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Charge carrier holes and Majorana fermions

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Understanding Luttinger holes in low dimensions is crucial for numerous spin-dependent phenomena and nanotechnology. In particular, hole quantum wires proximity-coupled to a superconductor is a promising system for observation of Majorana fermions. Earlier treatments of confined Luttinger holes ignored a mutual transformation of heavy and light holes at the heteroboundaries. We derive the effective hole Hamiltonian in the ground state. Mutual transformation of holes is crucial for Zeeman and spin-orbit coupling, and results in several spin-orbit terms linear in momentum in hole quantum wires. We discuss the criterion for realizing Majorana modes in charge carrier hole systems. GaAs or InSb hole wires shall exhibit stronger topological superconducting pairing, and provide additional opportunities for its control compared to InSb electron systems.

In recent years physicists realized that electron bandstructure and spin-orbit effects may lead to remarkable quantum matter¹⁻⁴. Many researchers studied charge carrier hole systems anticipating strong spin-orbit effects. However, in low-dimensional systems, in which spin-orbit interactions are well known for electrons, their understanding for holes is scarce and is just emerging^{5,6}.

Here we derive a two-dimensional (2D) hole Hamiltonian, including g-factor and spin-orbits constants crucial for spintronics and quantum computing. The difference between holes and electrons are not just parameters, holes are special physical species with different symmetry and different ways of tuning their properties. We consider holes in quantum wires, which are lithographically or electrostatically defined in quantum wells, or developed using cleaved edge overgrowth, which differ from hole epitaxial and core-shell nanowires^{7–9}.

Using our results for 2D holes we discuss Majorana bound states (MBS) in wires. Majorana particles are their own anti-particles obeying non-Abelian statistics and promissing for quantum computing^{10–12}. In condensed matter systems Majorana modes arise in p-wave¹³ spinless superconductors. Schemes generating such superconductivity in semiconductor-superconductor structures use three ingredients: proximity effects, time reversal symmetry breaking, and spin-orbit coupling^{3,4,14–18}. Strong spin-orbit interaction gives stronger p-wave pairing¹⁷. Both electrons and hole systems were suggested for realizing Majorana modes^{8,18–20}.

We show that in hole wires, the momentum-dependent Zeeman (spin-orbit) fields emerge in three spatial directions. This provides an opportunity to control the MBS by changing a relative orientation of spin-orbit and applied magnetic fields using electrostatic gates. Furthermore, at Zeeman energies $g\mu H$ satisfying conditions for topological state, holes exhibit sizable spin-orbit energies $E_{so} = \gamma^2 m > g\mu H$, where m is the effective mass and γ is the spin-orbit constant. Then the hole ground state has a camel back shape, Fig. 1b, making p-pairing much stronger than in electron settings.

Theory of low-dimensional holes is controversial. Most authors treat holes like electrons²⁰⁻²⁵: if the motion of



FIG. 1: (Color online). a: Transformation of holes reflected from the potential walls of the quantum wire: a heavy hole becomes heavy or light hole. b: Ground spin-orbit state energy at $E_{so} > g\mu H$. c: Ground state energy at $E_{so} < M_z$.

particles is quantized in direction i in a well of width d, their Hamiltonian is solved by replacing momentum p_i by zeros and p_i^2 by its expectation value in the ground state, $\langle \hat{p}_i^2 \rangle = (\frac{\hbar \pi}{d})^2$, and spin-orbit and Zeeman terms are found perturbatively. However, this approach is flawed. It does not account for a mutual transformation of heavy and light holes upon reflection from the heteroboundaries, Fig.1a. Although this effect can be evaluated perturbatively by including off-diagonal terms linear in k_i , it then requires summation of an infinite number of terms, which are parametrically all the same⁶. An alternative non-perturbative approach is known since the work of Nedorezov²⁶, but is seldom used^{6,27-29}. We show that in hole wires, this phenomenon strongly affects effective masses, g-factor and spin-orbit constants.

a. The effective Hamiltonian in hole quantum wells and wires. The Luttinger Hamiltonian for bulk holes is:

$$H_L = (A + \frac{5}{4}B)p^2 - \sum_i BJ_i^2 p_i^2 + D[J_i J_{i+1}]p_i p_{i+1}], \quad (1)$$

where **J** is the spin 3/2 operator, i = x, y, z, constants A, B, D are related to Luttinger constants $\gamma_1, \gamma_2, \gamma_3$. In an infinite symmetric well, the wavefunctions of Eq.(1), $\varphi_+(z, \mathbf{r})$ and $\varphi_-(z, \mathbf{r}), \mathbf{r} = (x, y)$, are symmetric and antisymmetric with respect to $z \to -z$ reflection. In the basis of Bloch functions $u^{3/2}, u^{1/2}, u^{-1/2}, u^{-3/2}$ of bulk holes, $\varphi_{+,-}^{\mathbf{k}}(z, \mathbf{r}) = \varphi_{+,-}^{\mathbf{k}}(z)exp(i\mathbf{k}\cdot\mathbf{r})$, and²⁹:

$$\varphi_{+}^{\mathbf{k}}(z) = \begin{pmatrix} A_0 C_z \\ -iA_1 S_z e^{i\phi_k} \\ A_2 C_z e^{2i\phi_k} \\ -iA_3 S_z e^{3i\phi_k} \end{pmatrix}, \varphi_{-}^{\mathbf{k}}(z) = \begin{pmatrix} iA_3 S_z e^{-3i\phi_k} \\ A_2 C_z e^{-2i\phi_k} \\ iA_1 S_z e^{-i\phi_k} \\ A_0 C_z \end{pmatrix},$$
(2)

where the wavevector $\mathbf{k} \perp \hat{z}$, ϕ_k is the angle between \mathbf{k} and \hat{x} , $S_z = sin(q_h z) - (s_h/s_l)sin(q_l z)$, $C_z = cos(q_h z) - (c_h/c_l)cos(q_l z)$, where $s_h = sin(q_h d/2)$, $s_l = sin(q_l d/2)$, $c_h = cos(q_h d/2)$, $c_l = cos(q_l d/2)$. At $k \ll \pi/d$, the heavy and light hole ground state longitudinal wave vectors $q_h \sim \pi/d$ and $q_l = \sqrt{\nu}q_h$, $\nu = m_l/m_h$, m_l and m_h are light and heavy effective masses. Then in a spherical approximation the coefficients $A_0 = \sqrt{d/2}$, $A_1 = -\sqrt{3}kA_0/2q_h$, $A_2 = \sqrt{3}A_0k^2/4q_h^2$, $A_3 = 3A_0k^3/8\nu q_h^3$. Thus, two standing waves describe the 2D holes, reflecting their mutual transformation at interfaces, Fig.1.

Next we project the Hamiltonian of the system

$$H_h = H_L(\mathbf{K}) + H_1 + H_2 + U_v(z, \mathbf{r}) + \tilde{M}_{1z}J_z + \tilde{M}_{2z}J_z^3 \quad (3)$$

on the doublet $\varphi_{\mathbf{k},-}^{\mathbf{k}}(z,\mathbf{r})$. Here $U_v(z,\mathbf{r})$ is the potential confining holes including its asymmetric part, $\mathbf{K} = \mathbf{k} - \frac{e}{\hbar c} \mathbf{A}$, \mathbf{A} is the vector-potential. Zeeman coupling of 2D holes to magnetic field $\mathbf{B} = curl\mathbf{A}$ comes from the orbital effect of magnetic field in the $(\hat{\mathbf{J}} \cdot \hat{\mathbf{p}})^2$ term of (1) and from pure Zeeman effects, $\tilde{M}_{1z} = \kappa \mu_B B$, $\tilde{M}_{2z} = q\mu_B B$, where κ and q are Luttinger parameters, and μ_B is the electron Bohr magneton. We consider $\mathbf{B}||z$. The Dresselhaus coupling H_1 gives linear in k 2D terms^{5,6,28}

$$H_1 = \frac{1}{2} \delta \alpha_v \sum_j V_j p_j \left(p_j^2 - \frac{1}{3} p^2 \right) - J_j^3 \kappa_j \qquad (4)$$

Here $V_z = J_x J_z J_x - J_y J_z J_y$, $\kappa_z = k_z (k_x^2 - k_y^2)$, and cyclic permutation of indices x, y, z defines other V_i and κ_i components. The term H_2 in (3) is due to admixture of conduction electrons to holes,

$$H_2 = \zeta(\mathbf{J} \times \mathbf{p}) \cdot \partial_{\mathbf{r}} U_e(z, \mathbf{r}), \qquad (5)$$

where $U_e(z, \mathbf{r})$ is the potential acting on electrons, $\zeta = -P^2/3E_g^2$, P is the Kane constant, E_g is the band gap. Eq. (5) gives k^3 2D terms, which become linear in k upon quantization in a 1D wire. In Eqs. (4,5), we omit small terms $\propto J_i^3$ which are due to distant bands and result in much smaller spin-orbit coupling^{5,30,31}.

Our principal result is the effective 2D Hamiltonian

$$\mathcal{H} = \frac{p^2}{2m} + V_{\mathbf{r}} + \tilde{\alpha}\sigma_z [\nabla_{\mathbf{r}}\tilde{V}_{\mathbf{r}} \times \mathbf{p}]_z + u(\sigma_x p_x + \sigma_y p_y) + \sum_n \beta_n p^3(\sigma_x \sin n\phi - (n-2)\sigma_y \cos n\phi) + g\mu_B B\sigma_z, (6)$$

n = 1, 3. The effective 2D mass m and g-factor are

$$\frac{n_0}{m} = \gamma_1 + \gamma_2 - 3a^2\gamma_2 + 3a^2(\gamma_1^2 - 4\gamma_2^2)^{1/2}f, \quad (7)$$

$$g = 6\kappa + \frac{27}{2}q - 6a^2\gamma_2 + 6a^2(\gamma_1^2 - 4\gamma_2^2)^{1/2}f, \quad (8)$$

 m_0 is a free electron mass, $f = \cot \frac{\pi}{2} \sqrt{\frac{\gamma_1 - 2\gamma_2}{\gamma_1 + 2\gamma_2}}$, $a = \frac{\gamma_3}{\gamma_2}$. Two last terms in (8) emerge as off-diagonal terms $\hat{p}_z(p_x[J_zJ_x] + p_y[J_zJ_y])$ contribute to symmetric state energy as $\propto p_-p_+ = p^2 + i(p_xp_y - p_yp_x)$, and give antisymmetric state energy $\propto p_+p_- = p^2 - i(p_xp_y - p_yp_x)$. At $B \neq 0, i(p_xp_y - p_yp_x) \rightarrow \frac{\hbar eB}{c}$, making the two last terms in (8) twice those in (7). This simple picture confirms g-factor obtained using Landau quantization⁶.

There are three spin-orbit terms in the ground state Hamiltonian (6). The Dresselhaus term is given by

$$u = \frac{1}{2} \left(\frac{\pi}{d}\right)^2 \delta \alpha_v \left[1 - a \left(1 - \sqrt{\nu} \frac{\gamma_1}{\gamma_2} f\right)\right], \qquad (9)$$

where $a = \frac{\gamma_3}{\gamma_2}$. The Rashba term is defined by β_1, β_3 :

$$\beta_n = \frac{3eFd^4}{4\hbar^3\pi^4} \left[A_n \left(\frac{4f/\sqrt{\nu}}{1-\nu} - \frac{3+\nu}{4\nu} \right) + \tilde{\zeta}_n \right].$$
(10)

Here $A_n = a(a+n-2)$, and the asymmetric part of the external electric field and doping potential eFz, $|z| < \frac{d}{2}$, is assumed equal for valence and conduction electrons. Distinct offset potentials, U_c for electrons and U_v for holes, give nonzero $\tilde{\zeta}_n = \pi^2 \hbar \zeta (n-1) (U_c - U_v) / (2d^2 U_v)$. For the ground state, β_1 and β_3 describe p^3 Rashba coupling. The newly predicted β_1 term has the symmetry of the first harmonics in **p**. It affects the hole transport, e.g., weak antilocalization³². We note that the term $\propto A_n$ in (10) is due to the matrix element $\langle \pm | eFz | \mp \rangle$ and accounts for infinite number of perturbative terms of the same order. Calculation³³ included terms with just two excited states and contributed only to β_3 .

The σ_z -term in Eq.(6) results in 2D holes skew scattering, but our interest here is such term due to the wire confinement potential. The effective potentials in Eq. (6) that define 2D transport and spectra of wires are

$$\tilde{V}_{\mathbf{r}} = \frac{3}{2d} \int_{-d/2}^{d/2} \left[U_v(z, \mathbf{r}) S_z^2 + \frac{\zeta \pi^2 \hbar}{d^2} U_e(z, \mathbf{r}) C_z^2 \right] dz, \quad (11)$$

 $V_{\mathbf{r}} = \frac{2}{d} \int_{-d/2}^{d/2} U_v(\mathbf{r}, z) C_z^2 dz, \text{ and the constant } \tilde{\alpha} = d^2 / \pi^2 \hbar.$

For hole wires, in which the wire width in x-direction $w \gg d^{25,34-36}$, the 1D Hamiltonian is

$$H_{1D} = \frac{p_y^2}{2m} + \alpha \sigma_z p_y + u \sigma_y p_y + \beta \sigma_x p_y + M_z \sigma_z.$$
(12)

Here $M_z = g\mu_B B/2$, $\beta = (\beta_1 + 3\beta_3)(\pi\hbar/w)^2$. We find α in a model with $U_{v,e}(z, \mathbf{r})$ being products of functions depending only on z and only on x. We take hole and electron symmetric wire potential $U_v^{(s)}(x) =$

 $U_v^{(w)}\theta(x)$ and $U_e^{(s)}(x) = U_e^{(w)}\theta(x)$, correspondingly, with $\theta(x) = -1$ at |x| < w/2 and $\theta(x) = 0$ otherwise. In electric field F_x acting on both electrons and holes, $\alpha = 3\zeta eF_x(1 - U_e^{(w)}/U_v^{(w)})$. Offset-dependent α and β_3 and α independent of \tilde{V} stem from the Ehrenfest theorem on vanishing average gradient of a potential in confined states. Thus, for the cleaved edge overgrowth wires α can be sizable, while for lithographically defined wires $\alpha = 0$.

A gap separates ground and excited states of an inplane and z-direction quantization in a wire. Eq. (12) fully accounts for hole physics via the modified mass, gfactor and spin-orbit constants. For MBS, this electronlike Hamiltonian allows to use methods of 16,37,38.

b. The existence of Majorana modes. After spin rotations around z and x axis, Eq. (12) becomes

$$H_{1D} = \frac{p^2}{2m} + \gamma \sigma_y p + M_z (\cos\theta\sigma_z + \sin\theta\sigma_y), \quad (13)$$

where index y of p is dropped, $\gamma = \sqrt{\alpha^2 + \beta^2 + u^2}$ describes the spin-orbit coupling and $\sin\theta = \frac{\alpha}{\sqrt{\alpha^2 + \beta^2 + u^2}}$ measures the alignment of the Zeeman and spin-orbit fields. The ground state wavefunctions of (13) are labeled + and -. The superconducting pairing arises due to the proximity effect^{35,40-45}. For ground band holes in the wire, the superconducting Hamiltonian is $H_{SC} = \int d\mathbf{r} \Delta e^{i\phi} \hat{c}^{\dagger}_{+} \hat{c}^{\dagger}_{-} + H.c.$, where \hat{c}^{\dagger}_{\pm} are the creation operators adding holes to + and - states, and $\Delta e^{i\phi}$ is the pairing potential. The BdG Hamiltonian in the Nambu τ -space reads:

$$H_{BdG} = \left(\frac{p^2}{2m} - \mu + \gamma \sigma_y p\right) \tau_z + M_z (\cos\theta\sigma_z + \sin\theta\sigma_y) + \Delta \cos\phi\tau_x - \Delta \sin\phi\tau_y.$$
(14)

To show the existence of MBS, we prove that there is a non-degenerate solution at E = 0 of the BdG equation $H_{BdG}\Psi = E\Psi^{37}$. Due to the particle-hole symmetry, this solution has the form $\Psi = (\psi, i\sigma_y\psi^*), \psi$ is a two-spinor. We have

$$[(\frac{p^2}{2m} - \mu + \gamma \sigma_y p) + M_z (\cos\theta\sigma_z + \sin\theta\sigma_y)]\psi + \Delta e^{i\phi} i\sigma_y \psi^* = 0.$$
(15)

MBS exist for any of the choices of the order parameter ϕ , $M_z \sin\theta = \lambda \Delta \sin\phi$, where $\lambda = \pm 1$. Writing $\psi = \psi_R + i\psi_I$, from Eq. (15), for the functions ψ_R ($\lambda = 1$) or ψ_I ($\lambda = -1$) we obtain:

$$\begin{pmatrix} \frac{p^2}{2m} - \mu + M_z \cos\theta & \lambda \Delta \cos\phi - i\gamma p\\ -\lambda \Delta \cos\phi + i\gamma p & \frac{p^2}{2m} - \mu - M_z \cos\theta \end{pmatrix} \psi_{R/I} = 0.$$
(16)

We note that the sign of the Zeeman term in the Eq. (59) of³⁷ should be +, not -, and equations for Ψ_I and Ψ_R cannot be both decoupled by a unique choice of ϕ .

At $\psi_{I/R} \sim e^{-\tau y}$ a secular equation for τ is

$$\frac{\tau^4}{4m^2} + \left(\frac{\mu}{m} + \gamma^2\right)\tau^2 + 2\lambda\gamma\Delta\cos\phi\tau + C_0 = 0, \quad (17)$$



FIG. 2: (Color online) The BdG energy spectra E_n in a 2 $\mu m \log$ GaAs quantum wire. B = 0.8T, $E_{so} = 0.2meV$. a: $\mu = 0.5M_z, \Delta = 0.6M_z$, $sin\theta = 0$. The zero energy solution exists and is well separated by a gap from the excited states. Inset: Majorana zero mode is localized at the boundary of the quantum wire. b,c,d: Parameters: b - $\mu = 0.5M_z, \Delta = 0.6M_z$, $sin\theta = 0.7$; c - $\mu = 0.5M_z, \Delta = M_z$, $sin\theta = 0$; d - $\mu = 0.9M_z, \Delta = 0.6M_z$, $sin\theta = 0.7$. There are no zero energy solutions. Insets: Wavefunctions of the lowest-lying states. Majorana zero modes disappear in cases b,c,d.



FIG. 3: (Color online) a: the BdG ground state energy E_s for different Δ . $M_z = 0.2meV$, $E_{so} = 0.2meV$, $\mu = 0.6M_z$ and $sin\theta = 0.2$. $E_s \neq 0$ at $|\Delta| < 0.2M_z$ or $|\Delta| > 0.8M_z$, which correspond to $\Delta < M_z sin\theta$ and $M_z^2 < \mu^2 + \Delta^2$, respectively. b: E_s for different $sin\theta$ ($\mu = 0.5M_z$, $\Delta = 0.7M_z$). E_s is nonzero at $\Delta < M_z sin\theta$. Inset: Excitation gap versus M_z . $\Delta =$ 0.1meV, $\mu = 0$. The gap closes at $M_z = \Delta$ or $\Delta/M_z = sin\theta$.

where $C_0 = \mu^2 + \Delta^2 - M_z^2$. Using Vieta's formulas, for $C_0 < 0$ we find 3 roots with $Re[\tau] > 0$ and 1 root with $Re[\tau] < 0$ for $\lambda = -1$, or 1 root with $Re[\tau] > 0$ and 3 roots with $Re[\tau] < 0$ for $\lambda = 1$. For $C_0 > 0$ there are two roots with $Re[\tau] \leq 0$. Due to one normalization and four boundary conditions, a unique bound state exists at the boundary between the topological phase with $C_0 =$

 $\Delta^2 + \mu^2 - M_z^2 < 0$ and a trivial phase with $C_0 > 0,^{4,15}$. Once $\psi_{R/I}$ is found from Eq. (16) for a given ϕ , $\psi_{I/R}$ can be found from Eq.(15) providing the other equation coupling $\psi_{R/I}$ and $\psi_{I/R}$. At E = 0 these $\psi_{I/R}$ define the wavefunction of the MBS. Hence the criterion for the topological superconductivity in hole wires is

$$M_z^2 > \mu^2 + \Delta^2. \tag{18}$$

Deriving (18) we used $M_z \sin\theta = \pm \Delta \sin\phi$. Therefore the existence of MBS for arbitrary ϕ requires

$$|\Delta| \ge |M_z \sin\theta|. \tag{19}$$

A question is whether MBS exist when Eqs. (15) cannot be decoupled. We show that for arbitrary ϕ the constraint $|\Delta| > |M_z sin\theta|$ is necessary for existence of a topological superconductor. If $\sin\theta = 1$, i.e. the Zeeman and spin-orbit fields are aligned, MBS do not exist. If $sin\theta = 0$, they arise if Eq. (18) is satisfied. Furthermore, the MBS exist at $M_z \sin\theta = \pm \Delta \sin\phi$, for "intermediate" θ . This precludes the possibility that only $\sin\theta = 0$ case, i.e. when the BdG equations are equivalent to those with real coefficients, gives MBS, while other θ do not. Thus, a critical angle $\theta_c \neq 0$ exists when topological superconductivity emerges. Solving the BdG equation numerically, we find that this critical angle is given by $\Delta = M_z \sin\theta_c$, Fig.2. We observe that the MBS exist only when both (18) and (19) are satisfied, and disappear when one of the conditions is not fullfilled. The extra constaint allows to control topological superconductivity tuning the σ_z -term by electrostatic gates at arbitrary direction of the magnetic field. In electron cases discussed $in^{4,15,37,46}$, the constraint is on the direction of the magnetic field. Fig.3 shows the ground state BdG energies for different Δ and $sin\theta$.

We find that hole wires in GaAs or InSb structures are favorable for MBS detection. In these systems a surface pinning of the Fermi level can be close to the valence band giving a small Schottki barrier for electrostatic control of charge carrier density. For w = 80nm nanowire, lithographically developed from an unstrained d = 20nmquantum well in a AlGaAs/GaAs/AlGaAs Carbon-doped heterostructure grown along [001], at $\gamma_1 = 6.8$, $\gamma_2 = 2.1$, $\gamma_3 = 2.9$, $\kappa = 1.2$, q = 0.04, P = 10eVÅ, $E_g = 1.52eV$ and⁵ $\delta \alpha_v = 76.7$ eV Å³, assuming $eF_z = 2 \times 10^4 V/cm$, we obtain m = 0.15 m₀ ($m = 0.25m_0$ when adjustments are made for the effects of finite depth of the well and one-sided doping), g = 5, and $\gamma = 70$ meV Å. At 2D density $n_s = 2 \times 10^{10} cm^{-2}$, $\mu = 0.14 meV$, and holes are only in the ground subband in the wire. For superconductivity caused by proximity to NbN, $\Delta \sim 0.1 meV$, and the transition between topological and nontopological superconducting order occurs at $B \sim 0.7T$. Then $E_{so} = 0.2 meV > M_z$, and the lowest single-hole state is of camel-back type, Fig1.b, i.e., spin-orbit coupling is strong.

For a similar InSb wire in InSb/AlInSb structure, at $\gamma_1 = 40.1$, $\gamma_2 = 18.1$, $\gamma_3 = 19.2$, $\kappa = 17.0$, q = 0.5, P = 9.6eVÅ, $E_g = 0.23eV$ and³⁰ $\delta \alpha_v = 70$ eV Å³, we get $\gamma \sim 250meV$ Å, and $g \sim 90$. Due to strain in this system, $m = 0.04m_0^{47}$ [according to (7) at zero strain, $m = 0.018m_0$]. Then $E_{so} \sim 0.4meV$. In proximity with NbN at $\Delta \sim 0.15meV$, $n_s = 2 \times 10^{10} cm^{-2}$, we find the transition between topological and non-topological superconductivity in the InSb hole wire at $B \sim 0.4T$. Then $M_z > E_{so}$, and the ground state of (13) has single-minimum Fig.1c shape, which is also the case in an electron InSb wire⁴⁰ with E_{so} 4 times smaller than here.

Conclusion. We treated hole wires non-perturbatively, including the effect of mutual transformation of heavy and light holes at heteroboundaries, and derived the hole g-factor and spin-orbit interactions. We found that Majorana settings in GaAs and InSb hole quantumwell-based wires exhibit considerably stronger p-type proximity-induced superconducting pairing compared to InSb electron system. For topological quantum computing, quantum-well-based wires could be of special importance because they may provide a natural path for construction of networks of high-mobility wires for braiding Majorana modes. We discussed a criterion for transition from non-topological to topological superconducting order, showing that Majorana modes arise even if the Bogoliubov-De Gennes equations for real and imaginary parts of the wavefunction cannot be decoupled. Beyond Majorana context, our results are important for the field of spin-based electronics, for generation, manipulation and transmission of spin currents.

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