Controlling the superconducting transition by rotation of an inversion symmetry breaking axis

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Using the ballistic-limit Bogoliubov–de Gennes framework on a cubic lattice, we consider the superconducting phase transition of a hybrid structure in which a layer with Rashba-like spin-orbit coupling is proximity-coupled to a conventional superconductor. We predict that the superconducting critical temperature $T_c$ can be tuned by rotating the vector $\mathbf{n}$ characterizing the axis of broken inversion symmetry. Specifically, we find that $T_c$ is suppressed when $\mathbf{n}$ is rotated from out-of-plane to in-plane relative to the spin-orbit layer. This is explained by the conversion of $s$-wave singlet Cooper pairs into other types of correlations, among these $s$-wave odd-frequency pairs which are robust to impurity scattering. Moreover, we find that $T_c$ varies even for purely in-plane rotations of $\mathbf{n}$. These results demonstrate a conceptually different way in which $T_c$ can be tuned compared to the previously studied variation of $T_c$ in magnetic hybrid structures via rotation of the magnetization $\mathbf{m}$.

Introduction.— Over the last years, research on combining superconducting and magnetic materials has shown that the physical properties of the resulting hybrid structure may be drastically altered compared to those of the individual materials [1–3]. In a conventional superconductor (S), electrons combine into $s$-wave singlet Cooper pairs [4]. A decrease in the $s$-wave singlet amplitude of the superconducting material leads to a loss of superconducting condensation energy, and thus also a suppression of the superconducting critical temperature, $T_c$. Such a decrease can be obtained by leakage of Cooper pairs into a non-superconducting material in proximity to the superconductor, and by conversion of $s$-wave singlets into different singlet and triplet Cooper pairs [2, 3]. For the latter to happen, the non-superconducting material must introduce some symmetry breaking additional to the translational invariance perpendicular to the interface [5]. This is the case in superconductor/ferromagnet hybrids where the spin-splitting of the energy bands of the homogeneous ferromagnetic material (F) leads to the creation of opposite-spin triplets [2].

The rotational invariance of a single, homogeneous ferromagnet cannot cause a variation in the $s$-wave singlet amplitude under rotations of the magnetization $\mathbf{m}$. However, experiments [6–10] have demonstrated that the critical temperature of F/S/F and S/F/F structures can be modulated by changing the relative orientation of the magnetization of the two homogeneous ferromagnets. In these hybrids, the rotational invariance is broken by the additional ferromagnetic layer in which opposite-spin triplets are rotated into equal-spin triplets when the ferromagnets are misaligned. While the opposite-spin triplets are subjected to pair-breaking by alignment of spins along the magnetization direction, the equal-spin triplets instead remain coherent for a longer distance into the ferromagnet, leading to a stronger decrease in the superconducting condensation energy.

Theoretical [11–15] and experimental [14] work has shown that a modulation of $T_c$ can be obtained by rotating the magnetization of a single homogeneous ferromagnet if thin heavy normal-metal layers are added in order to boost the Rashba spin-orbit coupling at the interface. The spin-orbit coupled layer (SOC) introduces inversion symmetry breaking perpendicular to an axis, here characterized by the vector $\mathbf{n}$, and thus breaks the rotational invariance.

While ferromagnetism only leads to a spin-splitting of the energy bands of spin-up and spin-down electrons, Rashba spin-orbit coupling is in addition odd under inversion of the momentum component perpendicular to $\mathbf{n}$. This raises an interesting question. While the proximity effect and accompanying change in $T_c$ in a S/F bilayer is invariant under rotations of $\mathbf{m}$, is it possible that $T_c$ in a S/SOC bilayer is not invariant under rotations of $\mathbf{n}$ (see Fig. 1)?

Motivated by this, we explore the possibility of a modulation of $T_c$ under reorientations of the inversion symmetry breaking vector $\mathbf{n}$ in a bilayer consisting of a conventional superconductor and a material with Rashba-like spin-orbit coupling. We choose this as a simple model to illustrate the concept of tuning $T_c$ via rotation of $\mathbf{n}$. We discover a suppression of the critical temperature when rotating $\mathbf{n}$ from an out-of-plane (OOP) to an in-plane (IP) orientation. Moreover, we demonstrate a variation in $T_c$ even when $\mathbf{n}$ is varied solely in the plane of the spin-orbit layer. We find that the difference in critical temperature for IP and OOP orientations of $\mathbf{n}$ can at least partly be accounted for by the absence of $s$-wave odd-frequency triplets for an OOP orientation of $\mathbf{n}$. Since $s$-wave triplets are robust with respect to impurity scattering, we expect our prediction of an IP suppression of the critical temperature to be observable not only in the ballistic limit covered by our theoretical framework, but also in the diffusive limit.

The lattice Bogoliubov–de Gennes framework.— We consider a 3D cubic lattice structure of size $N_x \times N_y \times N_z$.
consisting of a conventional superconductor and a spin-orbit coupled layer. The inversion symmetry breaking in the non-superconducting layer is accounted for by the existence of a Rashba spin-orbit coupling term in the Hamiltonian. The interface normal is directed along the $x$ axis. We use the ballistic-limit tight-binding lattice Bogoliubov–de Gennes (BdG) framework, following a similar approach to that in Refs. [15][17]. Our Hamiltonian is given by

$$H = -t \sum_{(i,j),\sigma} c_{i,\sigma}^\dagger c_{j,\sigma} - \sum_{i} \mu_{i} c_{i,\sigma}^\dagger c_{i,\sigma} - i \sum_{i} \lambda_{i} c_{i,\sigma}^\dagger n_i \cdot \{ \sigma \times \left[ \frac{1}{2} (1 + \zeta) (d_{i,j,x} + (d_{i,j,y})) \right] \} \alpha,\beta,$$

(1)

Above, $t$ is the hopping integral, $\mu_{i}$ is the chemical potential at lattice site $i$, $U_{i} > 0$ is the attractive on-site interaction giving rise to superconductivity, $\lambda$ is the Rashba spin-orbit coupling constant taken to be constant inside the spin-orbit coupled layer, $\sigma$ is the vector of Pauli matrices, $d_{i,j}$ is the vector from site $i$ to site $j$, and $(d_{i,j,x})$ and $(d_{i,j,y})$ are its projections onto the $x$ and $y$ plane, respectively. $\zeta = 1$ if site $i$ and $j$ are both inside the SOC layer, and $\zeta = 0$ if site $i$ and $j$ are on opposite sides of the interface. $c_{i,\sigma}^\dagger$ and $c_{i,\sigma}$ are the second quantization electron creation and annihilation operators at site $i$ with spin $\sigma$, and $n_{i,\sigma} \equiv c_{i,\sigma}^\dagger c_{i,\sigma}$ is the number operator. We describe $n \equiv \cos(\phi) (\sin(\theta), \sin(\phi) (\sin(\theta), \cos(\theta))$ by the azimuthal angle $\phi$ and the polar angle $\theta$ with respect to the $z$ axis. The terms of the Hamiltonian are only nonzero in their respective regions. We treat the superconducting term by a mean-field approach, assuming $c_{i,\sigma}^\dagger c_{i,\sigma} = \langle c_{i,\sigma}^\dagger c_{i,\sigma} \rangle + \delta$ and neglecting terms of second order in $\delta$. In the above Hamiltonian, the Rashba term is symmetrized in order to allow for in-plane components of $n$ while ensuring a hermitian Hamiltonian, rather than using the non-symmetrized Rashba term used for OOP $n$ in Refs. [15][17]. We derive the second quantization Rashba term above from the symmetrized first quantization Rashba operator $\frac{1}{2} (\mu \times \mathbf{d}) \cdot \{ \lambda (\mu) \}, \mathbf{d}$ is the momentum operator. The derivation is outlined in the supplemental material. In the following, we scale all energies to the hopping element $t$, and all lengths to the lattice constant $a$. We also set the reduced Planck constant $\hbar$ and the Boltzmann constant $k_B$ equal to 1. It follows that all temperatures are scaled by $t/k_B$ in the presentation of the results.

We assume periodic boundary conditions in the $y$ and $z$ directions, and introduce the Fourier transform along the $y$ and $z$ axes, $c_{k,\sigma} \equiv (N_y/N_z)^{-1/2} \sum_{k_y,k_z} c_{k_y,k_z,\sigma} \exp \{ ik_y y + ik_z z \}$, where the sum is taken over the allowed $k_y$ and $k_z$ inside the first Brillouin zone. In the following, we also use the relation $(N_m)^{-1} \sum_{m} \exp \{ i (k_m - k'_m) m \} = \delta_{k_m,k'_m}$, where $m = y,z$. By choosing the basis $B_{i,\sigma} \equiv \{ c_{k_y,k_z,\sigma}^\dagger, c_{-k_y,k_z,\sigma}^\dagger, c_{-k_y,-k_z,\sigma}^\dagger, c_{k_y,-k_z,\sigma}^\dagger \}$, and applying the Fourier transform, we rewrite the Hamiltonian as $H = H_0 + \frac{1}{2} \sum_{i,j,x,y,z} B_{i,x,y,z}^\dagger H_{i,j,x,y,z} B_{i,x,y,z}$, $H_0$ is a constant term of no importance for our further calculations, and

$$H_{i,j,x,y,z} = \epsilon_{i,x,y,z} \epsilon_{j,x,y,z} \tau_3 \delta_{0} + (\Delta_{i,x,y,z} + \Delta_{i,j,x,y,z} \tau_3) \delta_{y} \delta_{i,j} - \{ \sin(k_x) \tau_0 \delta_{x} - \sin(k_x) \tau_y \delta_{y} \} x - \{ \sin(k_y) \tau_x \delta_{y} - \sin(k_y) \tau_y \delta_{x} \} \lambda_{i,j} \delta_{i,j} + i \lambda (1 + \zeta) (\tau_0 \delta_{x} - \tau_y \delta_{y} \tau_z) \delta_{i,j}-1, \delta_{i,j}-1),$$

(2)

where $\tau^\pm = (\tau_1 \pm i \tau_2)/2$, $\tau_0 \delta_{x} = \tau \delta_{x}$ is the Kronecker product of the Pauli matrices spanning Nambu and spin space, $\epsilon_{i,x,y,z} \epsilon_{j,x,y,z} = \{ -2t[\cos(k_y) + \cos(k_z)] - \mu_{i,x,y,z} - t(\delta_{i,x,y,z} - 1) \}$, and $\Delta_{i,x,y,z}$ is the superconducting gap at site $i$. By rewriting the Hamiltonian in terms of the basis $W_{i,k_y,k_z}^\dagger = [B_{i,k_y,k_z,1}^\dagger, \ldots, B_{i,k_y,k_z,N_z}^\dagger, \ldots, B_{i,k_y,k_z,N_z}^\dagger]$, we assume periodic boundary conditions in $y$ and $z$ axes, rewriting to the new quasi-particle operators, and using that $\langle \gamma_{n,k_y,k_z} \gamma_{m,k_y,k_z} \rangle = f(E_{n,k_y,k_z}/2) \delta_{n,m}$, we find that the gap is given by $\Delta_{i,x,y,z} = \sum_{m} \langle \gamma_{n,k_y,k_z} \gamma_{m,k_y,k_z} \rangle = f(E_{n,k_y,k_z}/2)$, where $f(E_{n,k_y,k_z}/2)$ is the Fermi-Dirac distribution.

The superconducting critical temperature is found by a bi-nomial search [18]. In each of the $n_{i,x,y,z}$ iterations, we determine whether $T_c$ is contained within the upper or lower half of our temperature interval. This is done by determining whether $\Delta_{i,x,y,z}$ increases towards a superconducting solution or decreases towards a normal state solution from the initial guess after recalculating $\Delta_{i,x,y,z}$ times. We choose an initial guess with a similar $x$ dependence as the gap just below $T_c$, and with a magnitude $\Delta_0/1000$, where $\Delta_0$ is the zero-temperature superconducting gap.

The even-frequency $s$-wave singlet amplitude is given by $S_{i,x,y,z} = 2 \Delta_{i,x,y,z}/U_{i,x,y,z}$. As a measure of the total singlet amplitude of the superconductor, we introduce the quantity $S_x \equiv \sum_{i} \sum_{x} |S_{i,x,y,z}|$, where the sum is taken over the superconducting region only. We also define the opposite- and equal-spin odd-frequency $s$-wave triplet amplitudes $S_{0,\sigma}(\tau) = \langle c_{i,\sigma}^\dagger(\tau)c_{i,\sigma}(0) \rangle + \langle c_{i,\sigma}^\dagger(\tau)c_{i,\sigma}(0) \rangle$, and $S_{\sigma}(\tau) = \langle c_{i,\sigma}(\tau)c_{i,\sigma}(0) \rangle$, where the time-dependent electron annihilation operator is given by $c_{i,\sigma}(\tau) = e^{iH\tau} c_{i,\sigma} e^{-iH\tau}$ [19].

The influence of the spin-orbit coupled layer on $T_c$ is ex-
predicted to be strongest when the superconducting coherence length $\xi \equiv \hbar v_F / \pi \Delta_0$ is comparable to thickness of the superconductor. $v_F \equiv \left. \frac{dE}{dk} \right|_{k=k_F}$ is the normal-state Fermi velocity, $E_k$ is the normal-state eigenenergies when introducing periodic boundary conditions along all three axes, and $k_F$ is the corresponding Fermi momentum averaged over the Fermi surface. We round $\xi$ down to the closest integer number of lattice points.

The superconducting critical temperature.—By following the above approach, we plot $T_c/T_{c,S}$ and $\tilde{S}_s / \tilde{S}_{s,S}$ in Fig. 2. To ensure that the effect is robust, we use two different parameter sets: $N_{x,S} = 7$, $N_{x,HM} = 3$, $N_{y} = N_{z} = 85$, $\mu_{S} = 1.9$, $\mu_{HM} = 1.7$, $U = 2.1$, $\lambda = 0.8$, $n_{a,T} = 20$, and $N_{\Delta} = 35$ (panels (a) and (b)), and $N_{x,S} = 5$, $N_{x,HM} = 2$, $N_{y} = N_{z} = 100$, $\mu_{S} = 1.9$, $\mu_{HM} = 1.7$, $U = 1.9$, $\lambda = 0.2$, $n_{a,T} = 25$, and $N_{\Delta} = 40$ (panels (c) and (d)). This gives coherence lengths $\xi = 4$ and $\xi = 7$ for the first and second set of parameters, respectively. $T_c$ is the critical temperature and $\tilde{S}_{s,S}$ the total singlet amplitude of the superconducting layer without proximity to the SOC layer.

For both parameter sets, we see a suppression of the critical temperature for an IP $n$ compared to an OOP $n$ (see panels (a) and (c)). From panels (b) and (d), we see that there is also an IP variation in $T_c$, that may give the strongest in-plane suppression either when $n$ is oriented at a $\pi/4$ angle with respect to the cubic axes, or when $n$ is oriented along the cubic axes. As we find a similar variation in the normal-state free energy, which only depends on the eigenenergy spectrum of the system, this varying modulation of the IP component of the critical temperature is likely to be caused by band-structure effects due to the crystal structure of the cubic lattice.

$\tilde{S}_{s}/\tilde{S}_{s,S}$ is plotted at a temperature slightly below $T_c$, in order to explain the variation in the critical temperature. We see that the variation in the total singlet amplitude is of a similar form as the variation in $T_c$. The $T_c$ modulation can thus be attributed to the variation of the $s$-wave singlet amplitude in the superconducting region. Note that the slight deviation between $T_c/T_{c,S}$ and $\tilde{S}_s / \tilde{S}_{s,S}$ in Fig. 2 is caused by $\tilde{S}_s$ being calculated at $T < T_c$.

If we further investigate the triplet amplitudes present for different orientations of $n$, we find that the $s$-wave odd-frequency anomalous triplet amplitude is absent for $n = x$, i.e. when $n$ has no IP component. For all other orientations of $n$, the $s$-wave odd-frequency anomalous triplet amplitude is nonzero. This suggests that the OOP to IP change in the superconducting critical temperature is at least partly caused by the increase in the $s$-wave triplet amplitude from zero when $n$ points OOP to an increasing finite value as the IP component of $n$ increases. The $s$-wave triplet amplitude is of particular interest as it is the only triplet amplitude robust to impurity scattering. We may therefore expect an IP suppression of the critical temperature also in diffusive materials. Below, we perform analytical calculations which prove that odd-frequency pairing is absent when $n$ points OOP.

The continuum Bogoliubov–de Gennes framework.—In order to explain the absence of $s$-wave odd-frequency triplets when $n$ is OOP, we consider two 2D continuum systems that can be treated analytically within the BdG framework [20–27]: a SOC/S bilayer with an OOP $n = x$, and a F/S bilayer with magnetization $m \parallel z$. We use conventions similar to those in Refs. [26,27] (see also Ref. [28]). We choose our 2D systems to be located in the $xy$ plane, and the interface normal to be oriented along the $z$ axis with the interface at $x = 0$.

We find the scattering wave functions [29] $\Psi_{m}(r_1, t_1) \propto e^{-iE_{1}t_1}$ and $\Psi_{m}(r_2, t_2) \propto e^{iE_{T}t_2}$ from the time-independent Schrödinger equations [26,27] $H(k)\Psi_{m}(r_1, t_1) = E\Psi_{m}(r_1, t_1)$ and $H^{*}(-k)\Psi_{m}(r_2, t_2) = E\Psi_{m}(r_2, t_2)$, respectively, where

$$H(k) = \left( \frac{k^2}{\eta - \mu} \right) \tilde{\tau}_3 \tilde{\sigma}_0 + \Delta i \tilde{\tau}_+ \tilde{\sigma}_y - \Delta^* i \tilde{\tau}_- \tilde{\sigma}_y - \lambda (n_x k_y - n_y k_x) \tilde{\tau}_0 \tilde{\sigma}_z - \lambda n_z k_y \tilde{\tau}_0 \tilde{\sigma}_x + h_x \tilde{\tau}_3 \tilde{\sigma}_x + h_y \tilde{\tau}_0 \tilde{\sigma}_y + h_z \tilde{\tau}_3 \tilde{\sigma}_z.$$  

Above, $k = (k_x, k_y)$ is the wave vector, $\eta \equiv 2m/\hbar^2$, and $h = (h_x, h_y, h_z)$ is the magnetic exchange field. The terms are only nonzero in their respective regions. The four components of the scattering wave functions correspond to spin-up and spin-down electrons, and spin-up and spin-down holes, respectively. The indices $n$ and $m$ refer to the eight possible wave functions describing scattering of (quasi-)particles incoming from the left ($n, m = \{1, 2, 3, 4\}$) and from the right ($n, m = \{5, 6, 7, 8\}$). $\Psi_{m}(r, t)$
satisfies the boundary conditions \[ \Psi_n(r, t) \big|_{z=0^+} = \psi_n(r, t) \big|_{z=0^-}, \] and \[ \partial H(k_x) \rightarrow -\partial \psi_n(r, t) \big|_{z=0^-}, \] where \( \psi \equiv \partial H(k_x) \rightarrow -\partial \psi_n(r, t) \big|_{z=0^-} \) is the velocity operator. \( \Psi_m(r, t) \) satisfies a similar set of boundary conditions with \( \psi \equiv \partial H^*(k_x) \rightarrow i\partial \psi_n(r, t) \big|_{z=0^-} \). Note that the symmetrization of the Rashba term enters through these boundary conditions rather than through the Hamiltonian.

From the scattering wave functions, we construct the retarded Green's function in Nambu \( \otimes \) spin space \([26,27]\).

\[
[G^r(r_1, r_2; t_1, t_2)]_{x_1,x_2} = \theta(t_1 - t_2) \cdot \sum_{n,m=1}^4 \alpha_{nm} \Psi_n(r_1, t_1) \tilde{\Psi}^T_{m+4}(r_2, t_2),
\]

\[
[G^r(r_1, r_2; t_1, t_2)]_{x_1,x_2} = \theta(t_1 - t_2) \cdot \sum_{n,m=1}^4 \beta_{nm} \Psi_{n+4}(r_1, t_1) \tilde{\Psi}^T_m(r_2, t_2).
\]

We Fourier transform the retarded Green's function in the relative coordinates \( y \equiv y_1 - y_2 \) and \( t = t_1 - t_2 \), using \( G^r(x_1, x_2, p_y; \omega) = \int_{-\infty}^{\infty} dy e^{-ip_y y} \int_{-\infty}^{\infty} dt e^{i\omega t} G^r(x_1, x_2, y; t) \). The coefficients \( \alpha_{nm} \) and \( \beta_{nm} \) are found from the boundary conditions of the retarded Green's function at \( x_1 = x_2 \) \([26,27]\).

\[
[G^r(x_1 > x_2, p_y; \omega)]_{x_1,x_2} = [G^r(x_1 < x_2, p_y; \omega)]_{x_1,x_2}, \quad \partial_x G^r(x_1 > x_2, p_y; \omega)]_{x_1=x_2} - \partial_x G^r(x_1 < x_2, p_y; \omega)]_{x_1=x_2} = \eta \gamma_3 \gamma_0.
\]

The even-odd-frequency singlet and triplet retarded anomalous Green's functions are given by \([26,27]\).

\[
f^{r,E(O)}_0(x_1, x_2, p_y; \omega) = \left[ f^{r}_0(x_1, x_2, p_y; \omega) \right] / 2,
\]

\[
f^{r,E(O)}_i(x_1, x_2, p_y; \omega) = \left[ f^{r}_i(x_1, x_2, -p_y; \omega) \right] / 2,
\]

where \( f^{r}_0(x_1, x_2, p_y; \omega) \) represents the singlet amplitude, and \( f^{r}_i(x_1, x_2, p_y; \omega), \) \( i = 1, 2, 3 \), represents the spin-triplet amplitudes. Their parities under inversion of \( x \equiv x_1 - x_2 \) and \( p_y \) determines the spatial symmetry of the singlet and triplet amplitudes. Although the \( s \)-wave and \( d_{x^2-y^2} \)-wave triplets have the same parities along the \( x \) and \( y \) axis, we may prove the presence of the \( s \)-wave triplet by obtaining a nonzero result when integrating over all spatial coordinates.

Singlet and triplet amplitudes.— Applying the above method, we find that \( s \)- and \( p_x \)-wave singlets, and \( p_y \)- and \( d_{x^2-y^2} \)-wave opposite-spin triplets are present in the 2D SOC/S system when \( n = \sigma \). There may also be \( d_{x^2-y^2} \)-wave singlets in the system. At the first glance, it might seem strange that the odd-frequency \( s \)-wave triplet amplitude is zero, when it is nonzero for a 2D F/S structure with magnetization along the \( z \) axis. Although the Hamiltonians of these systems are of a similar form, they allow for the existence of different triplet amplitudes. The crucial difference leading to a generation of \( p_y \)- and \( d \)-wave triplets in the SOC/S system rather than \( s \)- and \( p_x \)-wave triplets as in the F/S system, is the \( k_y \) dependence of the Rashba term. As seen in the lengthy analytical expressions provided in the supplementary information, this is ultimately the reason for why the odd-frequency amplitude does not occur in the SOC/S case when \( n \) is oriented OOP.

We have also investigated a 2D SOC/S structure for an IP orientation \( n = z \) numerically and find additional equal-spin triplets which have an odd-frequency symmetry. For a 3D SOC/S system with \( n \) OOP, the Rashba term depends on both \( k_y \) and \( k_z \). Similarly as in 2D, we expect this to allow for triplets that are odd under inversion of \( k_y \) and \( k_z \), and therefore cause of the absence of \( s \)-wave triplet amplitudes.

Experimental realization.— We finally briefly comment on the possibilities of an experimental realization of the predicted \( T_c \) variation upon changing the direction of \( n \). We suggest cleaving a non-centrosymmetric metal, e.g. BiPd \([31,33]\), in different directions and growing a superconductor on the surface, or to deposit superconductors on the surface of a curved non-centrosymmetric material with a long edge (several mm) \([34]\). In both of these scenarios, different samples would have their inversion symmetry breaking axis in different directions, corresponding to a systematic rotation of \( n \) from in-plane to out-of-plane. We underline that although \( n \) rotates along with the lattice in the non-superconducting region in this way, the difference in \( T_c \) as \( n \) changes from IP to OOP is robust. The reason is that the corresponding change in the proximity effect, causing the variation in \( T_c \), exists even in a continuum model without the underlying lattice, as our Green function analysis demonstrates. The ideal scenario, albeit challenging, would be to induce an \( in \text{situ} \) rotation of \( n \) in the non-superconducting region via electric gating in different directions which induces an inversion-symmetry breaking field. In this way, the IP variation of \( T_c \) with \( n \) could also be observed.

Concluding, we have shown that the superconducting transition temperature \( T_c \) can be altered by rotating the inversion symmetry breaking axis \( n \) in a proximate material, providing a conceptually different way of controlling \( T_c \) compared to previous studies.

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SUPPLEMENTAL MATERIAL TO: CONTROLLING THE SUPERCONDUCTING TRANSITION BY ROTATION OF AN INVERSION SYMMETRY BREAKING AXIS

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I. THE LATTICE BOGLIUBOV–DE GENNES FRAMEWORK

A. Symmetrization of the Hamiltonian

If the inversion symmetry breaking axis directed along \( \mathbf{n} \) has an in-plane component, a Rashba Hamiltonian of the form
\[
\frac{1}{2}\sum_{\langle i,j \rangle, \alpha, \beta} \lambda c_i^\dagger \sigma \cdot \mathbf{n} \cdot \langle \sigma \times \mathbf{d}_{i,j} \rangle_{\alpha, \beta} c_j \text{ is in general non-Hermitian.}
\]
This term is the second quantized form of [35] \( \lambda \) acts as a step function at the interface. It follows that the symmetrized spin-orbit coupling contribution to the Hamiltonian is
\[
H_\lambda = -\frac{i}{2} \sum_{\langle i,j \rangle, \alpha, \beta} \lambda c_i^\dagger \sigma \cdot \mathbf{n} \cdot \{ \sigma \times (\mathbf{d}_{i,j})_{\alpha, \beta} c_j \}. \tag{8}
\]
Above, \( \mathbf{d}_{i,j} \) is decomposed into a part perpendicular to the interface \( (\mathbf{d}_{i,j})_x \), and a part parallel to the interface \( (\mathbf{d}_{i,j})_\parallel \).

ζ = 1 if site \( i \) and \( j \) are both inside the heavy-metal, and \( \zeta = 0 \) if site \( i \) and site \( j \) are on opposite sides of the interface.

II. THE CONTINUUM BOGLIUBOV–DE GENNES FRAMEWORK

The continuum Bogoliubov–de-Gennes framework [20–27] allows us to obtain analytical expressions for the singlet and triplet retarded anomalous Green’s functions of the 2D SOC/S system with \( \mathbf{n} = \hat{x} \) and the 2D F/S system with \( \mathbf{m} \parallel \hat{z} \).

We have not given these expressions in the paper, as we are mainly interested in their symmetries under spatial inversion. Here, we show the analytical expressions for the wave functions and the singlet and triplet retarded anomalous Green’s functions for these two systems, as well as the wave functions for the 2D SOC/S system with \( \mathbf{n} = \hat{z} \), derived by the method outlined in the paper.

A. The scattering wave functions

In the following, we give expressions for the scattering wave functions inside a 2D superconductor, a 2D material with Rashba-like spin-orbit coupling for \( \mathbf{n} = \hat{x} \) and \( \mathbf{n} = \hat{z} \), and a 2D ferromagnet with \( \mathbf{h} = h \hat{z} \), treating each material separately. We choose the superconducting region to be located at \( x > 0 \), while the non-superconducting region is located at \( x < 0 \).

1. The superconducting region

The scattering wave functions on the superconducting side of the interface are
\[
\Psi_n(r, t) = \Psi_{in,n}(r, t)
\]
\[
+ c_{n,1} [0, 0, u_0] T e^{i q_x x + i k_y y - i E t} + c_{n,2} [0, -u_0, 0] T e^{i q_x x + i k_y y - i E t}
\]
\[
+ d_{n,1} [0, 0, u_0] T e^{-i q_x x + i k_y y - i E t} + d_{n,2} [0, u_0, 0] T e^{-i q_x x + i k_y y - i E t}, \quad x > 0,
\]
\[
\tilde{\Psi}_m(r, t) = \tilde{\Psi}_{in,m}(r, t)
\]
\[
+ \tilde{c}_{m,1} [0, 0, u_0] T e^{i q_x x + i k_y y + i E t} + \tilde{c}_{m,2} [0, -u_0, 0] T e^{i q_x x + i k_y y + i E t}
\]
\[
+ \tilde{d}_{m,1} [0, 0, u_0] T e^{-i q_x x + i k_y y + i E t} + \tilde{d}_{m,2} [0, u_0, 0] T e^{-i q_x x + i k_y y + i E t}, \quad x > 0, \tag{9}
\]
where the quasi-particles incoming from the right are described by the wave functions

\[
\begin{align*}
\Psi_{m,5}^R(r, t) &= [u_0 \ 0 \ 0 \ v_0]^T e^{-i q x y + i k_y y - i E t}, \\
\Psi_{m,6}^R(r, t) &= [0 - u_0 \ 0 \ v_0]^T e^{-i q x y + i k_y y - i E t}, \\
\Psi_{m,7}^R(r, t) &= [0 - v_0 \ 0 \ u_0]^T e^{i q x y + i k_y y - i E t}, \\
\Psi_{m,8}^R(r, t) &= [v_0 \ 0 \ 0 \ u_0]^T e^{i q x y + i k_y y - i E t},
\end{align*}
\]  

and

\[
\begin{align*}
\tilde{\Psi}_{m,5}^R(r, t) &= [u_0 \ 0 \ 0 \ v_0]^T e^{-i q x y + i k_y y + i E t}, \\
\tilde{\Psi}_{m,6}^R(r, t) &= [0 - u_0 \ 0 \ v_0]^T e^{-i q x y + i k_y y + i E t}, \\
\tilde{\Psi}_{m,7}^R(r, t) &= [0 - v_0 \ 0 \ u_0]^T e^{i q x y + i k_y y + i E t}, \\
\tilde{\Psi}_{m,8}^R(r, t) &= [v_0 \ 0 \ 0 \ u_0]^T e^{i q x y + i k_y y + i E t}.
\end{align*}
\]

The region with Rashba spin-orbit coupling,

\[
\Psi_{m,5}^L(r, t) = \Psi_{m,6}^L(r, t) = \Psi_{m,7}^L(r, t) = \Psi_{m,8}^L(r, t) = 0.
\]

We reserve the indices \(n, m = \{1, 2, 3, 4\}\) for scattering processes with particles or quasi-particles scattering at the interface from the left. Above, \(q_x = \{-k_y^2 + \eta|\mu \pm \sqrt{E^2 - |\Delta|^2}\}^{1/2}\) are the allowed \(k_x\) values, \(E = \pm \sqrt{k^2/\eta - \mu^2 + |\Delta|^2} < |\Delta|\) are the corresponding eigenenergies, \(u_0^2 = \frac{1}{2} \left[1 + \sqrt{E^2 - |\Delta|^2} / E \right]\), and \(v_0^2 = \frac{1}{2} \left[1 - \sqrt{E^2 - |\Delta|^2} / E \right].\)

2. The region with Rashba spin-orbit coupling, \(n = \hat{z}\)

The scattering wave functions on the side of the interface with Rashba-like spin-orbit coupling are

\[
\begin{align*}
\Psi_n(r, t) &= \Psi_{m,n}^L(r, t) \\
&= \Psi_{m,n}^L(r, t) \\
&\quad + a_{n,1} [1 \ 0 \ 0 \ 0]^T e^{-i k_x^R x + i k_y y - i E t} \\
&\quad + a_{n,2} [0 \ 1 \ 0 \ 0]^T e^{-i k_x^R x + i k_y y - i E t} \\
&\quad + b_{n,1} [0 \ 0 \ 1 \ 0]^T e^{i k_x^R x + i k_y y - i E t} \\
&\quad + b_{n,2} [0 \ 0 \ 0 \ 1]^T e^{i k_x^R x + i k_y y + i E t}, \ x < 0,
\end{align*}
\]

\[
\begin{align*}
\tilde{\Psi}_m(r, t) &= \tilde{\Psi}_{m,n}^L(r, t) \\
&= \tilde{\Psi}_{m,n}^L(r, t) \\
&\quad + \tilde{a}_{m,1} [1 \ 0 \ 0 \ 0]^T e^{-i k_x^R x + i k_y y + i E t} \\
&\quad + \tilde{a}_{m,2} [0 \ 1 \ 0 \ 0]^T e^{-i k_x^R x + i k_y y + i E t} \\
&\quad + \tilde{b}_{m,1} [0 \ 0 \ 1 \ 0]^T e^{i k_x^R x + i k_y y + i E t} \\
&\quad + \tilde{b}_{m,2} [0 \ 0 \ 0 \ 1]^T e^{i k_x^R x + i k_y y + i E t}, \ x < 0,
\end{align*}
\]

if \(n = \hat{x}\), where the particles incoming from the left are described by

\[
\begin{align*}
\Psi_{m,1}^L(r, t) &= [1 \ 0 \ 0 \ 0]^T e^{i k_x^L x + i k_y y - i E t}, \\
\Psi_{m,2}^L(r, t) &= [0 \ 1 \ 0 \ 0]^T e^{i k_x^L x + i k_y y - i E t}, \\
\Psi_{m,3}^L(r, t) &= [0 \ 0 \ 1 \ 0]^T e^{-i k_x^L x + i k_y y - i E t}, \\
\Psi_{m,4}^L(r, t) &= [0 \ 0 \ 0 \ 1]^T e^{-i k_x^L x + i k_y y - i E t},
\end{align*}
\]

and

\[
\begin{align*}
\tilde{\Psi}_{m,1}^L(r, t) &= [0 \ 1 \ 0 \ 0]^T e^{i k_x^L x + i k_y y + i E t}, \\
\tilde{\Psi}_{m,2}^L(r, t) &= [1 \ 0 \ 0 \ 0]^T e^{i k_x^L x + i k_y y + i E t}, \\
\tilde{\Psi}_{m,3}^L(r, t) &= [0 \ 0 \ 1 \ 0]^T e^{-i k_x^L x + i k_y y + i E t}, \\
\tilde{\Psi}_{m,4}^L(r, t) &= [0 \ 0 \ 0 \ 1]^T e^{-i k_x^L x + i k_y y + i E t}.
\end{align*}
\]

3. The region with Rashba spin-orbit coupling, \(n = \hat{z}\)

The scattering wave functions on the side of the interface with Rashba-like spin-orbit coupling are

\[
\begin{align*}
\Psi_n(r, t) &= \Psi_{m,n}^L(r, t) \\
&+ a_{n,1} [1 \ i e^{i \phi} \ 0 \ 0]^T e^{-i k_x^R x + i k_y y - i E t} \\
&+ a_{n,2} [-1 \ i e^{i \phi} \ 0 \ 0]^T e^{-i k_x^R x + i k_y y - i E t} \\
&+ b_{n,1} [0 \ 0 \ 1 \ 0]^T e^{i k_x^R x + i k_y y - i E t} \\
&+ b_{n,2} [0 \ 0 \ 0 \ 1]^T e^{i k_x^R x + i k_y y + i E t}, \ x < 0,
\end{align*}
\]

\[
\begin{align*}
\tilde{\Psi}_m(r, t) &= \tilde{\Psi}_{m,n}^L(r, t) \\
&+ \tilde{a}_{m,1} [1 \ i e^{-i \phi} \ 0 \ 0]^T e^{-i k_x^R x + i k_y y + i E t} \\
&+ \tilde{a}_{m,2} [-1 \ i e^{-i \phi} \ 0 \ 0]^T e^{-i k_x^R x + i k_y y + i E t} \\
&+ \tilde{b}_{m,1} [0 \ 0 \ 1 \ 0]^T e^{i k_x^R x + i k_y y + i E t} \\
&+ \tilde{b}_{m,2} [0 \ 0 \ 0 \ 1]^T e^{i k_x^R x + i k_y y + i E t}, \ x < 0,
\end{align*}
\]

if \(n = \hat{z}\), where the particles incoming from the left are described by

\[
\begin{align*}
\Psi_{m,1}^L(r, t) &= [1 \ i e^{i \phi} \ 0 \ 0]^T e^{i k_x^L x + i k_y y - i E t}, \\
\Psi_{m,2}^L(r, t) &= [-1 \ i e^{i \phi} \ 0 \ 0]^T e^{i k_x^L x + i k_y y - i E t}, \\
\Psi_{m,3}^L(r, t) &= [0 \ 0 \ 1 \ 0]^T e^{-i k_x^L x + i k_y y - i E t}, \\
\Psi_{m,4}^L(r, t) &= [0 \ 0 \ 0 \ 1]^T e^{-i k_x^L x + i k_y y - i E t}
\end{align*}
\]
where

\[ \Psi_{m,1}(r, t) = [1 \ 0 \ 0 \ 0] e^{i k_x^\alpha x + i k_y y + i t E} \]
\[ \Psi_{m,2}(r, t) = [0 \ 1 \ 0 \ 0] e^{i k_x^\alpha x + i k_y y + i t E} \]
\[ \Psi_{m,3}(r, t) = [0 \ 0 \ 1 \ 0] e^{-i k_x^\alpha x - i k_y y + i t E} \]
\[ \Psi_{m,4}(r, t) = [0 \ 0 \ 0 \ 1] e^{-i k_x^\alpha x + i k_y y + i t E} \]

(17)

\[ \Psi_{m,5}(r, t) = \Psi_{m,6}(r, t) = \Psi_{m,7}(r, t) = \Psi_{m,8}(r, t) = 0. \]

Above, \( k_x^\alpha \) are the allowed \( k_x \) values, where \( k_x = \pm \sqrt{\eta^2 / 2 + \eta (\mu \pm E)} \) are the corresponding eigenenergies, where \( \pm \) corresponds to electrons and holes, respectively, and \( \pm' \) corresponds to the two different spin-mixed states. We define \( k_x^\alpha \) to be positive by setting \( \phi \in [-\pi/2, \pi/2] \).

4. The ferromagnetic scattering wave functions

The scattering wave functions on the ferromagnetic side of the interface are

\[ \Psi_n(r, t) = \Psi_{n,m}(r, t) = \Psi_{n,1}(r, t) = \Psi_{n,2}(r, t) = \Psi_{n,3}(r, t) = \Psi_{n,4}(r, t) = 0. \]

\[ \Psi_{n,5}(r, t) = \Psi_{n,6}(r, t) = \Psi_{n,7}(r, t) = \Psi_{n,8}(r, t) = 0. \]

\[ \Psi_{n,5}(r, t) = \Psi_{n,6}(r, t) = \Psi_{n,7}(r, t) = \Psi_{n,8}(r, t) = 0. \]

(18)

5. The single and triplet retarded anomalous Green’s functions

We find the retarded anomalous Green’s functions by the method outlined in the paper, i.e. by solving the boundary conditions of the wave functions, constructing the retarded Green’s function from the wave functions, and solving the boundary conditions of the retarded Green’s function.

Before identifying the singlet and triplet even- and odd-frequency anomalous contributions to the retarded Green’s function, we rewrite the coordinates to relative coordinates \( x \equiv x_1 - x_2, y \equiv y_1 - y_2, t \equiv t_1 - t_2 \), and the center of mass coordinate \( X \equiv (x_1 + x_2) / 2 \), and apply the Fourier transform in the relative \( y \) coordinate, \( f_{n, \beta}(x_1, x_2, y; \omega) \equiv \int_{-\infty}^{\infty} dy \ e^{-i p_y y} f_{n, \beta}(x_1, x_2, y; \omega) \).

The definitions of the singlet and triplet anomalous contributions to the retarded Green’s functions that we use below are

\[ f_{n, \beta}^s(x_1, x_2, y; \omega) \equiv \{ [G^s(x_1, x_2, p_y; \omega)]_{11} - [G^s(x_1, x_2, p_y; \omega)]_{23} \} / 2 \]

for the singlet amplitude, \( f_{n, \beta}^t(x_1, x_2, p_y; \omega) \equiv \{ G^t(x_1, x_2, p_y; \omega) \} / 13 \), and \( f_{n, \beta}^{23}(x_1, x_2, p_y; \omega) \equiv \{ G^s(x_1, x_2, p_y; \omega)]_{14} + [G^s(x_1, x_2, p_y; \omega)]_{23} \} / 2 \) for the opposite-spin triplet amplitude.

1. The SOC/S system, \( n = \hat{z} \)

On the side of the interface with Rashba-like spin-orbit coupling, where \( x_1, x_2 < 0 \), the nonzero even- and odd-frequency singlet and triplet retarded anomalous Green’s functions are given by
where $D_{1(2)} = u_0^2 (k_{e1(2)} + q_x^+) (k_{h1(2)} + q_x^-) + v_0^2 (k_{e1(2)} - q_x^+) (-k_{e1(2)} + q_x^-)$. On the superconducting side of the interface, where $x_1, x_2 > 0$, the nonzero even- and odd-frequency

singlet and triplet retarded anomalous Green's functions are given by

\[
\begin{align*}
\psi_{0,E}(X, x, p_y; \omega) = & \frac{\phi'}{2} u_0 v_0 (g_x^+ + q_x^-) \delta(p_y - k_{h}) \frac{1}{\omega - E + i\delta^+} \cdot \left\{ \frac{1}{D_1} (k_{e1} + k_{h1}) + \frac{1}{D_2} (k_{e2} + k_{h2}) \right\} \cdot e^{i(q_x^- - q_x^+) x} \cos((q_x^+ + q_x^-) x/2) \\
\psi_{0,O}(X, x, p_y; \omega) = & \frac{\phi'}{2i} u_0 v_0 \delta(p_y - k_{h}) \frac{1}{\omega - E + i\delta^+} \cdot \left\{ \frac{1}{D_1} (k_{e1} + k_{h1}) + \frac{1}{D_2} (k_{e2} + k_{h2}) \right\} \cdot e^{i(q_x^- - q_x^+) x} \sin((q_x^+ + q_x^-) x/2) \\
\psi_{1,E}(X, x, p_y; \omega) = & \frac{\phi'}{2} u_0 v_0 \delta(p_y - k_{h}) \frac{1}{\omega - E + i\delta^+} \cdot \left\{ \frac{1}{D_1} (k_{e1} + k_{h1}) + \frac{1}{D_2} (k_{e2} + k_{h2}) \right\} \cdot e^{i(q_x^- - q_x^+) x} (u_0^2 - v_0^2) \sin((q_x^+ + q_x^-) x/2) \\
\psi_{1,O}(X, x, p_y; \omega) = & \frac{\phi'}{2i} u_0 v_0 \delta(p_y - k_{h}) \frac{1}{\omega - E + i\delta^+} \cdot \left\{ \frac{1}{D_1} (k_{e1} + k_{h1}) + \frac{1}{D_2} (k_{e2} + k_{h2}) \right\} \cdot e^{i(q_x^- - q_x^+) x} \sin((q_x^+ + q_x^-) x/2) \\
\psi_{2,E}(X, x, p_y; \omega) = & \frac{\phi'}{2} u_0 v_0 \delta(p_y - k_{h}) \frac{1}{\omega - E + i\delta^+} \cdot \left\{ \frac{1}{D_1} (k_{e1} + k_{h1}) + \frac{1}{D_2} (k_{e2} + k_{h2}) \right\} \cdot e^{i(q_x^- - q_x^+) x} (u_0^2 - v_0^2) \sin((q_x^+ + q_x^-) x/2) \\
\psi_{2,O}(X, x, p_y; \omega) = & \frac{\phi'}{2i} u_0 v_0 \delta(p_y - k_{h}) \frac{1}{\omega - E + i\delta^+} \cdot \left\{ \frac{1}{D_1} (k_{e1} + k_{h1}) + \frac{1}{D_2} (k_{e2} + k_{h2}) \right\} \cdot e^{i(q_x^- - q_x^+) x} \sin((q_x^+ + q_x^-) x/2)
\end{align*}
\]

where $E_{1(2)} = u_0^2 (-k_{e1(2)} + q_x^+) (k_{h1(2)} + q_x^-) + v_0^2 (-k_{h1(2)} - q_x^+) (-k_{e1(2)} + q_x^-)$, and $F_{1(2)} = u_0^2 (k_{e1(2)} + q_x^+) (-k_{h1(2)} + q_x^-) + v_0^2 (k_{h1(2)} - q_x^+) (k_{e1(2)} + q_x^-)$. There are no equal-spin triplets in the system.

2. The F/S system

On the ferromagnetic side of the interface, where $x_1, x_2 < 0$, the nonzero even- and odd-frequency singlet and triplet retarded anomalous Green’s functions are given by
where \( C_{12(21)} \equiv u_0^2(k_{e1(2)} + q_x^+) (k_{h2(1)} + q_x^-) + v_0^2(k_{h2(1)} - q_x^+) (-k_{e1(2)} + q_x^-) \). On the superconducting side of the interface, where \( x_1, x_2 > 0 \), the nonzero even- and odd-frequency singlet and triplet retarded anomalous Green’s functions are given by

\[
\begin{align*}
   f_{0}^{r,E}(X, x, p_y; \omega) &= \frac{u_0 v_0}{2} \frac{1}{u_0^2 - v_0^2} \frac{1}{\omega - E + i\delta^+} \\
   &\cdot \left\{ \frac{1}{C_{21}} (k_{e2} + k_{h1}) + \frac{1}{C_{12}} (k_{e1} + k_{h2}) \right\} \cdot e^{i(q_x^+ - q_x^-)X} \cos((q_x^+ + q_x^-)x/2) \\
   &\quad - \left\{ \frac{1}{4q_x^2} e^{iq_x^+|x|} + \frac{1}{4q_x^-} e^{-iq_x^-|x|} \right\} + \frac{1}{2} \left( A_{21} + A_{12} \right) + \frac{1}{2q_x} e^{2iq_x^+ x} + \frac{1}{2} \left( \frac{B_{21}}{C_{21}} + \frac{B_{12}}{C_{12}} \right) \frac{1}{q_x} e^{-2iq_x^- x} \right\}, \\
   f_{0}^{r,O}(X, x, p_y; \omega) &= \frac{u_0 v_0}{2i} \frac{1}{u_0^2 - v_0^2} \frac{1}{\omega - E + i\delta^+} \\
   &\cdot \left\{ \frac{1}{C_{21}} (k_{e2} + k_{h1}) + \frac{1}{C_{12}} (k_{e1} + k_{h2}) \right\} \cdot e^{i(q_x^+ - q_x^-)X} \sin((q_x^+ + q_x^-)x/2) \\
   &\quad - \left\{ \frac{1}{4q_x^2} e^{iq_x^+|x|} + \frac{1}{4q_x^-} e^{-iq_x^-|x|} \right\} + \frac{1}{2} \left( A_{21} - A_{12} \right) + \frac{1}{2q_x} e^{2iq_x^+ x} + \frac{1}{2} \left( \frac{B_{21}}{C_{21}} - \frac{B_{12}}{C_{12}} \right) \frac{1}{q_x} e^{-2iq_x^- x} \right\}, \\
   f_{3}^{r,E}(X, x, p_y; \omega) &= \frac{u_0 v_0}{2} \frac{1}{u_0^2 - v_0^2} \frac{1}{\omega - E + i\delta^+} \\
   &\cdot \left\{ \frac{1}{C_{21}} (k_{e2} + k_{h1}) - \frac{1}{C_{12}} (k_{e1} + k_{h2}) \right\} \cdot e^{i(q_x^+ - q_x^-)X} (v_0^2 - u_0^2) \sin((q_x^+ + q_x^-)x/2) \\
   &\quad + \frac{1}{2} \left( A_{21} - A_{12} \right) \frac{1}{q_x^2} e^{2iq_x^+ x} + \frac{1}{2} \left( \frac{B_{21}}{C_{21}} - \frac{B_{12}}{C_{12}} \right) \frac{1}{q_x} e^{-2iq_x^- x} \right\}, \\
   f_{3}^{r,O}(X, x, p_y; \omega) &= \frac{u_0 v_0}{2i} \frac{1}{u_0^2 - v_0^2} \frac{1}{\omega - E + i\delta^+} \\
   &\cdot \left\{ \frac{1}{C_{21}} (k_{e2} + k_{h1}) - \frac{1}{C_{12}} (k_{e1} + k_{h2}) \right\} e^{i(q_x^+ - q_x^-)X} (v_0^2 - u_0^2) \sin((q_x^+ + q_x^-)x/2) \\
   &\quad + \frac{1}{2} \left( A_{21} - A_{12} \right) \frac{1}{q_x^2} e^{2iq_x^+ x} + \frac{1}{2} \left( \frac{B_{21}}{C_{21}} - \frac{B_{12}}{C_{12}} \right) \frac{1}{q_x} e^{-2iq_x^- x} \right\}.
\end{align*}
\]

where \( A_{12(21)} \equiv u_0^2(k_{e1(2)} - q_x^+) (k_{h2(1)} + q_x^-) + v_0^2(k_{h2(1)} + q_x^+) (-k_{e1(2)} + q_x^-) \). There are no equal-spin triplets in the system.

C. The symmetries of the singlet and triplet retarded anomalous Green’s functions

Finally, we investigate the spatial symmetries of the singlet and triplet retarded anomalous Green’s functions of the
SOC/S systems with \( n = \hat{x} \) and \( n = \hat{z} \) and the F/S system with \( mn \) in the \( \hat{z} \) direction. \( P \) is inversion of the relative coordinate, \( x \rightarrow -x \). \( P_x \) describes inversion of the momentum along the \( y \) axis, \( p_y \rightarrow -p_y \). \( P \) is total spatial inversion, and must be 1 for \( f^E_0 \) and \( f^O_3 \), and -1 for \( f^E_3 \) and \( f^O_0 \), according to the Pauli principle. For \( P = 1 \), we may have \( P_x = P_y = 1 \), which describes an \( s \)- or a \( d_{x^2-y^2} \)-wave amplitude, or \( P_x = P_y = -1 \), which describes a \( d_{xy} \)-wave amplitude. For \( P = -1 \), we may have \( P_x = 1 \) and \( P_y = -1 \), which describes a \( p_y \)-wave amplitude, or \( P_x = -1 \) and \( P_y = 1 \), which describes a \( p_x \)-wave amplitude. Considering \( P, P_x \), and \( P_y \) is sufficient for determining whether a Green’s function has an \( s \)-wave or a \( d_{x^2-y^2} \)-wave symmetry. In order to prove the presence of \( s \)-wave singlets and triplets, we apply the Fourier transform,

\[
\hat{G} = \int_{-\infty}^{\infty} dx \hat{r}_{\mu}(x) e^{-ipx_x} \tag{22}
\]

for the nonzero singlet and triplet even- and odd-frequency retarded anomalous Green’s functions given in Eqs. (23) and (24).

| \( P_x \) | \( P_y \) | \( P \) |
|---|---|---|
| 1 | 1 | 1 |
| -1 | 1 | 1 |
| -1 | -1 | -1 |

Table I. The above table shows the parities of the SOC/S system with \( n = \hat{z} \) under \( x \rightarrow -x \) and \( p_y \rightarrow -p_y \), and total spatial inversion (P) for the nonzero singlet and triplet even- and odd-frequency retarded anomalous Green’s functions given in Eqs. (21) and (22).

The symmetries of Green’s functions in Eqs. (21) and (22) under \( P_x \), \( P_y \) and \( P \) are given in Table I. We see from the table that \( f^E_0 \) can represent \( s \)- and \( d_{x^2-y^2} \)-wave singlets, \( f^O_3 \) represents \( p_x \)-wave singlets, \( f^E_3 \) represents a \( p_y \)-wave opposite-spin triplet, and \( f^O_0 \) represents \( d_{xy} \)-wave opposite-spin triplets. By integrating over all space, we find that \( s \)-wave singlets are present.

2. The SOC/S system, \( n = \hat{z} \)

The symmetries of Green’s functions of the SOC/S system for \( n = \hat{z} \) are shown in Table II. These were found numerically by the same approach as for the two other systems. We see that the same singlet and opposite-spin triplet amplitudes are present as for \( n = \hat{x} \). In addition, we have nonzero equal-spin triplet amplitudes, that are a mix of triplet amplitudes with different symmetries under \( P_x \) and \( P_y \). \( f^E_1 \) and \( f^O_2 \) are therefore a mix of \( p_x \)- and \( p_y \)-wave even-frequency triplets, while \( f^O_1 \) and \( f^O_3 \) are a mix of \( s \)- and \( d \)-wave triplets.

| \( P_x \) | \( P_y \) | \( P \) |
|---|---|---|
| 1 | 1 | 1 |
| 1 | -1 | 1 |
| -1 | -1 | -1 |
| 1 | 1 | 1 |

Table II. The above table shows the parities of the SOC/S system with \( n = \hat{z} \) under \( x \rightarrow -x \) and \( p_y \rightarrow -p_y \), and total spatial inversion (P) for the nonzero singlet and triplet even- and odd-frequency retarded anomalous Green’s functions present in the system. In addition, we have nonzero equal-spin triplet amplitudes with mixing (-) of the possible symmetries in \( P_x \) and \( P_y \).

3. The F/S system

Table III shows the symmetries of Eqs. (23) and (24) under \( P_x \), \( P_y \), and \( P \). Due to the lack of symmetry breaking in the \( y \) direction, we must conclude that there are no \( p_y \)- or \( d \)-wave symmetries present. The nonzero singlet and triplet retarded anomalous Green’s functions are therefore the \( s \)-wave even-frequency singlet, the \( p_x \)-wave odd-frequency singlet, the \( p_y \)-wave even-frequency opposite-spin triplet and the \( s \)-wave odd-frequency opposite-spin triplet.

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