Surface Bound States and Spin Currents in Noncentrosymmetric Superconductors

A. B. Vorontsov,1,* I. Vekhter,1 and M. Eschrig2

1Department of Physics and Astronomy, Louisiana State University, Baton Rouge, Louisiana, 70803, USA
2Institut für Theoretische Festkörperphysik and DFG-Center for Functional Nanostructures, Universität Karlsruhe, D-76128 Karlsruhe, Germany

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We investigate the ground state properties of a noncentrosymmetric superconductor near a surface. We determine the spectrum of Andreev bound states due to surface-induced mixing of bands with opposite spin helicities for a Rashba-type spin-orbit coupling. We find that the order parameter suppression qualitatively changes the bound state spectrum. The spin structure of Andreev states leads to a spin supercurrent along the interface, which is strongly enhanced compared to the normal state spin current. Particle and hole coherence amplitudes show Faraday-like rotations of the spin along quasiparticle trajectories.

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The role of chirality and spin-orbit coupling in materials and nanostructures is a very active and promising subject in the fields of spintronics, superconductivity, and magnetism [1–3]. The unusual properties of noncentrosymmetric (NCS) materials originate from the crystal structure that lacks a center of inversion, allowing for pronounced spin-orbit (SO) coupling that is odd in the electron momentum, and leading to a chiral ground state. The resulting two-band nature of NCS metals leads to effects reminiscent of semiconductor physics, such as birefringence and spin polarization of the electron wave packet [4]. Especially promising is the presence of charge-neutral spin currents in the ground state [5,6].

Since understanding of interface physics is one of the foundations for all potential applications, it is of pivotal interest to investigate how the physical properties of NCS materials are modified near surfaces. The key point here is that interface scattering in materials with strong spin-orbit effects is spin active. Spins dominate the surface physics, and any successful theoretical treatment must take this into account.

The recently discovered class of NCS superconductors [7–10] combines the strong SO coupling that governs the metallic bands with a nontrivial spin structure of the superconducting (SC) order parameter [11–13] due to lack of parity. As a result, one may expect that spin transport in the SC phase exhibits novel features compared to usual superconductors. These features are especially prominent near surfaces and interfaces, where the physics is controlled by the Andreev bound states (ABS), built as a result of particle-hole coherent scattering. ABS are crucially important in unconventional superconductors [14], where the phase variation of the order parameter (OP) on the Fermi surface [15] and the pairbreaking near interfaces lead to a midgap peak in the density of states (DOS) at the surface. The ABS states control thermodynamic properties and stability of the surface phases [16,17], and govern transport across interfaces [18–20].

In this Letter we study the Andreev states and spin currents at the surface of a NCS superconductor. We show that due to the nontrivial spin structure of the superconducting order, (i) a finite-bias peak appears in the surface DOS, and (ii) Andreev states acquire spin polarization and carry a spin supercurrent. Spin currents are enhanced near the surface already in the normal state, but the spin current in the SC phase has a significantly greater magnitude. We develop a detailed theory of these effects, and compare them with the previously studied spin currents in metallic and semiconducting systems.

For a noncentrosymmetric material it is convenient to perform a canonical transformation from a spin basis (with fermion annihilation operators $c_{k\mu}$ for spin $\mu = \uparrow, \downarrow$) to the so-called helicity basis $(b_{k\uparrow}, b_{k\downarrow})$ with helicity $s = \pm$, that diagonalizes the kinetic part of the Hamiltonian,

$$H_{\text{kin}} = \sum_{k\mu\nu} c_{k\mu}^\dagger \left( \xi_k + \alpha_k \sigma_{\mu\nu} c_{k\nu} \right) - \sum_{k,s} \varepsilon_k b_{k\uparrow}^\dagger b_{k\downarrow}. \quad (1)$$

Here, $\xi_k$ is the band dispersion relative to the chemical potential in the absence of SO interaction, $\alpha$ is the SO coupling strength, $\sigma$ is the vector of Pauli matrices, and $g_k = -g_{-k}$ is a normalized (see below) SO vector [11,12], Fig. 1. The helicity band dispersion is $\varepsilon_{k\pm} = \xi_k \pm \alpha |g_k|$. In each helicity band the orientation of the quasiparticle spin is fixed with respect to its momentum.

The Hamiltonian (1) is time reversal invariant but lifts the spin degeneracy. The transformation from spin to helicity basis, $U_k$, is defined by $U_k(g_k \sigma) U_k^\dagger = |g_k| \sigma_3$, and determined by the direction of the $g$ vector in $k$ space,

$$U_k = e^{-i(k \cdot \varepsilon_k/2) n_g \sigma_3}, \quad n_g = g_k / |g_k| \times \hat{z}, \quad (2)$$

where $\hat{z}$ is the unit vector in the $z$ direction, and $\theta_g$ is the polar angle between $g_k$ and $\hat{z}$ [12].

To describe superconductivity we use the Nambu-Gor’kov formalism modified for a helical basis. We define the helical counterpart $B_k^\dagger = (b_{k\uparrow}^\dagger, b_{k\downarrow}^\dagger, b_{k\uparrow}, b_{k\downarrow})$ to the
The Pauli matrix in the particle-hole space. Using energy scales (transition temperature functions in the helicity basis, grand canonical average, and Fermi surface and propagate coherently along a common Nambu spinor components, with normalization

\[ \langle \gamma, \alpha | \gamma', \beta \rangle = \delta_{\gamma \gamma'} \delta_{\alpha \alpha'} \]

We choose a separable pairing interaction consistent with \( v \) and the fermionic anticommutation energies via the surface amplitudes in the helicity basis \( k \) under reflection changes sign, \( \langle \ldots \rangle_{\text{AS}} \) is a grand canonical average, and \( \theta \) is the usual step function.

We employ the quasiclassical method [21] for treating the inhomogeneous surface problem. In the materials of interest \( \alpha | \gamma_k | \ll E_f \) for any Fermi momentum \( k_f \), where \( E_f \) is the Fermi energy. In addition, the superconducting energy scales (transition temperature \( T_c \) and the gap \( \Delta \)) are much smaller than \( E_f \). Under these conditions quasiparticles with different helicity can be assigned to a common Fermi surface and propagate coherently along a common classical trajectory over distances much longer than the Fermi wavelength. We utilize \( g_k, \langle g_k^\dagger \rangle = 1 \), where \( \langle \ldots \rangle \) denotes a Fermi surface average. The quasiclassical propagator is then obtained as \( g_k(k_f, R, \epsilon, t) = \tilde{\tau}_3 \int d\xi_k \times \int (d\sigma) e^{i(Q \cdot \sigma \cdot r)} \hat{G}_{k+1/2-k-1/2}(t + \tau, t) \) where \( \tilde{\tau}_3 \) is the Pauli matrix in the particle-hole space. Using

\[ U_k^{-1} = g_k \sigma \]

and the fermionic anticommutation symmetry relations for the 2 \( \times 2 \) Nambu matrix components, \( g(e, k_f)_{22} = \left[ (n_k \sigma) g(-e, -k_f) \right]_{11} \) and \( g(e, k_f)_{21} = \left[ (n_k \sigma) g(-e, -k_f) \right]_{12} \). Standard procedure [21] yields the Eilenberger equation in the helicity basis,

\[ [\epsilon \hat{\tau}_3 - \alpha \hat{\nabla}_{SO} - \Delta, \hat{g}] + i\gamma \hat{\nabla}\hat{g} = 0 \]

with normalization \( \hat{g}^2 = -\sigma^2 \hat{1} \). Here, \( \epsilon \) is the energy, \( \hat{\nabla}_{SO} = |g_k| \sigma_3 \hat{\tau}_3 \), and \( \Delta \) is the superconducting OP. The velocity renormalization of order \( \alpha / E_f \ll 1 \) is neglected. We choose a separable pairing interaction consistent with the form of the gap, and determine \( \Delta \) self consistently with \( \hat{g} \). In NCS superconductors the OP is a mixture of spin singlet (\( \Delta_s \)) and triplet (\( \Delta_t \)) components [13,22]. In the real gauge it is given by

\[ \hat{\Delta} = \sqrt{\Delta_s} (\Delta_s (R) \hat{1} + \Delta_t (R) \hat{\sigma}_3) \hat{1}, \]

where the basis function \( \sqrt{\Delta_s} (k_f) \) transforms according to one of the irreducible representations of the crystal point group, and \( \langle \Delta_s (k_f) \rangle = 1 \). With the gap functions in the helicity bands, \( \Delta_s = \Delta_s \), the order parameter is \( \Delta = (\Delta_s \Delta_s^* - \Delta_t \Delta_t^*) \sqrt{\Delta_s} \).

We parametrize the Green’s function by the coherence functions for particles and holes, \( \gamma \) and \( \tilde{\gamma} \) (2 \( \times 2 \) spin matrices), which allow a very intuitive physical interpretation of the Andreev scattering processes [23],

\[ \tilde{g} = -i\gamma \left( \begin{array}{cc} 1 - \gamma \tilde{\gamma} & 0 \\ 0 & 1 - \gamma \tilde{\gamma} \end{array} \right)^{-1} \left( \begin{array}{cc} 1 + \gamma \tilde{\gamma} & 2 \gamma \\ -2\gamma & -1 - \gamma \tilde{\gamma} \end{array} \right) \]

Fundamental symmetry relates \( \gamma \) and \( \tilde{\gamma} \) in the helicity basis by \( \tilde{\gamma} (e, k_f) = \left[ (n_k \sigma) g(-e, -k_f) \right] (i \sigma_2) \). In the bulk, \( \gamma = \gamma_0 \Delta^* + \gamma_0 \Delta^0 \), and \( \tilde{\gamma} = \tilde{\gamma}_0 \Delta^0 \Delta^0 \), with \( \gamma_0 \) and \( \tilde{\gamma}_0 \) transforming according to \( \gamma_0 = \gamma_k \) and \( \tilde{\gamma}_0 = \tilde{\gamma}_k \).

The surface bound states are determined by the poles of the Green’s function, Eq. (5). We consider specular reflection, whereby the component of \( k \) normal to the surface changes sign, \( \gamma_k \rightarrow k \); see Fig. 1. We find \( \gamma_k \) by integrating forward (backward) along the incoming, \( k \), (outgoing, \( k \)) trajectory starting from the values in the bulk [23]. In contrast, \( \gamma_k \) and \( \tilde{\gamma}_k \) are determined from the boundary conditions at the surface. Since the interface is nonmagnetic, \( \tilde{g} \) in the spin basis, \( \tilde{g}_k = \hat{U}_k \tilde{g}_k \hat{U}_k \), is continuous at the surface. This leads to a surface-induced mixing of the helicity bands according to \( U_k^0 \gamma_k U_k^0 = \gamma_k \) and \( U_k^0 \tilde{\gamma}_k U_k^0 = \tilde{\gamma}_k = U_k^0 \gamma_k U_k^0 \)

\[ \text{Eq. (5), the bound states correspond to the zero eigenvalues of the matrix } 1 - \gamma_k \tilde{\gamma}_k \]

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From Eq. (5), the bound states correspond to the zero eigenvalues of the matrix \( 1 - \gamma_k \tilde{\gamma}_k \) and \( 1 - \gamma_k \gamma_k \).

To derive our final equation for the ABS energies via the surface amplitudes in the helicity basis

\[ (1 + \gamma \tilde{\gamma}_s)(1 + \gamma \tilde{\gamma}_s) = -(1 + \gamma \tilde{\gamma}_s)(1 + \gamma \tilde{\gamma}_s) \]

\[ \mathfrak{M} \]

The “mixing” factor \( \mathfrak{M} \) is determined by the change of \( g_k \) under reflection \( k \rightarrow -k \) at the surface,

\[ \mathfrak{M} = \cos^2 \frac{\theta_g \phi_g}{2} + \cos^2 \frac{\phi_g}{2} \tan^2 \frac{\phi_g}{2} \]

where \( \theta_g, \phi_g, \phi_g \) are the polar and azimuthal angles of \( g_k \). In NCS superconductors with no SO coupling. The limit \( \mathfrak{M} \rightarrow \infty \) describes pure interband scattering. For a general Fermi surface and an arbitrary vector \( g_k \) (\( A \rightarrow A' \) in Fig. 1) a finite \( \mathfrak{M} \) determines the
results \[24,25\]. Experimentally accessing this peak by gap at a finite energy, in qualitative contrast to earlier respect to the interface \[16\]. Crucially, self-consistency in other unconventional superconductors misaligned with direction confirms this. Note that contributors the most to the subgap DOS.

To obtain insight in the role of the OP suppression, we consider first a simple model where \( \Delta = 0 \) in a layer of width \( W \) next to the surface; see Fig. 2. Trajectories incident at an angle \( \phi \) travel through a non-SC region of an effective width \( 2D = 2W/\cos \phi \). In this case Eq. (7) reads \( M = \cot^2 \phi \), the surface coherence amplitudes gain a phase factor, \( \gamma_s = \gamma_0 e^{2i\pi D/v_f} \), \( \gamma_s \) = \( \gamma_0 e^{2i\pi D/v_f} \), Eq. (5) yields \( \text{Im}^2(\gamma_s^0 e^{2i\pi D/v_f}) = \text{Re}^2(\gamma_0^0 e^{2i\pi D/v_f})M \), and the bound states are given by

\[
e^2 - \epsilon^2 = -\tan(2\pi e/\epsilon f \cos \phi \pm \phi).
\] (8)

Solutions of this equation are shown in Fig. 2. The “principal” modes with energies away from the continuum edge contribute the most to the subgap DOS. \( W = 0 \) (no gap suppression) reproduces the result of Ref. \[24\]: each incoming trajectory yields a bound state at a different energy. For \( W \neq 0 \) the main mode \( \epsilon_{\text{in}}(\phi) \) develops a maximum at \( \epsilon^* < \Delta_0 \), and we expect a peak in the surface DOS near \( \epsilon^* \) due to abundance of trajectories contributing to \( N(\epsilon^*) \).

The fully self-consistent solution, shown in Fig. 3(b), confirms this. Note that \( \Delta \neq 0 \) at the surface, Fig. 3(a), as in other unconventional superconductors misaligned with respect to the interface \[16\]. Crucially, self-consistency does yield a strong peak in the surface DOS below the gap at a finite energy, in qualitative contrast to earlier results \[24,25\]. Experimentally accessing this peak by point contact tunneling requires a sufficiently wide tunneling cone as the feature arises from the trajectories at intermediate incident angles; see Fig. 2.

These ABS have unusual spin structure. Figures 3(c) and 3(d) show the spin-resolved density of states, \( N_s(\epsilon, k_f) \) (dark) and \( N_s(\epsilon, k_f) \) (light) correspond to dark and light branches in Fig. 2.

Spin currents exist in NCS materials because the spin is not conserved, and consequently precession terms enter the continuity equation, \( \partial_t S^\alpha(x) + \nabla \cdot \Pi^\alpha(x) = P^\alpha(x) \) \[5\]. Here, the spin density, \( S^\alpha(x) = \frac{1}{2} \text{Tr} f d\epsilon \sigma^\alpha G(\epsilon, x) \), the spin current, \( \Pi^\alpha(x) = \frac{1}{2} \text{Tr} f d\epsilon [\sigma^\alpha, v_k] G(\epsilon, x) \), and the precession \( P^\alpha(x) = \frac{1}{2} \text{Tr} f d\epsilon [\sigma^\alpha, v_k - k] G(\epsilon, x) \), where \([\bullet, \bullet]\) is a commutator, and \( v_k = k/k_f + \alpha_R(\hat{\epsilon} \times \hat{\sigma}) \) (the band velocity), are all given in terms of Green’s functions at imaginary relative time \( \tau = -i \delta \). For the Rashba case, the precession terms are related to spin currents via the relations \( P^X = -2m_R \Pi^X \), \( P^Y = -2m_R \Pi^Y \), \( P^Z = 2m_R \alpha_R(\Pi^X \times \Pi^Y) \) \[26\].

We first consider the spin currents in the normal state. The bulk value, \( \Pi^Y = -\Pi^X = \Pi^\text{spin} = m^2 \epsilon^3 / 3 \pi \) agrees with Ref. \[5\]. To determine the surface spin currents we find the Green’s function for a surface modeled as a \( \delta \)-function barrier at \( x = 0 \) of strength \( U \). The Dyson equation in \( 2 \times 2 \) spin space reads \( G^{-1} = [G(0)]^{-1} - \epsilon \delta(x) \), where \( [G(0)]^{-1} = \epsilon - \xi_k - \alpha_R(\hat{\epsilon} \times \hat{\sigma}) \) for an impenetrable surface \( (U \rightarrow \infty) \) the solution is (for fixed \( \xi_k \) \[27\].

![FIG. 2 (color online). Bound state energy as a function of the impact angle for different widths \( W \) (in units of \( v_f / 2\Delta_0 \)) of the order parameter suppression region. Dark (light) lines correspond to the plus (minus) sign in Eq. (8). Solid lines: principal mode; broken lines: higher multiple reflection modes.](image2)

![FIG. 3 (color online). Structure of the surface states for a Rashba triplet superconductor \( \Delta_+ = -\Delta_- \). (a) Order parameter suppression; (b) DOS at locations indicated in (a); the large subgap peaks are due to the suppression of \( \Delta \). Inset: DOS for a homogeneous order parameter; note the absence of any subgap features. (c, d) Spin-resolved surface DOS for two trajectories: \( N_s(\epsilon, k_f) \) (dark) and \( N_s(\epsilon, k_f) \) (light) correspond to dark and light branches in Fig. 2.](image3)
We found that the Rashba-type spin-orbit coupling. We predicted that large in amplitude and slowly decaying spin currents with out of plane spin polarization are generically carried by these surface states. Our prediction opens the route to future investigations and applications of spin transport in systems containing superconductors without center of inversion, and for their use in spin-based devices.

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*Present address: Department of Physics, University of Wisconsin, Madison, WI, USA.


[27] Note, our last equation differs from Eq. (33) of this paper.
