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We show that the Hamiltonian of a multi-band spin-orbit coupled semiconductor nanowire with Zeeman splitting and *s*-wave superconductivity is approximately chiral symmetric. The chiral symmetry becomes exact when only one pair of confinement bands is occupied and the Zeeman splitting is parallel to the nanowire. In this idealized case the Hamiltonian symmetry class is BDI allowing an arbitrary integer number of zero energy Majorana fermion modes *at each end*. In the realistic case of multi-band wires (Zeeman splitting still parallel to length) the chiral symmetry is approximate and results in multiple near-zero-energy end states with increasing Zeeman splitting. The existence of such low energy end states implies vanishing of the minigap with increased Zeeman splitting which can only be restored by breaking the approximate chiral symmetry by a second Zeeman field.

Rashba spin-orbit (SO) coupled semiconductors in dimensions $d = 2, 1$ with a Zeeman field and proximity-induced *s*-wave superconductivity have recently attracted a lot of attention [1–17]. Under suitable external conditions these systems can support Majorana fermion (MF) excitations (defined by second quantized operators $\gamma^\dagger = \gamma$) whose statistics is non-Abelian. In $d = 2$ the particle-hole (p-h) symmetric Bogoliubov-de Gennes (BdG) Hamiltonian of the Rashba-coupled semiconductor with *s*-wave superconductivity and a Zeeman field in the *z*-direction (semiconductor plane being $(x - y)$) is in the topological class D [18, 19] with an integer $\mathbb{Z}$ topological invariant which counts the number of gapless chiral Majorana modes on the boundary. From dimensional reduction, i.e., by putting one of the wave-vectors (say k_y) to zero [20], the gapless boundary Majorana modes in $d = 2$ reduce to zero-energy *end* Majorana modes in a $d = 1$ nanowire. The dimensional reduction argument suggests that the number of possible end Majorana modes in a SO coupled nanowire should also in principle be an integer. In this paper, we first discuss an inherent chirality symmetry of the nanowire Hamiltonian with only a single pair of occupied confinement-induced bands (i.e., large confinement energy) and use it to map the problem on the general theoretical framework for chiral symmetric Hamiltonians [21, 22]. Based on this we argue that the Hamiltonian for the idealized case of a single-band (by 'single-band' we mean a single pair of spin-split sub-bands [13]) nanowire with proximity induced *s*-wave superconductivity and a parallel Zeeman field is in the topological class BDI with a $\mathbb{Z}$ invariant which gives the number of zero-energy Majorana modes on a given end [18–22]. We discuss the algebraic form of the $\mathbb{Z}$ invariant [21, 22] and its relation with the more-frequently-used $\mathbb{Z}_2$ invariant [23, 24] which gives only the parity of the number of end Majorana modes. For realistic *multi-band* nanowires we show that the exact chiral symmetry of single band wires is broken by the inter-band Rashba couplings and thus, the realistic nanowires are not in the

topological class BDI. Nevertheless, the experimentally realistic inter-band Rashba couplings increase the energies of the zero energy end states only slightly, resulting in multiple *near-zero-energy* end states. Since the chiral symmetry is only weakly broken by the interband Rashba couplings, we call the multi-band nanowires *approximately chiral symmetric*. We show that the approximate chiral symmetry of the multi-band wires results in multiple near-zero-energy end states on a given end with increasing parallel Zeeman field. The existence of such multiple low energy states on a given end implies vanishing of the minigap above the Majorana fermion end states which can only be restored to experimentally realistic values by externally breaking the approximate chiral symmetry by a second Zeeman field.

The topological class of the SO coupled semiconductor is analogous to that of a spinless $p_x + ip_y$ superconductor. In $d = 2$ the spinless $p_x + ip_y$ superconductor, with broken time reversal (TR) invariance (due to the presence of i in the order parameter), is in class D characterized by a $\mathbb{Z}$ invariant [25, 26]. It is also possible to define a $\mathbb{Z}_2$ invariant which only counts the parity of the number of boundary Majorana modes [24]. Dimensional reduction arguments suggest that the number of possible end MFs in a $d = 1$ spinless superconductor should also be an integer and this has recently been shown explicitly [27]. Therefore, the Hamiltonian should be in the topological class BDI with a $\mathbb{Z}$ invariant in $d = 1$. Note, however, that $d = 1$ Hamiltonians in class BDI are supposed to be TR-invariant while the spinless $p_x + ip_y$ superconductor explicitly breaks TR symmetry in $d = 2$. The key to this difference is that, in $d = 1$, the Hamiltonian can be made completely real [27] while it is necessarily complex in $d = 2$. Redefining the time-reversal operator only in terms of the complex conjugation operator $\mathcal{K}$, it follows that in $d = 2$ this symmetry is broken (class D) but it remains intact in $d = 1$ (class BDI). More generally, we show below that the emergence of the reality condition in $d = 1$ changes the symmetry class of the spinless *p*-

wave superconductor as well as the single-band Rashba spin-orbit coupled system from D in $d = 2$ to BDI in $d = 1$. After discussing the $\mathbb{Z}$ invariant for the single-band Rashba coupled BDI system using the framework for chiral symmetric Hamiltonians [18–22], we discuss the more general experimentally realistic multi-band Rashba coupled wires and show how the *approximate* chiral symmetry results in the vanishing of the minigap with increasing Zeeman fields.

To understand the difference between complex and real Hamiltonians let us start from the Hamiltonian of a spinless $p_x + ip_y$ superconductor in $d = 2$,

$$H_1(\mathbf{k}) = (\epsilon_{\mathbf{k}} - \mu)\tau_z + \Delta_x k_x \tau_x - \Delta_y k_y \tau_y, \qquad (1)$$

where $\mathbf{k}$ is a two-dimensional wave-vector, μ is the chemical potential, and Δ_x, Δ_y are superconducting pair potentials along the x, y directions, respectively. Here we have used the p-h basis $(c_{\mathbf{k}}^\dagger, c_{-\mathbf{k}})$ and its hermitian conjugate, and the τ matrices in Eq. 1 are defined in this basis. Writing this Hamiltonian in terms of the Anderson pseudo-spin vector [28] $\vec{d}(\mathbf{k})$ as $H_1(\mathbf{k}) = \vec{d}(\mathbf{k}).\vec{\tau}$, we see that for spinless $p_x + ip_y$ superconductor in $d = 2$ all three components of $\vec{d}$ are non-zero. The group of topological invariant is then $\mathbb{Z}$ which is the relevant homotopy group $\pi_2(S^2)$ of the mapping from the two-dimensional k space to the 2-sphere of the 3-component unit vector $\hat{d} = \vec{d}/|\vec{d}|$ [25, 26]. On the other hand, in $d = 1$, since the corresponding Hamiltonian can be made purely real (Δ_x drops out from Eq. (1) for the system along the y-axis), the vector $\vec{d}$ has only two components. Noting that the k-space now is also one-dimensional, the topological invariant must again be in $\mathbb{Z}$ (class BDI) since $\pi_1(S^1) = \mathbb{Z}$. This invariant is simply the winding number,

$$N = \frac{1}{2\pi} \int_0^{2\pi} d\theta(k), \qquad (2)$$

where $\theta(k)$ is the angle the unit vector $\hat{d}$ makes with, say, the z-axis on the $y-z$ plane. It is clear that only with the breakdown of the reality condition of the BdG Hamiltonian the symmetry class of the spinless p-wave superconductor can change from BDI to D (which is characterized by a $\mathbb{Z}_2$ invariant) even in $d = 1$.

In $d = 2, 1$ the 4×4 BdG Hamiltonian $H_2(\mathbf{k})$ of a single-band Rashba-coupled semiconductor with Zeeman coupling and proximity induced s-wave superconductivity is given by,

$$H_2(\mathbf{k}) = (\epsilon_{\mathbf{k}} - \mu)\tau_z + V_Z \hat{\boldsymbol{S}} \cdot \boldsymbol{\sigma} \tau_z + \alpha k_x \sigma_y \tau_z$$
$$- \alpha k_y \sigma_x + \Delta_0 \sigma_y \tau_y, \qquad (3)$$

where we have used the 4-component p-h spinor $(u_\uparrow(\boldsymbol{r}), u_\downarrow(\boldsymbol{r}), v_\uparrow(\boldsymbol{r}), v_\downarrow(\boldsymbol{r}))$ (with quasiparticle operators given by $d^\dagger = \sum_\sigma (u_\sigma(r)c_\sigma^\dagger(r) + v_\sigma(r)c_\sigma(r)))$, and the Pauli matrices $\sigma_{x,y,z}, \tau_{x,y,z}$ act on the spin and particle-hole

spaces, respectively. In Eq. (3), the vector $\hat{\boldsymbol{S}}$ is a suitably chosen direction of the applied Zeeman spin splitting V_Z (e.g., $\hat{\boldsymbol{S}} = \hat{z}$ in $d = 2$ for $\mathbf{k} = (k_x, k_y)$, $\hat{\boldsymbol{S}} = \hat{x}$ in $d = 1$ for $\mathbf{k} = k_x$), μ is the chemical potential, α is the Rashba SO coupling constant, and Δ_0 is an s-wave superconducting pair-potential. It is clear that in $d = 2$ the Hamiltonian cannot be made real because of the complex Rashba term. In contrast, in $d = 1$ H_2 can be made purely real, and one can define a pseudo TR operator in terms of $\mathcal{K}$ alone. Then, in $d = 1$ H_2 preserves both p-h as well as the new 'time reversal' symmetry and hence is in class BDI characterized by a $\mathbb{Z}$ invariant. Note, however, that in contrast to the case of a spinless p-wave superconductor, the components of the $\vec{d}$-vector in the present 4×4 Hamiltonian are themselves 2×2 matrices. More generally, the BdG Hamiltonian of a TS system in $d = 1$, despite being real (thus preserving the chiral symmetry), can be a large $2N \times 2N$ square matrix so that the components of the $\vec{d}$-vector are $N \times N$ matrices.

Let us now show that in general real BdG Hamiltonians such as the Hamiltonian for the single-band Rashba spin-orbit coupled superconductor (Eq. 3) in $d = 1$, are chiral symmetric i.e. can be unitarily transformed to an off-diagonal matrix [20]. Since in the p-h space the matrix H in Eq. 3 can be written as $H = H_0 \tau_z + i\Delta \tau_y$ it can be made purely off-diagonal by a rotation in the p-h space by the unitary transformation $U = e^{-i\frac{\pi}{4}\tau_y}$. It follows that the rotated Hamiltonian

$$UH(k)U^\dagger = \begin{pmatrix} 0 & A(k) \\ A^T(-k) & 0 \end{pmatrix} \qquad (4)$$

is off-diagonal and therefore chiral-symmetric. Moreover, the transformed Hamiltonian is symmetric with the matrix $A = H_0 + \Delta$ being real i.e. it satisfies $A(k) = A^*(-k)$. The off-diagonal form of the transformed Hamiltonian is a result of the chiral symmetry [18–20] defined as $S = \mathcal{K} \cdot \Lambda$ (with $\Lambda = \tau_x \cdot \mathcal{K}$ in this basis), under which the Hamiltonian is invariant.

We now review the procedure [21, 22, 29, 30] for constructing the $\mathbb{Z}$-invariant associated with chiral-symmetric Hamiltonians. The topological $\mathbb{Z}$-invariant associated with chiral-symmetric Hamiltonians is obtained by writing the Hamiltonian in k-space as

$$UH(k)U^\dagger = \begin{pmatrix} 0 & A(k) \\ A^T(-k) & 0 \end{pmatrix}, \qquad (5)$$

where $A(k)$ is the momentum space representation of A. Since, $Det(UH(k)U^\dagger) = Det(A(k))Det(A^T(-k))$, $Det(A(k))$ can only vanish if $H(k)$ has a vanishing determinant or equivalently a zero-eigenvalue. Therefore, Hamiltonians $H(k)$, with a gap at zero-energy, are characterized by a complex function $z(k) = \exp(i\theta(k)) = Det(A(k))/|Det(A(k))|$, of modulus $|z(k)| = 1$. For $d = 1$, where the wave-vector k is periodic from $k = 0$ to $k = 2\pi$, so that the existence of the function $z(k)$ leads

to a natural association of a winding number W with H, which is written as $W = \frac{-i}{2\pi}\int_{k=0}^{k=2\pi}\frac{dz(k)}{z(k)}$. Since the matrix A, from which $A(k)$ was derived, was real in Eq. 4 as a consequence of the particle-hole symmetry of H,

$$Det(A(k)) = Det(A(-k))^*. \tag{6}$$

Therefore the winding number W can be written as

$$W = \frac{-i}{\pi}\int_{k=0}^{k=\pi}\frac{dz(k)}{z(k)}. \tag{7}$$

Even though the calculation of W requires an integral over the half of the Brillouin zone, in practice the value of the integrand shows any significant variation only near $k = 0$ for the spin-orbit coupled nanowire [31]. This justifies the use of the $(k \cdot p)$-type Hamiltonian Eq. (3) to calculate the integer invariant W defined over the entire Brillouin zone.

Now we derive a formula connecting the $\mathbb{Z}$ invariant W and the Pfaffian $\mathbb{Z}_2$ invariant [23, 24] more frequently used for a semiconductor nanowire. The Pfaffian $\mathbb{Z}_2$ invariant is defined for any BdG matrix H_{BdG} with a particle-hole symmetry of the form $\tau_x H_{BdG} = -H_{BdG}^*\tau_x$ (note that $\Lambda = \mathcal{K}\cdot\tau_x$) where $\tau_x = \tau_x^T$ is the symmetric particle-hole transformation matrix satisfying $\tau_x\tau_x^* = 1$. Then the matrix $H_{BdG}\tau_x$ is anti-symmetric i.e $(H_{BdG}\tau_x)^T = \tau_x H_{BdG}^* = -H_{BdG}\tau_x$. This allows us to define a Pfaffian $Pf(H_{BdG}\tau_x)$ associated with the BdG Hamiltonian as

$$Q = \text{sign}[\frac{Pf(H(k=\pi)\tau_x)}{Pf(H(k=0)\tau_x)}], \tag{8}$$

where $k = 0, \pi$ are the particle-hole symmetric k-points in the Brillouin zone.

For chiral-symmetric matrices, the Pfaffian of $H(k)$ at the particle-hole symmetric k-points $k = 0, \pi$ can be simplified as

$$Pf[H(k)\tau_x] = Pf[U^\dagger\begin{pmatrix} 0 & A(k) \\ A^T(-k) & 0 \end{pmatrix}U\tau_x U^T U^*]$$
$$= Pf[\begin{pmatrix} 0 & A(k) \\ -A^T(-k) & 0 \end{pmatrix}] = Det(A(k)), \tag{9}$$

where we have used the fact that $Det(U) = 1$. Computing the Pfaffian invariant in Eq. 8 using the above result, we obtain that the $\mathbb{Z}_2$ invariant for chiral symmetric Hamiltonian is given by

$$\text{sign}[\frac{Det(A(k=\pi))}{Det(A(k=0))}] = \frac{z(k=\pi)}{z(k=0)} = e^{i\pi W} = (-1)^W. \tag{10}$$

The second pair of equalities follow from the definition of the winding number W in Eq. 7. Therefore the familiar $\mathbb{Z}_2$ Pfaffian invariant of the $d = 1$ systems is simply the parity of the more general $\mathbb{Z}$ invariant of a chiral Hamiltonian.

We now consider the case of a single-band SO-coupled semiconductor nanowire with a parallel Zeeman coupling and a proximity-induced s-wave superconductivity. In this case, from Eq. (3) we have, $H_0 = (\epsilon_k-\mu)+\alpha f(k)\sigma_y+V_Z\sigma_x$ and $\Delta = i\Delta_0\sigma_y$ so that $A(k) = (\epsilon_k-\mu)+\alpha f(k)\sigma_y+V_Z\sigma_x+i\Delta_0\sigma_y$. Here we have generalized the SO coupling term to have a general wave-vector dependence with the constraint $f(k\to\pm\pi)\to 0$. We find that

$$Det(A(k)) = (\epsilon_k-\mu)^2+\Delta_0^2-V_Z^2-\alpha^2 f^2(k)+2i\Delta_0\alpha f(k) \tag{11}$$

has a winding number $W = 1$ whenever the Pfaffian of the Hamiltonian $(\epsilon_k-\mu)^2+\Delta_0^2-V_Z^2-\alpha^2 f^2(k)$ has a single zero as k ranges from $k = 0$ to $k = \pi$. This corresponds to the regime where the $\mathbb{Z}_2$ Pfaffian invariant in Eq. 8 is non-trivial. In the limit of small Δ, this corresponds to a single band crossing the fermi-level at a pair of points $\pm k_F$. By considering the trajectory of $Det(A(k))$ in Eq. 11 in the complex plane as k changes from 0 to π, and noting that $Det(A(k)) \neq 0$ and $Det(A(k))$ moves from a point on the positive real axis to the negative real axis while crossing the imaginary axis exactly once, it is clear the winding number $W = \pm 1$ depending on the sign of $f(k)$ when $Re(Det(A(k))) = 0$.

Now we consider a quasi-1D nanowire (lengths $L_x \gg L_y \gg L_z$) with multiple occupied bands with a parallel Zeeman field (i.e., in x-direction) and proximity induced s-wave superconductivity. For a wire of infinite length, the BdG Hamiltonian of the multiband system has the form,

$$H_{nm}(k) = [\epsilon_{nm}(k) - \mu\delta_{nm}]\tau_z + V_Z\delta_{nm}\sigma_x\tau_z$$
$$+ \alpha k\delta_{nm}\sigma_y\tau_z - i\alpha_y q_{nm}\sigma_x + \Delta_{nm}\sigma_y\tau_y, \tag{12}$$

where $k = k_x$, n, m label different confinement bands with wave functions $\phi_n(y) \propto \sin(n\pi y/L_y)$, and the induced superconducting pairing Δ_{nm} contains non-vanishing inter-band components. The inter-band Rashba coupling α_y comes with matrix elements $q_{nm} \propto \langle\phi_n|\partial/\partial y|\phi_m\rangle$ which couple transverse states with opposite parity. As we show below a finite α_y breaks the exact chirality symmetry of $\widetilde{H}_{nm} = H_{nm}(\alpha_y = 0)$ to only an approximate one for H_{nm}.

To discuss the chirality symmetry of the multi-band nanowire we first consider the Hamiltonian $\widetilde{H}_{nm}$. It can be seen by explicit construction that $\widetilde{H}_{nm}$ anticommutes with a unitary operator $\mathcal{S} = \tau_x$,

$$\{\widetilde{H}_{nm}, \mathcal{S}\} = 0. \tag{13}$$

Here, the chirality operator $\mathcal{S} = \tau_x$ with the p-h operator $\Lambda = \tau_x \cdot \mathcal{K}$. It is easy to check explicitly that $\widetilde{H}_{nm}$ commutes with the complex conjugation operator $\mathcal{K}$ and anticommutes with the p-h transformation operator Λ, and hence it anticommutes with the chirality operator $\mathcal{S} = \mathcal{K}\cdot\Lambda = \tau_x$. The existence of all three symmetries - 'time reversal', particle-hole, and chirality - ensures that

$\widetilde{H}_{nm}$ is in the BDI symmetry class [18–20] characterized by an integer invariant W. From Eq. (13) it follows that the large square matrix Hamiltonian $\widetilde{H}_{nm}$ can be off-diagonalized in a basis in which the unitary operator $\mathcal{S}$ is diagonal:

$$ U\widetilde{H}_{nm}(k)U^{\dagger} = \begin{pmatrix} 0 & A(k) \\ A^T(-k) & 0 \end{pmatrix}. \qquad (14) $$

Defining the variable $z(k) = \exp(i\theta(k)) = Det(A(k))/|Det(A(k))|$ and following Eq. (7), we can now calculate the invariant W which is an integer ($W \in Z$) including zero. The integer W gives the number of zero energy Majorana modes on any given end of the nanowire described by the hamiltonian $\widetilde{H}_{nm}$. As has been shown in detail in Ref. [31], on the $(\mu - V_Z)$ plane W increases in integer steps with increasing V_Z (for fixed μ), indicating quantum phase transitions to phases with multiple Majorana modes on a given end with increasing Zeeman coupling.

In a real quasi-1D nanowire with finite α_y, $H_{nm}(\alpha_y \neq 0)$ does not anti-commute with τ_x. Hence, the Hamiltonian matrix is no longer off-diagonalizable in the diagonal basis of $\mathcal{S}$ and the number W can no longer be defined. A finite α_y thus breaks the chirality symmetry. Nevertheless, since $\alpha_y = \alpha \sim 0.1eV\mathring{A}$ makes only a minute contribution $\sim 10^{-2}E_{qp}$ ($E_{qp} \sim 1K$ is the expected bulk quasiparticle gap in InAs wires in proximity to Nb) to the energies of the end states, the integer invariant for $\widetilde{H}_{nm}$ (i.e., with $\alpha_y = 0$) can still be used to describe the phase diagram of $H_{nm}(\alpha_y = \alpha)$ with the integer W now indicating the number of *near-zero energy* end states on a given end. The different topological phases of the full Hamiltonian $H_{nm}(\alpha_y = \alpha)$ characterized by different numbers of near-zero-energy end states can be characterized by different values of the integer W calculated for the corresponding reduced Hamiltonian $H_{nm}(\alpha_y = 0)$. It is also important to note [31] that the multiple near-zero-energy end states on a given end of a realistic nanowire are robust to all perturbations including disorder as long as the chirality symmetry of $H_{nm}(\alpha_y = 0)$ is unbroken. The exact chiral symmetry of $H_{nm}(\alpha_y = 0)$ (which is only approximate for $H_{nm}(\alpha_y = \alpha)$) thus leads to an effective vanishing of the minimum topological gap (minigap) in realistic quasi-1D nanowires with increasing V_Z. It then becomes difficult (although not impossible [32]) to probe the physics of isolated MFs with increasing V_Z at experimentally accessible temperatures [32, 33].

The small minigap problem of quasi-1D multi-band nanowires can be resolved by applying an additional *transverse* Zeeman field $V_Z^y = g^*\mu_B B_y/2$ in addition to the longitudinal one needed to create the TS state itself. With this term, the BdG Hamiltonian of the nanowire becomes,

$$ H'_{nm}(k) = H_{nm}(k) + V_Z^y \delta_{nm}\sigma_y. \qquad (15) $$

In $H'_{nm}(k)$ the terms with coupling constants V_Z^y and α_y cannot be made fully off-diagonal even in the basis in which $\mathcal{S} = \tau_x$ is diagonal. It is not possible to construct *any* unitary symmetry operator with the available discrete symmetries (time reversal, particle-hole, complex conjugation, etc)) that anticommutes with H'_{nm}. It follows that V_Z^y *externally* breaks the chiral symmetry hidden in $\widetilde{H}_{nm}$. It can be shown that [31], with no V_Z^y if the number of near-zero modes is even, the transverse field creates a gap for all of them resulting in no Majorana edge mode. If the number of zero modes is odd for $V_Z^y = 0$, the transverse field opens a gap for all of them except one, resulting in only one non-degenerate Majorana end mode at each end. The energy gap above the non-degenerate Majorana mode is the minigap which is now tunable by the external transverse Zeeman field breaking the approximate chirality symmetry of the multi-band wire. As shown in Ref. [31] the minigap can be lifted to experimental temperature regimes ($\sim 0.1E_{qp} = 100mK$) by external breaking of the chiral symmetry of $H_{nm}(\alpha_y = 0)$ with a reasonable second Zeeman splitting orthogonal to the wire.

In summary we show that the Hamiltonian of a 1D single-band SO-coupled semiconductor nanowire with s-wave superconductivity and a parallel Zeeman field is chiral symmetric and in the topological class BDI with an integer $\mathbb{Z}$ topological invariant. The familiar Z_2 invariant of this system only gives the parity of the integer invariant. For realistic quasi-1D multi-band nanowires the chiral symmetry is only approximate, nevertheless it results in multiple near-zero-energy end states on any given end with increasing values of the parallel Zeeman splitting. The results derived here have important implications for the topological minigap and robustness of MF modes in semiconductor nanowires [31]. In particular the approximate chiral symmetry implies that the minigap of a realistic multi-band wire almost vanishes with the increase of the parallel Zeeman field and can only be restored to experimentally accessible values by a second Zeeman field orthogonal to the wire which breaks the approximate chiral symmetry. The results here have also been recently shown to be important for Majorana flat bands in $(p\pm ip)$ superconductors [34] and edge MF modes in semiconductor wires with long SO coupling lengths [35, 36].

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