorite candidate for the SC state in the stripe phase found in some high-T_c cuprates, especially Nd-doped $La_{2-x}Sr_xCuO_4$ [17] and $La_{2-x}Ba_xCuO_4$ for $x = 1/8$ [18–21]. A solution of a pairing Hamiltonian with finite momentum pairing in the absence of magnetic field was provided only recently [22].

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2. hc/e periodicity in unconventional superconductors

All physical properties of a loop, the interior of which is threaded by a magnetic flux Φ, are periodic in Φ with the period of the flux quantum $\Phi_0 = hc/e$. This is a direct consequence of the gauge invariance of the many-particle wave function in a multiply connected geometry. If the loop is in the SC state, it is actually $\Phi_0/2$ periodic in general, as shown experimentally by Little and Parks [2] and explained theoretically by Byers and Yang [5] and by Brenig [6]. The additional periodicity of $\Phi_0/2$ is in fact caused by the existence of two distinct classes of SC wave functions. The members of the first class can be mapped by a gauge transformation onto the wave function representing electron pairing with zero COM angular momentum, whereas the members of the second class are related to pairing with COM momentum $\hbar$ [7].

If these classes of wave functions are so radically different, then why is it that the SC state has a flux period of $\Phi_0/2$ and not just the basic period Φ_0? The first class of wave functions generates minima in the free energy at integer values of the dimensionless flux $\phi = \Phi/\Phi_0$, and the second class minima at half-integer values of ϕ, thus the flux dependent free energy has minima spaced equally in steps of $hc/2e$. In the thermodynamic limit, these minima are degenerate and, consequently, the periodicity is $\Phi_0/2$.

This statement is challenged by the question: how large must the diameter of a ring be so that one can consider it to be "in the thermodynamic limit"? The answer to this question has to distinguish between conventional (s-wave) and unconventional superconductors. To illustrate this, we consider a discrete one dimensional (1D) SC ring with radius Ra, where a is the lattice constant, threaded by a flux ϕ. It has a single-particle kinetic energy of the form $\varepsilon_k = -2t\cos([k-\phi]2\pi/R)$, thus ε_k varies as a function of ϕ, which is called the "Doppler shift". In one dimension, we are restricted to s-wave superconductivity, with an OP $\Delta(k) \equiv \Delta$ that is k independent, and the dispersion relation reads

$$E_{\pm}(k) = \frac{\varepsilon_k - \varepsilon_{k+q}}{2} \pm \sqrt{\Delta^2 + \left(\frac{\varepsilon_k + \varepsilon_{k+q}}{2}\right)^2}. \quad (1)$$

The pair momentum in the ground state is given by $q = \text{floor}(2\phi + 1/2)$. The Doppler shift shifts the eigenenergies $E_{\pm}(k)$ to higher or lower energies, respectively, and has a maximum of $t/2R$ at those flux values where q changes to the next integer. Therefore, if $\Delta < t/2R$, the energy gap closes as a function of flux and superconductivity breaks down [23]. The critical radius above which superconductivity is not (or very little) affected by the flux is therefore $R_c = t/2\Delta = \xi_0/2$, where $\xi_0 = t/\Delta$ is the coherence length in a 1D superconductor.

The considerations above tell that the coherence length ξ_0 is the characteristic length scale for an *s*-wave superconductor, above which finite size effects become negligible and the flux periodicity is $hc/2e$. Such a scale is missing in unconventional superconductors with gap nodes, as in a pairing state with *d*-wave symmetry. In these systems, ξ_0 may be considered an average over all momenta $\mathbf{k}$, but, since the OP $\Delta(\mathbf{k})$ vanishes for certain directions of $\mathbf{k}$, it has divergent contributions and it is therefore not possible to reach a well defined thermodynamic limit. How this affects quantities such as the total energy and the supercurrent is shown in the following.

To investigate the flux dependence for a *d*-wave superconductor, we study a two dimensional (2D) multiply connected geometry. We start from a discrete 2D square lattice with a square hole cut from its center and open boundary conditions with boundaries along the *x*- and *y*-direction, respectively [8]. For this choice, the supercurrent is largest and consequently, the hc/e periodicity most pronounced. The spectrum of the current carrying states in this system is very robust against small deformations or insertion of impurities, because they typically generate bound states at the Fermi energy in a *d*-wave superconductor [24], which are almost flux independent. We obtain the eigenenergies of the SC state by solving the Bogoliubov–de Gennes equations. By applying the self-consistency for the OP resulting from a nearest-neighbor pairing interaction, we obtain the standard *d*-wave solution.

Fig. 1 shows the energy spectrum as a function of ϕ for the square frame geometry. The maximum energy gap Δ is here much larger than the maximum Doppler shift. Nevertheless, in the flux sectors corresponding to even q, there are nodal states with eigenenergies which shift towards the Fermi energy (at $E = 0$). The eigenenergies have a non-linear flux dependence, from which follows a non-linear flux dependence of the supercurrent $J(\phi)$ as shown in Fig. 2b, and a non-parabolic form of the total energy

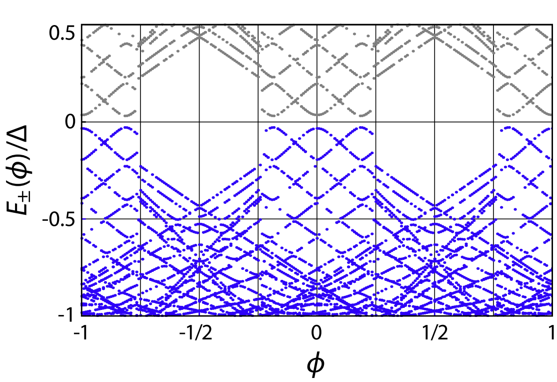

Fig. 1. Energy spectrum of the *d*-wave BCS model. The eigenenergies in the gap region are shown for a square 40×40 frame with a hole in its center with the size of 14×14 unit cells and a pairing interaction $0.3t$ as a function of flux ϕ. The energies are in units of the superconducting order parameter Δ for $\phi = 0 (\Delta \approx 0.22t)$. The reconstruction of the condensate occurs near $\phi = \pm(2n+1)/2$, where the eigenenergies jump abruptly.

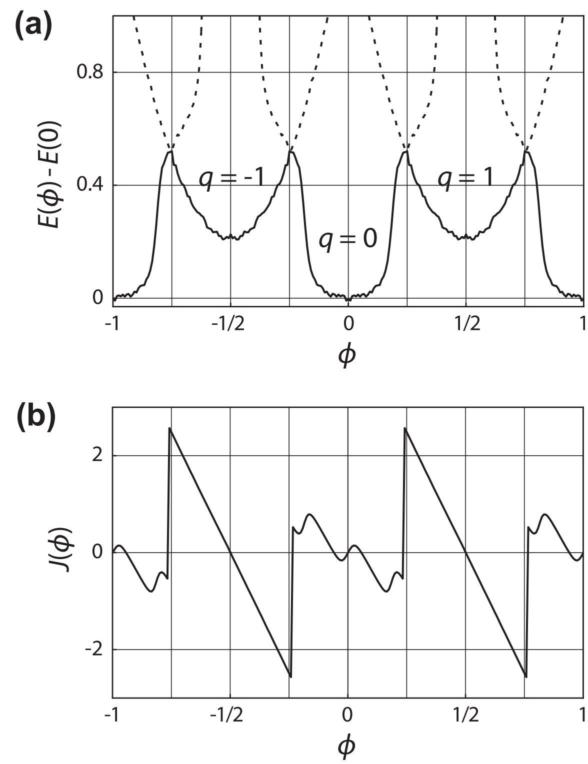

Fig. 2. Flux dependence of the total energy $E(\phi) - E(0)$ (a) and supercurrent $J(\phi)$ (b) for the square loop described in the caption of Fig. 1 at $T = 0$. J is given in units of et/hc. There is a clear difference between condensate states with an even and an odd winding number q of the OP, reflected e.g. in the deformation of the $q = 0$-parabola. The overall ϕ-periodicity for E and J is hc/e.

$E(\phi)$ (see Fig. 2a). In the odd q flux sectors, there is an effective energy gap, which is characteristic for the loop geometry. The energy levels have an essentially linear flux dependence, and so has the supercurrent. The difference of the total energy and the supercurrent in even and odd flux sectors leads to an effective flux periodicity of $\Phi_0 = hc/e$ for the *d*-wave superconductor.

The results shown in Figs. 1 and 2 exemplify that the SC states, belonging to the two distinct classes of wave functions for odd and even q introduced above, have different physical properties in general. We can quantify this difference by calculating the first component $J_{h/e}$ of the Fourier transform of the supercurrent $J(\phi)$. For an *s*-wave superconductor, $J_{h/e}$ vanishes exponentially with the radius R of the ring, once R exceeds ξ_0. To calculate the R dependence of $J_{h/e}$ for a *d*-wave superconductor, the real-space calculation based on the Bogoliubov–de Gennes equations is not ideal, because it is restricted to rather small systems, with unavoidable finite size effects. We can circumvent this problem by extending the analytical calculation for a 1D ring not to a square frame, but to a cylinder with finite height. This geometry has the advantage that the corresponding Hamiltonian is diagonal in momentum space, and by choosing a cylinder with circumference $2\pi Ra$, which is an even multiple of the height Ha, one obtains a spectrum qualitatively equivalent to the spectrum of the square frame. This allows for an approximate analytical calculation for the supercurrent by replacing the sum over the momenta $\mathbf{k}$ by a quasi continuous energy integration for large cylinders [11]. In this way one obtains the supercurrent density $j(\phi) = J(\phi)/H$ as

$$j(\phi) \approx -4\frac{t}{R}\frac{e}{hc}\begin{cases} \phi + 1/2 & \text{for} \quad -1/2 \leqslant \phi < -1/4, \\ \phi(1 - b\phi) & \text{for} \quad -1/4 \leqslant \phi < 1/4, \\ \phi - 1/2 & \text{for} \quad 1/4 \leqslant \phi < 1/2, \end{cases} \quad (2)$$

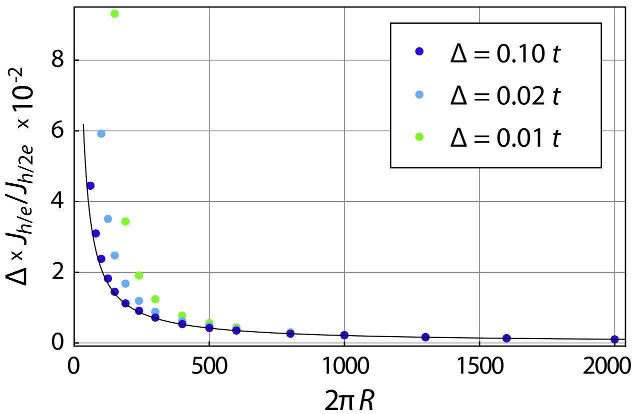

Fig. 3. Ratio of the first and the second Fourier component of the supercurrent density as a function of the cylinder radius R for fixed values of Δ. The height H of the cylinder is equal to $2\pi R$, which yields the maximum values for $J_{h/e}$. For $\Delta R \gg t$, the results of the exact evaluations compare very well to the approximate result in of Eq. (3) (black solid line).

Using Eq. (3) to estimate this ratio for a mesoscopic cylinder with a circumference $2\pi Ra = 2600a \approx 1\,\mu\text{m}$ and $\Delta/t = 0.01$, we obtain $j_{h/e}/j_{h/2e} \approx 0.03$. A comparison of this model to a numeric evaluation of the supercurrent in the cylinder is found in Fig. 3. It shows excellent agreement if $\Delta R \gg t$, which can be generalized to the statement that the hc/e periodic part of the supercurrent vanishes like $1/Ra$ if $Ra \gg \xi_0$.

The magnetic-flux-induced presence of hc/e periodic supercurrents affect many properties of unconventional superconductors. Of particular importance are a resulting enhancement of the London penetration depth and a weakening of the radiofrequency shielding. Furthermore, at any temperature, including $T = 0$, the condensation energies, the screening current densities, the kinetic inductances and the penetration depths of rings of nodal superconductors are hc/e periodic, the relative intensity of the hc/e Fourier component decreasing with $1/R$. The models presented above give an upper limit for these effects for clean systems.

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