Cooper Pair Shape in Normal-metal/Superconductor Junctions

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In s-wave superconductors the Cooper pair wave function is isotropic in momentum space. This property may also be expected for Cooper pairs entering a normal metal from a superconductor due to the proximity effect. We show, however, that such a deduction is incorrect and the pairing function in a normal metal is surprisingly anisotropic because of quasiparticle interference. We calculate angle resolved quasiparticle density of states in NS bilayers which reflects such anisotropic shape of the pairing function. We also propose a magneto-tunneling spectroscopy experiment which could confirm our predictions.

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It is well known that Cooper pairs consisting of two electrons are characterized by electric charge 2e, macroscopic phase, internal spin, and by time and orbital structures \( \theta \). The charge 2e manifests itself in various experiments, like Shapiro steps, flux quantization and excess current due to the Andreev reflection. The macroscopic phase generates the Josephson current \( \phi \). The internal spin structure is classified into spin-triplet and spin-singlet states which can be identified by nuclear magnetic resonance. Further, based on a symmetry with respect to the internal time, superconducting state can belong to the even-frequency or the odd-frequency symmetry class \( \lambda \). The orbital degree of freedom is described by an angular momentum quantum number \( l \). In s-wave superconductors with \( l = 0 \), the Cooper pair wave function is spherically symmetric on the Fermi surface, i.e. an angular structure of a Cooper pair is isotropic in momentum space. The shape of Cooper pairs in \( p \)-wave \((l = 1)\) and \( d \)-wave \((l = 2)\) superconductors is characterized by two-fold and four-fold symmetries, respectively \( \sigma \). The well established properties listed above hold in bulk superconductors. The presence of perturbations like spin-flip or interface scattering may change the symmetry of Cooper pairs. For instance, unusual odd-frequency property of Cooper pairs in proximity structures was predicted in recent studies \( \Omega \). The shape of Cooper pair wave function in non-uniform systems like superconducting junctions is not necessarily the same as that in the bulk state. Despite the extensive study of the proximity effect during several past decades, rather little attention has been paid to the problem of Cooper pair shape in non-uniform superconducting systems \( \Delta \). This issue is quite important in view of current interest to the physics of superconducting nanostructures.

The aim of the present Letter is to clarify the consequences of breakdown of translational symmetry in superconductors on the Cooper pair shape. For this purpose, we study the proximity effect in quasi-two-dimensional normal metal/superconductor (N/S) junctions by solving the Eilenberger equation, treating self-consistently the spatial variation of the superconducting pair potential. We analyze the pairing function and the local density of states (LDOS) in N/S junctions with spin-singlet s-wave and spin-triplet \( p_x \)-wave superconductors. Surprisingly, the pairing function in a normal metal turns out to be strongly anisotropic even in junctions with s-wave superconductors. To detect the complex Cooper pair shape, we propose to use scanning tunneling spectroscopy in rotating magnetic field. We show that the calculated tunneling conductance exhibits complex patterns even in the s-wave case.

Let us consider a quasi-two dimensional N/S junction as shown in Fig. 1 which is the simplest example of non-uniform superconducting system, where the S region is semi-infinite and the normal metal has finite length \( L \). In the case of \( p_x \)-wave superconductor, we assume for simplicity that triplet Cooper pairs consist of two electrons with opposite spin projections on z-axis, i.e. \( S_z = 0 \). These assumptions do not limit the generality of the discussion below. We consider a perfect N/S interface with full transmissivity, while it can be shown that characteristic behavior of Cooper pairs remains qualitatively unchanged even in the presence of a potential barrier at the N/S interface.

The quasiclassical Green’s functions \( \Sigma \) in a normal metal \((N)\) and a superconductor \((S)\) are parameterized...
as
\[ g_{\pm}^{(i)} = f_{1\pm}^{(i)} \sigma_1 + f_{2\pm}^{(i)} \sigma_2 + g_{\pm}^{(i)} \sigma_3, \quad (g_{\pm}^{(i)})^2 = 1, \]
where a superscript \(i = N, S\) refers to N and S, \(\sigma_j\) \((j = 1 - 3)\) are the Pauli matrices, and \(\mathbb{1}\) is a unit matrix. The subscript \(+(-)\) denotes a moving direction of a quasiparticle in the \(x\) direction \([8]\), and \(\Delta_\pm(x)\) \((\Delta_\pm(x))\) is the pair potential for a left (right) going quasiparticle. In a normal metal, \(\Delta_\pm(x)\) is set to zero because the pairing interaction is absent there. The Green’s functions can be expressed in terms of the Riccati parameters \([9]\),
\[
\begin{align*}
J_{1\pm}^{(i)} &= \mp v_\nu [\Gamma_{\pm}^{(i)}(x) + \zeta_{\pm}^{(i)}(x)]/[1 + \Gamma_{\pm}^{(i)}(x) \zeta_{\pm}^{(i)}(x)], \\
J_{2\pm}^{(i)} &= i[\Gamma_{\pm}^{(i)}(x) - \zeta_{\pm}^{(i)}(x)]/[1 + \Gamma_{\pm}^{(i)}(x) \zeta_{\pm}^{(i)}(x)], \\
\bar{g}_{\pm}^{(i)} &= [1 - \Gamma_{\pm}^{(i)}(x) \zeta_{\pm}^{(i)}(x)]/[1 + \Gamma_{\pm}^{(i)}(x) \zeta_{\pm}^{(i)}(x)],
\end{align*}
\]
with \(v_\nu = 1\) for \(i = S\) and \(v_\nu = -1\) for \(i = N\). The parameters \(\Gamma_{\pm}^{(i)}(x)\) and \(\zeta_{\pm}^{(i)}(x)\) obey the Eilenberger equation of the Riccati type \([9]\),
\[
\begin{align*}
v_F \kappa_\pm \partial_x \Gamma_{\pm}^{(i)}(x) &= -\Delta_{\pm}(x)[1 + (\Gamma_{\pm}^{(i)}(x))^2] + 2\epsilon \nu_\pm \Gamma_{\pm}^{(i)}(x), \\
v_F \kappa_\pm \partial_x \zeta_{\pm}^{(i)}(x) &= -\Delta_{\pm}(x)[1 + (\zeta_{\pm}^{(i)}(x))^2] - 2\epsilon \nu_\pm \zeta_{\pm}^{(i)}(x),
\end{align*}
\]
with \(\kappa_\pm = \epsilon + i\delta_0\) where \(\epsilon\) is the energy of a quasiparticle measured from the Fermi level and \(\delta_0\) is the inverse of the mean free time due to impurity scattering. In the clean limit, we consider \(\delta_0 \ll \Delta_0\). Boundary condition at \(x = -L\) is given by \(\zeta_\pm^{(N)}(-L) = -\Gamma_\pm^{(N)}(-L)\). Boundary condition at the N/S interface becomes \(\zeta_\pm^{(S)}(0) = -\Gamma_\pm^{(S)}(0)\) and \(\zeta_\pm^{(N)}(0) = -\Gamma_\pm^{(S)}(0)\). The pair potential \(\Delta_\pm(x)\) is expressed by \(\Delta_\pm(x) = \Delta(x) \Phi_\pm(\theta(x))\), where a form factor \(\Phi_\pm(\theta)\) is given by \(\Phi_\pm(\theta) = 1\) for \(s\)-wave symmetry and \(\pm \cos \theta\) for \(p_\sigma\)-wave one with \(\theta\) being an incident angle of a quasiparticle measured from the \(x\) direction. Bulk pair potential is \(\Delta(\infty) = \Delta_0\), and we determine the spatial dependence \(\Delta(x)\) in a self-consistent way.

For \(x \gg L_0\), the angular structure of \(f_{2\pm}^{(i)}\) follows that of the pair potential, whereas \(f_{1\pm}^{(i)}\) is zero with \(L_0 = v_F/2\pi T_C\) being a coherence length and \(T_C\) being the transition temperature. The pairing function \(f_{1\pm}^{(i)}\) is generated by inhomogeneity in a system and thus has a finite value only near the interface and in a normal metal. Recent study \([10]\) showed that \(f_{1\pm}^{(i)}\) has an odd-frequency symmetry. Generally speaking, functions \(f_{1\pm}^{(i)}\) and \(f_{2\pm}^{(i)}\) have opposite parities. If a superconductor has \(s\)-\((p_\sigma)\)-wave symmetry, the induced odd-frequency component has the odd (even) parity, respectively. Pairing function \(f_1\) is defined in the angular domain of \(-\pi/2 \leq \theta < 3\pi/2\). We denote \(f_1(\theta)\) by \(f_{1\pm}(\theta)\) in the angle range \(-\pi/2 \leq \theta < \pi/2\) and \(f_1(\theta) = f_{1-}(\pi - \theta)\) for \(\pi/2 \leq \theta < 3\pi/2\). The angular structure of functions \(f_{2\pm}\) and \(g\) is defined in the same manner. LDOS is given by the relation \(\rho_L(\theta) = \text{Real}[g(\theta)]\). In what follows, we fix
\[
\begin{align*}
f_{1N}^{(i)} &= \pm \Gamma \frac{1 - \alpha^2}{\Xi}, \\
f_{2N}^{(i)} &= i\Gamma \frac{1 + \alpha^2}{\Xi}, \\
g_N^{(i)} &= \frac{1 + \alpha^2 \Gamma^2}{\Xi},
\end{align*}
\]
with \(\Xi = 1 - \Gamma^2 \alpha^2\), \(\Gamma = \zeta_\pm^{(S)}(0)\), and \(\alpha = \exp[2i\epsilon L/(v_F \cos \theta)]\). For \(\epsilon \ll \Delta_0\), \(\Gamma \sim 1/i\) and \(f_{1\pm} \sim ig_{\pm}\) are satisfied. Thus shape of function \(f_1\) is similar to that of \(\rho_L\). This argument seems to be valid even for \(\epsilon = 0.1\Delta_0\) in Fig.2(e) and (f), and for \(\epsilon = 0.5\Delta_0\) in Fig.2(h) and (i). The oscillating behavior in \(f_1\), \(f_2\), and \(\rho_L\) is more remarkable at \(\epsilon = 0.5\Delta_0\). Although we do not present calculated results of \(f_1\) and \(f_2\) at \(x = -L/2\) for \(\epsilon = 0.5\Delta_0\), the butterfly-like pattern with many spikes in the pairing functions can be seen also in a normal metal. The directions of the spin projections in LDOS are characterized by small value of \(\Xi\), which has close relation to the formation of the bound states \([11]\). For \(\theta \sim \pm \pi/2\), \(\alpha\) oscillates rapidly with small variation of \(\theta\), which explains the fine structures in LDOS around \(\theta \sim \pm \pi/2\).
and ρ by red lines in Fig. 3(g), (h), and (i). Similar to ε = 0 and ε = 0.1 Δ₀ for (d), (e) and (f), and ε = 0.5 Δ₀ for (g), (h) and (i). The angle θ is measured from the x-axis.

The quasiparticle interference effect is a source of bound state formation in a normal metal. As a result, the circular shape of Cooper pairs in s-wave superconductor is modified into the butterfly-like pattern in a normal metal.

Next, we discuss the results for p±-wave junctions shown in Fig. 3 In a superconductor (x = ∞), functions f₂ and g are given by Δ₀ cos θ/√ε² − Δ₀² cos² θ and ε/√ε² − Δ₀² cos² θ, respectively. As shown by black lines in Fig. 3(d), (f), (g) and (i), the amplitudes of f₂ and g become large along the directions θ = cos⁻¹(ε/Δ₀). At ε = 0 and x = 0, formation of a mid-gap Andreev resonant state [12, 13] significantly enhances the amplitudes of f₁ and ρ₂ compared to that of f₂ as shown by red lines in Fig. 3(a), (b), and (c). For ε = 0 and ε = 0.1 Δ₀, the shapes of f₁ and ρ₂ at the N/S interface are similar to those in s-wave superconductor junctions (red lines in Fig. 3(b), (c), (e) and (f)). The shape of f₁ and f₂ in the N region is rather complex too. At ε = 0.5 Δ₀, f₁, f₂ and ρ₂ also exhibit the butterfly-like patterns as shown by red lines in Fig. 3(g), (h), and (i). Similar to s-wave case, functions f₁ and f₂ in N have a complex line shapes with many spikes. The butterfly-like pattern in angle resolved local density of states could be observed through the LDOS in magnetic fields.

Here, we propose an experimental setup of scanning tunneling spectroscopy (STS) in the presence of the magnetic field. As shown in Fig. 1, magnetic field is applied parallel to the N/S plane. Tunneling current at a fixed bias voltage is measured as a function of the angle φ between the x axis and the direction of magnetic field. The vector potential in this configuration is given by (Aₓ, Aᵧ) = −λ H (sin φ, cos φ) [14, 15]. We assume that thickness of a quasi two-dimensional superconductor is sufficiently small compared to the magnetic field penetration depth λ. Magnetic field shifts the quasiparticle energy ε to ε − H Δ₀ sin(φ − θ)/B₀ where B₀ = h/(2 e π² ξ λ) and ξ = h vₐ/F Δ₀. For typical values of ξ ∼ λ ∼ 100 nm, the magnitude of B₀ is of the order of 0.02 Tesla. Local density of state observed in STS experiments is given by, ρ(φ) = ∫₀^π/2 ρ₂(θ, φ) dθ.

In Fig. 4, ρ is plotted as a function of φ. For ε = 0, Δ₀ H/B₀ gives the effective energy of a quasiparticle. In an s-wave superconductor, it is evident that ρ is independent of φ and the amplitude of LDOS is vanishingly small, see curve A in Fig. 4(a). In a p±-wave superconductor,
as shown by curve A in Fig. 4(b), \( \rho \) decreases with \( \phi \) due to quasiparticle excitations near the nodal points at the Fermi surface [16]. At the N/S interface, \( \rho \) in the s-wave case has minima at \( \phi = \pi/2 \) and \( 3\pi/2 \) and maxima at \( \phi = 0 \) and \( \pi \), as shown by curve B in Fig. 4(a). On the other hand, in the \( p_x \)-wave case, \( \rho \) has maxima at \( \phi = \pi/2 \) and \( 3\pi/2 \), see curve B in Fig. 4(b). This behavior can be explained in the following way. Eq. (5) yields approximate expression for \( \rho \) at \( H \ll B_0 \)

\[
\rho \approx \int_{-\pi/2}^{\pi/2} \frac{2(1-a^2)}{1+a^2+2a\cos[C \sin(\theta-\phi)/\cos \theta]} \sin 2\theta \, d\theta,
\]

where \( a = \exp(-4L\delta_0/\hbar |v_F x|) \), \( C = 4LH/\hbar |v_F x| \), and the sign in the denominator is \( (+) \) for s-wave (\( p_x \)-wave) junctions. We note that \( a \) is a positive number almost independent of \( \theta \) and \( C \) is a small positive number. For \( \phi = n\pi + \pi/2 \) with integer \( n \), the magnitude of the argument of cosine function in the denominator becomes small and the denominator is reduced to \( (1 \pm a)^2 \) for s-wave (\( p_x \)-wave) case. When \( \phi \) deviates from \( n\pi + \pi/2 \), the cosine function decreases and therefore \( \rho \) has a dip (peak) at \( \phi = \pi/2 \) and \( 3\pi/2 \) for s-wave (\( p_x \)-wave) cases as shown by curve B in Fig. 4(a) ((b)). Similar argument also explains the maximum (minimum) of \( \rho \) at \( \phi = n\pi \) in s-wave (\( p_x \)-wave) junctions. When the field \( H \) is increased further (curves C in Figs. 4(a) and (b)), the shape of the \( \rho \) exhibits more complex behavior reflecting the butterfly-like pattern of \( \rho_L \) shown in Figs. 2 and 3 because the increase of \( H \) has qualitatively similar effect as the increase of \( \varepsilon \).

The complicated oscillating features are seen much more clear at \( \varepsilon = 0.5\Delta_0 \). As shown by curves C in Figs. 4(c) and (d), the period of oscillations becomes shorter than that in Figs. 4(a) and (b), reflecting the butterfly-like patterns in Figs. 2(i) and Figs. 3(i). At the same time, the magnitude of the oscillations at \( \varepsilon = 0.5\Delta_0 \) becomes smaller than that at \( \varepsilon = 0 \), since the integration with respect to \( \theta \) averages the butterfly-like pattern in \( \rho_L \). The discussed features in LDOS at the N/S interface differ strongly from those in a bulk superconductor. We conclude that STS experiments in magnetic field should resolve the remarkable deformation of Cooper pairs.

In summary, we have studied the Cooper pair shape in normal-metal/superconductor (N/S) junctions by using the quasiclassical Green’s function formalism. The quasiparticle interference leads to striking deformations in the shape of a Cooper pair wave function in a normal metal. As a consequence, the angle resolved local density of states exhibits the butterfly-like patterns. We also show that the anisotropic shape of Cooper pairs could be resolved by scanning tunneling spectroscopy experiments in magnetic field. The Cooper pair deformation is a common feature of non-uniform superconducting systems in the clean limit. This provides a key concept to explore new quantum interference phenomena in superconducting nanostructures.

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