

Unveiling in-gap states and Majorana zero modes in superconductor-topological insulator bilayer model

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Interfaces between topological insulators and superconductors (SCs) are promising platforms for realizing Majorana zero modes (MZMs) via the superconducting proximity effect. We introduce a bilayer model consisting of the surface states of a three-dimensional topological insulator (3DTI) coupled to an s -wave superconductor and systematically study the role of interlayer tunneling strength ($t_{\perp}$) motivated by the recent growth of the Fe(Te, Se)/Bi₂Te₃ heterostructure. We find that increasing $t_{\perp}$ shifts the proximity-induced (PrI) gap minimum away from the Γ point, giving rise to momentum-selective interference patterns that manifest as spatial oscillations in the in-gap states. We introduce an antidot with a magnetic vortex in the model and investigate the resulting in-gap states, including MZMs and Caroli–de Gennes–Matricon (CdGM) modes. With increasing hybridization strength, the energy separation between MZMs and CdGM states increases, enhancing the isolation of MZMs. Importantly, in the strong hybridization limit, the leading CdGM separation remains large in spite of the decrease in the PrI gap. Spin- and spatially resolved wavefunction analysis reveals angular momentum asymmetries absent in conventional s -wave systems. A direct comparison with a standalone s -wave superconductor confirms the emergence of distinct p -wave-like features in the bilayer geometry. Our results provide experimentally relevant predictions for tuning the stability of MZMs and their differentiation from the CdGM modes in SC-3DTI heterostructures and offer a theoretical framework for probing unconventional superconductivity in engineered topological systems.

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I. INTRODUCTION

The search for a suitable platform for topological quantum computing remains a challenge in condensed matter physics and materials science, with multiple pathways proposed with different materials and mechanisms [1]. The prominent pathways are as follows: (1) superconductor (SC) and three-dimensional topological insulator (3DTI) surface state (SS) interfaces realizing Majorana zero modes (MZMs) in materials [2,3], (2) spin-orbit coupled semiconductor nanowire proximitized by an SC [4,5], (3) quantum spin liquid in honeycomb Kitaev model [6–8], and (4) topological states in moiré platforms [9,10].

Vortices in p -wave superconductors have long been proposed to host Majorana zero modes [11–16], and a superconducting proximitized semiconductor surface can provide a natural pathway to realize such states [2,17,18]. However, the materials platforms for these remain a challenge in the design of topological qubits, considering the inherent complexity of the materials.

Following the original proposal by Kitaev to realize Majorana fermions in a p -wave paired nanowire [19], one-dimensional semiconductor wires proximitized by superconductors have been extensively investigated [4,5,20]. This effort led to significant progress in the design of topological states [21,22]. One of the major issues has been the long SC coherence length in Al, which can lead to fragile topology due to impurity scattering in Al [23]. Additionally, vortex states in bulk Fe-based superconductors have been extensively explored using, for example, scanning tunneling microscopy (STM) and scanning tunneling spectroscopy (STS) [24–28], following theoretical proposals of topological superconductivity in these materials [29]. More recently, platforms such as magnetic topological surface states [30,31], topological crystalline insulators [32] proximitized with SC, and SC-insulator-SC junction [33] have been explored as a host for Majorana modes.

A persistent challenge in interpreting STM experiments is distinguishing genuine MZMs from other in-gap states. Observed features may arise from conventional Andreev bound states (ABS) [34,35], Caroli–de Gennes–Matricon (CdGM) modes [36], or Yu-Shiba-Rusinov states [37–40], complicating the identification of true MZMs [41].

Compared to bulk compounds, engineered heterostructures such as the interface of 3DTI SS and s -wave superconductor offer tunability over physical parameters by changing growth conditions, stoichiometry, and annealing, enabling

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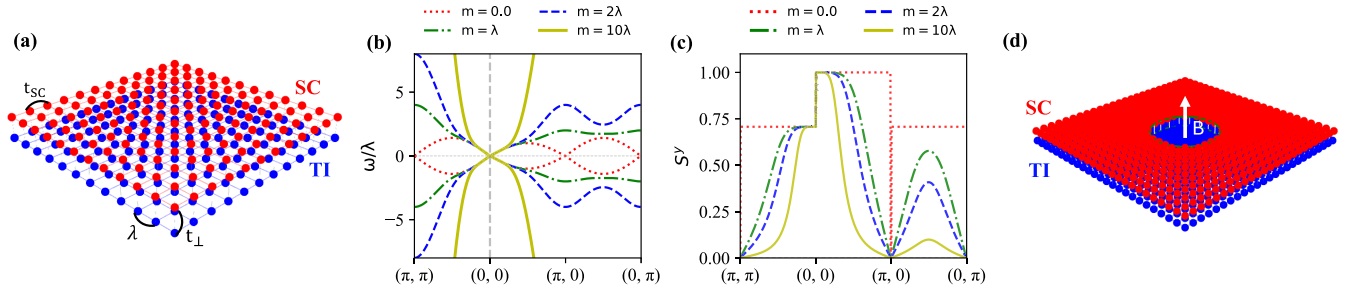


FIG. 1. Bilayer square lattice consisting of a 3DTI SS and SC. (a) Schematic of the SC-TI bilayer square lattice. (b) Band structures for the 3DTI SS for $m = \{0, \lambda, 2\lambda, 10\lambda\}$, illustrating the role of m in opening the gap at $X(\pi, 0)$, $Y(0, \pi)$, and $M(\pi, \pi)$ points in the BZ. (c) Spin polarization along the y direction in the 3DTI SS bands, showcasing the reduction of spin-momentum locking in the BZ away from the zone center due to m . Panel (d) shows the antidot geometry in the bilayer model.

more systematic characterization. Notably, $\text{Fe}(\text{Te}, \text{Se})/\text{Bi}_2\text{Te}_3$ heterostructures have been successfully synthesized [42,43], and vortices can be patterned in a controlled fashion using lithography [44]. With their large superconducting gap and high T_c , these systems provide a promising avenue for realizing Majorana bound states.

Recent angle-resolved photoemission spectroscopy (ARPES) experiments on the $\text{Fe}(\text{Te}, \text{Se})/\text{Bi}_2\text{Te}_3$ interface [45] have shown that these heterostructures contain essential ingredients for topological superconductivity: spin-momentum locking in the TI layer and strong interlayer coupling. Remarkably, superconductivity appears even at very low Se concentrations [45], in which disorder effects can be minimized [46]. However, a detailed microscopic understanding of the superconducting state in these heterostructures remains lacking.

Motivated by these developments, we introduce a bilayer consisting of 3DTI SS coupled to a two-dimensional s -wave superconductor, modeled after $\text{Fe}(\text{Se}, \text{Te})$ monolayers grown on Bi_2Te_3 [42,43,45], and investigate proximity-induced (PrI) superconductivity. Rather than imposing a momentum-independent pairing potential directly on the TI surface, as in the Fu-Kane model [2], we explicitly include a superconducting layer with finite dispersion and interlayer tunneling.

We find that large interlayer coupling shifts the PrI gap away from the Γ point due to the finite dispersion of the superconducting layer. This finite momentum produces Friedel-like oscillations in wavefunctions localized at lattice boundaries. Introducing an antidot, modeled by removing the SC layer within a finite region, we investigate the resulting in-gap bound states and MZMs. Similar antidot systems have been studied previously in both clean [15,16] and disordered [47–50] regimes, but primarily within the Fu-Kane framework. In contrast, our explicit bilayer model reveals that the superconducting layer plays a crucial role in shaping the in-gap spectrum and controlling the energy separation between MZMs and CdGM states, thereby facilitating the isolation of MZMs from other in-gap excitations. The SC-3DTI interface is thus highly sensitive to interlayer tunneling strength, exhibiting rich behavior that governs the formation, localization, and spectral properties of topological in-gap states.

The paper is organized as follows. Section II introduces the bilayer model and our implementation of an antidot. Section III presents the main results: an analysis of the PrI gap (Sec. III A); chiral edge modes (CEMs) (Sec. III B); and

in-gap bound states (Sec. III C) in the bilayer, contrasted with a vortex in an s -wave superconductor. Section III D outlines how to reproduce these findings within a single-layer model and clarifies its limitations. Section IV summarizes the work.

II. METHODS

We consider a bilayer system, containing 3DTI SS and a conventional s -wave superconductor, both modeled on a two-dimensional (2D) square lattice, as schematically illustrated in Fig. 1(a). The Hamiltonian is given by $\mathcal{H} = H_{\text{TI}} + H_{\text{SC}} + H_{\text{hyb}}$.

The first term H_{TI} describing 3DTI SS is given by [51]

$$H_{\text{TI}} = i\frac{\lambda}{2} \sum_{\mathbf{r}, \alpha} \psi_{\mathbf{r}}^\dagger \boldsymbol{\sigma} \cdot (\hat{\mathbf{z}} \times \boldsymbol{\alpha}) \psi_{\mathbf{r}+\alpha} + \sum_{\mathbf{r}} \psi_{\mathbf{r}}^\dagger \left(\frac{3}{2} m \sigma_z + \varepsilon_{\text{TI}} - \mu \right) \psi_{\mathbf{r}} - \frac{m}{8} \sum_{\mathbf{r}, \alpha} \psi_{\mathbf{r}}^\dagger (4\sigma_z \psi_{\mathbf{r}+\alpha} - \sigma_z \psi_{\mathbf{r}+2\alpha}). \quad (1)$$

Here, $\psi_{\mathbf{r}} = [c_{\mathbf{r}\uparrow} \ c_{\mathbf{r}\downarrow}]^T$ is the spinor at the lattice site $\mathbf{r} = (x, y)$ in the 3DTI and $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ is the vector of Pauli matrices. $\boldsymbol{\alpha} = \pm\hat{\mathbf{x}}, \pm\hat{\mathbf{y}}$ denotes the vector of nearest neighbors in units of the lattice constant, $\hat{\mathbf{x}}, \hat{\mathbf{y}}$, and $\hat{\mathbf{z}}$ being the unit vectors along the x , y , and z directions, respectively. The parameter λ represents the Rashba spin-orbit coupling (also equal to the Dirac velocity). ε_{TI} is the on-site potential for the TI layer, and μ is the chemical potential.

The parameter m introduces a Wilson mass term that lifts the degeneracy X, Y , and M points in the spectrum of the 3DTI SS, yielding a single gapless Dirac cone at the Γ point, as shown in Fig. 1(b) for a set of m values. This mass term is essential for isolating a single Dirac cone and thereby capturing the low-energy physics of a 3DTI surface, and avoids the need for more computationally expensive 3D slab model [52]. Notably, the inclusion of m circumvents the fermion doubling problem, which states that a lattice model preserving time-reversal symmetry (TRS) cannot host an odd number of Dirac points, as dictated by the Nielsen-Ninomiya theorem [53]. This mass term m , therefore, explicitly breaks the TRS in the model from the outset and allows for odd number of Dirac cones.

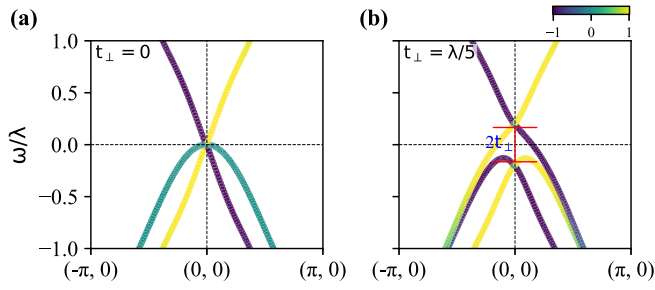


FIG. 2. Hybridization of the SC-layer metallic band with the 3DTI SS. (a) Band structure of the unhybridized system, showing the 3DTI SS and the metallic band from the SC layer. (b) Hybridized band structure for interlayer coupling $t_{\perp} = \lambda/5$. The color scale indicates spin polarization along the y direction $S_y^l(\mathbf{k})$, as defined in Eq. (5).

The second term H_{SC} describing the SC layer is given by

$$H_{SC} = t_{SC} \sum_{\mathbf{r}, \alpha} \xi_{\mathbf{r}+\alpha}^{\dagger} \xi_{\mathbf{r}} + (\varepsilon_{SC} - \mu) \sum_{\mathbf{r}} \xi_{\mathbf{r}}^{\dagger} \xi_{\mathbf{r}} + \sum_{\mathbf{r}} (\Delta_{\mathbf{r}} \xi_{\mathbf{r}}^{\dagger} \sigma_y \xi_{\mathbf{r}}^{\dagger} + \text{H.c.}), \quad (2)$$

where $\xi_{\mathbf{r}} = [d_{\mathbf{r}\uparrow} \quad d_{\mathbf{r}\downarrow}]^T$ and $\Delta_{\mathbf{r}}$ is the s -wave SC pairing potential. The parameters ε_{SC} and t_{SC} are the on-site potential and hopping amplitude (related to effective mass) in the SC lattice.

The last term H_{hyb} describing the interlayer coupling is given by

$$H_{hyb} = t_{\perp} \sum_{\mathbf{r}} (\xi_{\mathbf{r}}^{\dagger} \sigma_0 \psi_{\mathbf{r}} + \text{H.c.}), \quad (3)$$

$$\hat{h}_{\mathbf{k}} = \begin{bmatrix} \mathbf{d}_{TI}(\mathbf{k}) \cdot \boldsymbol{\sigma} & 0 & \sigma_0 t_{\perp} & 0 \\ 0 & -\mathbf{d}_{TI}(-\mathbf{k}) \cdot \boldsymbol{\sigma}^* & 0 & -\sigma_0 t_{\perp} \\ \sigma_0 t_{\perp} & 0 & \mathbf{d}_{SC}(\mathbf{k}) \cdot \boldsymbol{\sigma} & i\sigma_y \Delta \\ 0 & -\sigma_0 t_{\perp} & -i\sigma_y \Delta^* & -\mathbf{d}_{SC}(-\mathbf{k}) \cdot \boldsymbol{\sigma}^* \end{bmatrix}. \quad (4)$$

Here, $\mathbf{d}_{TI}(\mathbf{k}) = (\varepsilon_{TI} - \mu, -\lambda \sin k_y, \lambda \sin k_x, M_{\mathbf{k}})$, $\boldsymbol{\sigma} = (\sigma_0, \sigma_x, \sigma_y, \sigma_z)$ with $\mathbf{k} = (k_x, k_y)$, $M_{\mathbf{k}} = m[(2 - \cos k_x - \cos k_y) - \frac{1}{4}(2 - \cos 2k_x - \cos 2k_y)]$, and $\Delta = \Delta_0$.

In the limit $\mathbf{k} \rightarrow \Gamma$, $\mathbf{d}_{TI}(\mathbf{k}) \cdot \boldsymbol{\sigma} = \begin{bmatrix} \varepsilon_{TI} - \mu & -i\lambda k_- \\ i\lambda k_+ & \varepsilon_{TI} - \mu \end{bmatrix}$, where $k_{\pm} = k_x \pm ik_y$ and $|\mathbf{k}|^2 = k_x^2 + k_y^2$. Therefore, model preserves the TRS in this momentum region as $M_{\mathbf{k}}$ vanishes up to the cubic term. The energies are given by $\omega_{TI}^{\pm}(\mathbf{k}) = \varepsilon_{TI} - \mu \pm \lambda|\mathbf{k}|$, in the vicinity of Γ point. The eigenstates are given by $|V_{TI}\rangle_{\pm} = (\sqrt{k_-} c_{\mathbf{k}\uparrow}^{\dagger} \pm i\sqrt{k_+} c_{\mathbf{k}\downarrow}^{\dagger})|0\rangle$. For $\mathbf{k}$ along $(0, 0)$ to $(\pi, 0)$, the ω_{TI}^+ (ω_{TI}^-) dispersion have $\uparrow$ ($\downarrow$) spin along the y direction, where σ_x and σ_z vanish, as can be seen in Fig. 2(a).

In our model, the mass term $M_{\mathbf{k}}$ opens a large gap in the 3DTI SS bands at the Brillouin zone (BZ) boundaries [see Fig. 1(b)] and leads to a softening of the spin-momentum

where $t_{\perp}$ denotes the interlayer tunneling amplitude and σ_0 is the 2×2 identity matrix; thus, the hybridization is diagonal in the spin index. The spin-conserving interlayer tunneling is critical to preserving the spin-momentum locking of 3DTI SS in the PrI gap. Conversely, the spin active hopping can close the PrI gap.

We use the Bogoliubov–de Gennes (BdG) formalism [54,55], in which each lattice site will be described by an eight-dimensional Hamiltonian (2 TI particle + 2 TI hole + 2 SC particle + 2 SC hole). Therefore, the full Hamiltonian is given by $\mathcal{H} = \sum_{\mathbf{r}, \alpha} \phi_{\mathbf{r}}^{\dagger} h_{\mathbf{r}, \mathbf{r}+\alpha} \phi_{\mathbf{r}+\alpha}$, where $\phi_{\mathbf{r}} = [\psi_{\mathbf{r}} \quad \psi_{\mathbf{r}}^{\dagger} \quad \xi_{\mathbf{r}} \quad \xi_{\mathbf{r}}^{\dagger}]^T$ in the Nambu representation. Here, $\alpha = 0$ accounts for the on-site and SC pairing term and the interlayer hybridization, whereas $\alpha = \pm \hat{x}, \pm \hat{y}$ for the nearest-neighbor hopping, and $\alpha = \pm 2\hat{x}, \pm 2\hat{y}$ for next-nearest-neighbor hopping.

Throughout this work, we use the following parameters unless otherwise stated: lattice spacing as the unit length, $\lambda = 1$ as the unit energy, and consider $\mu = 0$, $\varepsilon_{TI} = 0$, and $m = 2\lambda$ for the TI layer; $\Delta_{\mathbf{r}} = \Delta_0 = \lambda/5$, $t_{SC} = 2\Delta_0$, and $\varepsilon_{SC} = -4t_{SC}$ for the SC layer. Parameter values are chosen to achieve a qualitative agreement with the electronic structure of Fe(Te, Se)/Bi₂Ti₃ interface [45], while also simplifying the model to facilitate efficient numerical calculations. In particular, by fixing $t_{SC} > 0$, we ensure that the SC layer near the Fermi level has a negative effective mass [see Fig. 2(a)], consistent with the holelike band observed near Γ point in Fe(Te, Se) [56]. ε_{SC} is chosen such that the band top at the Γ point in SC layer touches the Fermi level, which is globally set to zero energy.

To understand the interplay between the real and momentum space and present a comprehensive picture, we transform the bilayer Hamiltonian to the momentum space, which is then given by $\mathcal{H} = \sum_{\mathbf{k}} \phi_{\mathbf{k}}^{\dagger} \hat{h}_{\mathbf{k}} \phi_{\mathbf{k}}$, where $\phi_{\mathbf{k}} = [\psi_{\mathbf{k}} \quad \psi_{-\mathbf{k}}^{\dagger} \quad \xi_{\mathbf{k}} \quad \xi_{-\mathbf{k}}^{\dagger}]^T$ and

locking away from the zone center, as it polarizes spin along the z direction. Nevertheless, the locking persists throughout a wide momentum range, albeit with reduced magnitude, as shown in Fig. 1(c).

The SC part is given by $\mathbf{d}_{SC}(\mathbf{k}) = [\varepsilon_{SC} - \mu + 2t_{SC} \cos(k_x) + 2t_{SC} \cos(k_y), 0, 0, 0]$. In the limit $\mathbf{k} \rightarrow \Gamma$, $\mathbf{d}_{SC}(\mathbf{k}) \cdot \boldsymbol{\sigma} = \begin{bmatrix} \varepsilon_{SC} - \mu + 4t_{SC} - t_{SC}|\mathbf{k}|^2 & 0 \\ 0 & \varepsilon_{SC} - \mu + 4t_{SC} - t_{SC}|\mathbf{k}|^2 \end{bmatrix}$. Under the constraint $\varepsilon_{SC} - \mu = -4t_{SC}$ used in our work, the SC bands are given by $\omega_{SC}^{\pm}(\mathbf{k}) = \pm \sqrt{|\Delta|^2 + t_{SC}^2 |\mathbf{k}|^2}$ and will be gapped by the pair potential Δ .

The spin polarization in each band is evaluated using the relation

$$S_{\alpha}^l(\mathbf{k}) = \langle \phi_{\mathbf{k}} | \sigma_{\alpha}^l | \phi_{\mathbf{k}} \rangle. \quad (5)$$

Here, l corresponds to each particle and hole index of the 3DTI and SC layer, and $\alpha \in \{x, y, z\}$ components of the spin.

Antidot in the model

One of the key focuses of this work is to study the inhomogeneous bilayer configuration where the superconducting layer is locally removed to form an antidot of radius R , which traps a magnetic flux quantum [see Fig. 1(c)]. We consider the magnetic field $\mathbf{B} = (0, 0, B_0)$ distributed uniformly inside the antidot [50]. The corresponding vector potential is then given by

$$\mathbf{A}(\mathbf{r}) = \begin{cases} \frac{\Phi}{2\pi R^2}(-y, x, 0), & \text{for } r < R, \\ \frac{\Phi}{2\pi r^2}(-y, x, 0), & \text{for } r \geq R, \end{cases} \quad (6)$$

where $\Phi = N\Phi_0 = N\frac{h}{2|e|}$ is the total flux trapped in the antidot, with $-|e|$ the electron charge and Φ_0 the superconducting flux quantum. We assume that the magnetic-field penetration depth is negligible compared to R , so that the flux is confined within the antidot.

The magnetic field can be accounted for by using Peierls substitution in the hopping terms in both layers given by

$$c_{\mathbf{r}}^\dagger c_{\mathbf{r}'} \rightarrow c_{\mathbf{r}}^\dagger c_{\mathbf{r}'} e^{-i\frac{|e|\hbar}{2\pi} \int_{\mathbf{r}}^{\mathbf{r}'} \mathbf{A}(\mathbf{s}) \cdot d\mathbf{s}} = c_{\mathbf{r}}^\dagger c_{\mathbf{r}'} e^{iN\Phi_{\mathbf{r}\mathbf{r}'}}. \quad (7)$$

Peierls phase is given by

$$\Phi_{\mathbf{r}\mathbf{r}'} = \begin{cases} -(x' - x)y \frac{1}{2R^2}, & \text{for } r, r' < R \\ -\frac{1}{2} \left\{ \tan^{-1} \left(\frac{x'}{y} \right) - \tan^{-1} \left(\frac{x}{y} \right) \right\}, & \text{for } r, r' \geq R \end{cases} \quad (8)$$

for $\mathbf{r}$ and $\mathbf{r}'$ along the x direction, and

$$\Phi_{\mathbf{r}\mathbf{r}'} = \begin{cases} +(y' - y)x \frac{1}{2R^2}, & \text{for } r, r' < R \\ +\frac{1}{2} \left\{ \tan^{-1} \left(\frac{y'}{x} \right) - \tan^{-1} \left(\frac{y}{x} \right) \right\}, & \text{for } r, r' \geq R \end{cases} \quad (9)$$

for $\mathbf{r}$ and $\mathbf{r}'$ along the y direction, and $\mathbf{r} = (x, y)$ and $\mathbf{r}' = (x', y')$.

The above equations account for the Peierls phase in the hopping terms of both the TI and SC layers. Note, however, that inside the antidot region the SC layer is absent.

The magnetic flux also introduces a spatially varying phase into the superconducting pairing potential, which we write as

$$\Delta_{\mathbf{r}} = \begin{cases} 0, & r < R, \\ \Delta_0 e^{iN\varphi}, & r \geq R, \end{cases} \quad (10)$$

where (r, φ) are polar coordinates centered on the vortex, Δ_0 is the SC gap amplitude, and N denotes the number of flux quanta threading the antidot. The choice of this phase factor follows from gauge considerations, as detailed in Appendix A.

To characterize the chiral edge modes, Majorana zero modes, and other in-gap states in our model, we diagonalize the real-space Hamiltonian introduced above and analyze

the resulting eigenstates. The m th eigenvector of the real-space Hamiltonian is given by $|\Psi_m(\mathbf{r})\rangle = (u_{\mathbf{r}\uparrow}^{\text{TI}} c_{\mathbf{r}\uparrow}^\dagger + u_{\mathbf{r}\downarrow}^{\text{TI}} c_{\mathbf{r}\downarrow}^\dagger + v_{\mathbf{r}\uparrow}^{\text{TI}} c_{\mathbf{r}\uparrow} + v_{\mathbf{r}\downarrow}^{\text{TI}} c_{\mathbf{r}\downarrow} + \dots + v_{\mathbf{r}\downarrow}^{\text{SC}} d_{\mathbf{r}\downarrow})|0\rangle$. Here, u and v are the particle and hole components of the corresponding eigenvector of the Hamiltonian.

Using this eigenvector, the site-resolved probability density for a state (m) on TI is given by $n_{\text{TI}}^m(\mathbf{r}) = |u_{\mathbf{r}\uparrow}^{\text{TI}}|^2 + |u_{\mathbf{r}\downarrow}^{\text{TI}}|^2 + |v_{\mathbf{r}\uparrow}^{\text{TI}}|^2 + |v_{\mathbf{r}\downarrow}^{\text{TI}}|^2$. Similarly, the probability density on SC can be evaluated as $n_{\text{SC}}^m(\mathbf{r}) = |u_{\mathbf{r}\uparrow}^{\text{SC}}|^2 + |u_{\mathbf{r}\downarrow}^{\text{SC}}|^2 + |v_{\mathbf{r}\uparrow}^{\text{SC}}|^2 + |v_{\mathbf{r}\downarrow}^{\text{SC}}|^2$.

III. RESULTS AND DISCUSSION

We begin by exploring the bilayer model in momentum space without superconductivity, providing insight into the underlying band structure. Then, with BdG formalism, we introduce a pairing potential. Building on these momentum-space results, we next explore the system under open boundary conditions to examine edge phenomena. Finally, we introduce an antidot to investigate the emergence and structure of in-gap bound states.

Metallic band-3DTI SS hybridization. We briefly explore a bilayer model composed of (1) 3DTI SS and (2) a metallic band from the SC layer (without the pairing terms). The goal is to investigate how interlayer hybridization influences the band structure, the results for which are shown in Fig. 2.

Panel (a) displays the unhybridized bands ($t_{\perp} = 0$) of the two layers. 3DTI SS exhibits spin-momentum locking near the Dirac point, as can be seen in the dispersion (despite the model explicitly breaking the TRS away from the Γ point). The metallic band from the SC layer is spin-degenerate and unpolarized.

Panel (b) shows the hybridized band structure for a finite interlayer tunneling $t_{\perp} = \lambda/5$. At the crossing points, the spin-momentum-locked states of the 3DTI SS hybridize selectively with metallic states of the same spin, opening spin-dependent gaps. However, the other spin-momentum-locked band remains always gapless resulting in only partial gapping of the spectrum, which leads to a Rashba-like dispersion, consistent with inversion symmetry breaking. These features offer a sensitive probe of the interlayer coupling strength using spin-sensitive ARPES. In Fig. 4 of Ref. [45], ARPES data on Fe(Te, Se) films grown on Bi_2Te_3 show an emergent Dirac-like feature interpreted as quantum well states. Our band structure here also shows that the spin-dependent coupling leads to the doubling of Dirac-like points, but a more detailed comparison using spin-resolved ARPES will be needed to understand the nature of these features.

Away from the band crossing regions, the bands largely retain their character from the unhybridized limit. Importantly, the interlayer coupling enhances the spin-momentum-locked density of states (DOS) near zero energy, compared to the uncoupled 3DTI SS. Such an enhancement cannot be captured within a single-layer 3DTI SS model, where the density of states is governed solely by the TI layer.

A. Proximity-induced gap

We now introduce a pairing potential Δ in the SC layer and examine how coupling between the two layers modifies

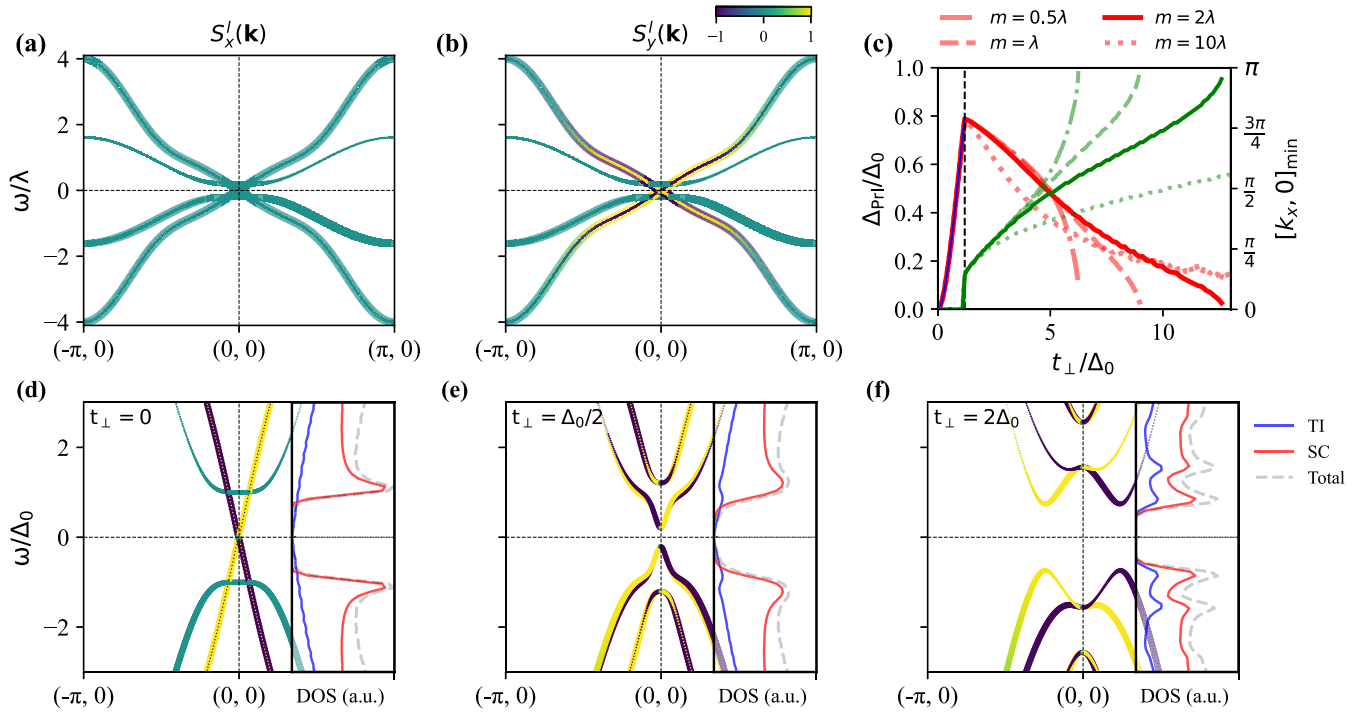


FIG. 3. Gap opening in the SC-3DTI SS bilayer. (a), (b) Spin-resolved spectral functions with spin projections along the x [$S'_x(\mathbf{k})$] and y [$S'_y(\mathbf{k})$] directions, respectively, for $t_\perp = 0$, with the spin projections defined by Eq. (5). Thickness of the bands denotes particle (thick) and hole (thin) components of the Bogoliubov quasiparticles. (c) Proximity-induced gap as a function of interlayer tunneling strength $t_\perp$ for a set of Wilson mass m , as indicated (solid lines indicate the case used in the paper, unless stated otherwise). Red lines represent numerical gap values. The blue line given by Eq. (11) shows the smallest gap opening at the Γ point. Green line tracks the momentum-space location of the minimum gap in the BZ. (d) Enlarged view of the low-energy spectral region from panel (b). Panels (e) and (f) display spectra for nonzero couplings $t_\perp = \Delta_0/2$ and $t_\perp = 2\Delta_0$, respectively, colored according to the spin projection in the y direction. The insets in panels (d)–(f) show the corresponding density of states.

the low-energy spectrum by solving the BdG Hamiltonian [Eq. (4)]. The interlayer coupling induces a PrI gap in the hybridized bands, as illustrated in Fig. 3.

Panels (a) and (b) show the spin-resolved band structure along the Γ -X direction in the BZ, with spin projections computed using Eq. (5) along the x and y axes, respectively. Bands span the range $[-4\lambda, 4\lambda]$ for $m = 2\lambda$, used in this work. As discussed below Eq. (1), large m gaps out the Dirac points except the one at Γ point and moves the band to $\pm 2m$ at $(0, \pm\pi)$ and $\pm 4m$ at $(\pm\pi, \pm\pi)$ [see Fig. 1(b)]. Near zero energy along Γ -X, the spin is locked in the transverse y direction, while the x component remains zero throughout the dispersion, consistent with the expected spin-momentum locking of the 3DTI SS.

The SC bands are gapped in the energy range $[-\Delta, \Delta]$, with dispersion in the interval $[\pm\Delta, \pm\sqrt{\Delta^2 + (4t_{\text{SC}})^2}]$. These bands are spin-degenerate. Their form is chosen to qualitatively resemble experimental SC band structures reported in Ref. [56]. Notably, the unhybridized bands preserve the TRS within the energy window of interest.

We now introduce interlayer coupling $t_\perp$ to investigate hybridization between the 3DTI SS and the SC bands, and to analyze the resulting PrI gap in the hybridized spectrum. The PrI gap is defined as the energy gap between the Fermi level and the nearest bulk states and is symmetric about the Fermi energy due to particle-hole symmetry

Panel (c) presents results for the PrI gap as the interlayer coupling increases for a set of Wilson mass term parameter values m , as indicated above the panel, and $m = 2\lambda$, used in this paper unless stated otherwise, is shown using solid lines. The red points indicate the numerically extracted PrI gap at the Γ point, while the blue curve shows the corresponding analytical estimate derived below.

For small $t_\perp$, the PrI gap is located at the Γ point for all the cases and is given by

$$\Delta_{\text{PrI}} = \sqrt{t_\perp^2 + \frac{|\Delta_0|^2}{2}} - \frac{|\Delta_0|}{2} \sqrt{4t_\perp^2 + |\Delta_0|^2}, \quad (11)$$

which is also plotted as the blue curve in panel (c). In this regime, Δ_{PrI} is fully determined by $t_\perp$ and Δ_0 . In the limit $t_\perp/|\Delta_0| \ll 1$, the expression simplifies to $\Delta_{\text{PrI}} \approx \frac{t_\perp^2}{\Delta_0}$, consistent with the expectation from second-order perturbation theory.

As $t_\perp$ increases beyond $1.2\Delta_0$, the location of the PrI gap shifts from the Γ point to a finite momentum, forming a ring-shaped contour of radius $|k_F|$ in momentum space [panel (f)]. This transition is shown by the green line in panel (c). We show the finite-momentum results till $(\pi, 0)$ in the BZ for all the cases. In this regime, the magnitude of PrI gap remains below Δ_0 and decreases monotonically.

The momentum-space transition is discontinuous: $|k_F|$, momentum of PrI gap, abruptly jumps from 0 to finite momentum, in all the cases at $t_\perp = 1.2\Delta_0$, and then increases monotonically with increasing $t_\perp$. This discontinuity in the gap location originates from the specific noninteracting metallic band structure assumed for the SC layer. The transition point itself is only weakly dependent on the Wilson mass m , although quantitative differences appear away from the transition.

These effects remain controlled provided that $|\lambda \sin k_F| \gg |M_{k_F}|$, and that the proximity-induced gap is sufficiently small, i.e., $\Delta_{\text{PrI}} \ll v_{\text{eff}}(k_{F,\text{max}} - k_F)$, where $v_{\text{eff}} = \lambda$ when the PrI gap is centered at Γ , and $v_{\text{eff}} = v_F$ when it opens at finite k_F . Here, v_F is the effective Fermi velocity of the hybridized band, and $k_{F,\text{max}}$ denotes the largest momentum for which the condition $|\lambda \sin k| \gg |M_k|$ remains satisfied. The PrI gap that develops near the Γ point remains parametrically smaller than the M_k -induced gap at the zone boundary, since throughout this work we consider the regime $t_\perp \ll m$ [see Figs. 3(b)–3(e)].

Throughout this work, we therefore focus on the regime $t_\perp \lesssim 2\Delta_0 \ll m$, where the hybridization occurs near the Γ point and remains well separated from the Wilson-mass-induced gap at the BZ boundaries. Within this parameter regime, the PrI gap and its finite-momentum shift are governed by low-energy hybridization and are insensitive to the high-energy Wilson regularization.

For $m = 2\lambda$ (case in this paper), the gap closes at X point in the BZ at $t_\perp \approx 13\Delta_0$. This in turn sets a large range of interlayer coupling where the PrI gap with finite momentum can be realized.

Panel (d) presents an enlarged view of the low-energy spectral region from panel (b) for the unhybridized case. Panels (e) and (f) illustrate the two characteristic regimes of PrI gap formation for interlayer couplings $t_\perp = \Delta_0/2$ and $t_\perp = 2\Delta_0$, respectively. For $t_\perp = \Delta_0/2$, the gap opens at the Γ point. In contrast, for $t_\perp = 2\Delta_0$, the gap shifts to a nonzero momentum, forming a ring-shaped contour centered away from Γ . The insets in the panels (d)–(f) show the corresponding density of states. We note that the DOS for Γ -point minima and finite-momentum minima have distinct one and two humps in the DOS, respectively, close to the gap.

These findings in the bilayer model can be mapped onto the single-layer models commonly explored in the literature, where the SC layer is integrated out [2,50]. The correspondence and differences are discussed further in Sec. III D. Notably, in the single-layer framework, the gap minimum shifts to finite momentum only when the on-site potential ε_{TI} is tuned, whereas in the explicit bilayer model this behavior arises naturally from interlayer hybridization.

B. Chiral edge modes

We next turn to edge phenomena under open boundaries and investigate chiral edge modes in the bilayer model. To this end, we solve the real-space Hamiltonian with open boundary conditions on an $L = 201$ square bilayer lattice, introduced in Sec. II, and schematically shown in Fig. 4(a).

Coupling the 3DTI SS to an s -wave superconductor preserves TRS, and the corresponding physical hybrid system is

therefore characterized by a vanishing Chern number $C = 0$. In contrast, our effective Hamiltonian carries a nonzero Chern number, $C = -1$, originating from the TRS-breaking regularization term M_k at high energies, even though its low-energy sector relevant for the proximity-induced gap remains approximately TRS preserving. Thus, the edge modes implied by bulk-boundary correspondence in the effective model are a by-product of the chosen regularization scheme, and should not be interpreted as physical edge states of a genuinely TRS-preserving system, such as a proximitized 3DTI slab or a proximitized TI region surrounded by an otherwise ungapped TI surface.

Nevertheless, a physically meaningful interpretation can be given by noting that the edge of the effective model is topologically equivalent to an interface between two distinct gapped regions of the 3DTI surface: one proximitized by a superconductor and the other by a magnetic insulator. In this sense, the edge modes studied here can be viewed as chiral Majorana boundary modes of such a hybrid structure, although quantitative details will depend on the specific realization of the interface.

Figure 4 summarizes our analysis of the CEMs. Panel (a) shows the schematic of the bilayer system, along with the spatial cut used in the analysis. Panel (b) presents the eigenenergies of the system as a function of interlayer hybridization strength $t_\perp$, shown along the horizontal axis. Color scale indicates the probability density localized at the edge of lattice for each eigenstate: bright yellow denotes strong edge localization, while dark blue corresponds to bulk states. The edge-localized states form a gapless branch, consistent with the topological protection. The bulk energy gap, highlighted by the pale blue background, agrees well with the PrI gap extracted from the momentum-space analysis in Fig. 3(c) for the corresponding values of $t_\perp$.

Interestingly, while the CEMs are nearly equally spaced in energy when the PrI gap minimum lies at the Γ point (e.g., $t_\perp = \Delta_0/2, \Delta_0$), the levels become increasingly dense near the bulk continuum when the gap minimum shifts to a finite-momentum ring (e.g., at larger $t_\perp$). The signature of which can be seen as increase in the density of states, (i.e., higher number of states in the same energy interval) shown near the bulk continuum for large $t_\perp$. This transition reflects a modification in the CEM's density of states across different hybridization regimes.

Panel (c) presents the spatial structure of the CEMs across both the SC and TI layers. The probability density $n(r)$ is shown separately for the TI $n_{\text{TI}}(r)$ and SC $n_{\text{SC}}(r)$ layers using solid and dashed lines, respectively. The results are shown for a representative edge-localized state near the Fermi level along a spatial cut indicated by the white dashed line in panel (a). Results are displayed for several values of $t_\perp$, annotated along the top of panel. The TI-layer density, shown as solid lines, peaks sharply at the boundary and exhibits a rapid decay into the bulk. As $t_\perp$ increases, the edge localization in the TI layer becomes more pronounced. In the SC layer (dashed lines), the density is generally suppressed deep in the bulk. A notable feature is the shift in the density maximum: At small $t_\perp$, the maximum is located away from the boundary but gradually shifts toward the edge as $t_\perp$ increases. This reflects

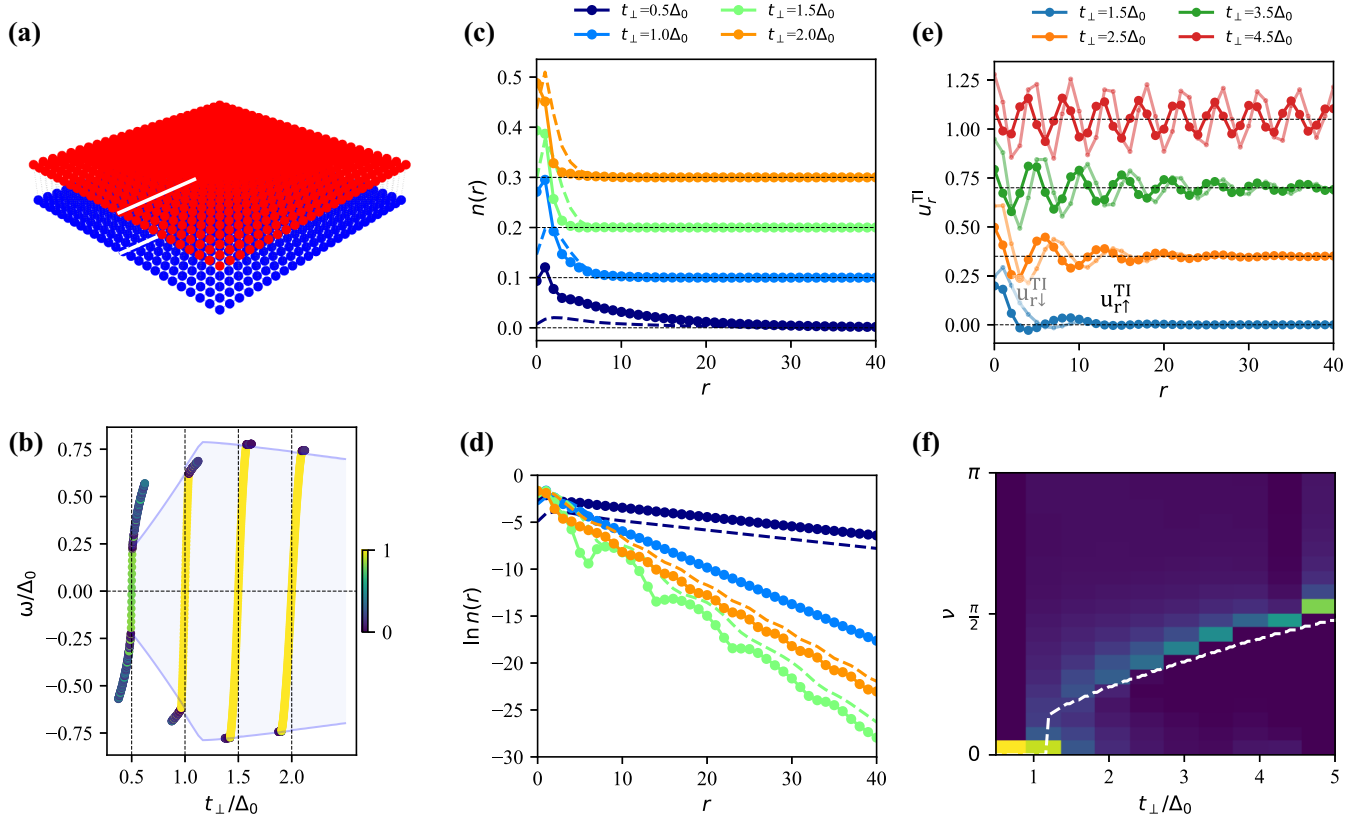


FIG. 4. Nature of chiral edge modes in the bilayer model. (a) Schematic of the SC-3DTI SS bilayer, with the spatial cut (white lines) used for analyzing edge-localized states. (b) The 250 closest eigenvalues near the Fermi level for interlayer couplings $t_{\perp}$ indicated below the panel. Eigenvalues are offset horizontally for clarity. Color scale denotes the degree of particle density localization at the edge. Blue lines denote the PrI gap from Fig. 3(c) ($\lambda = 1$), and the shaded region marks the corresponding gapped regime. (c) Spatial profile of the CEM probability density $n(r)$, shown separately for the TI $n_{\text{TI}}(r)$ and SC $n_{\text{SC}}(r)$ layers using solid and dashed lines, respectively. (d) Logarithmic plot of the probability density $n(r)$ from panel (c), highlighting the exponential decay into the bulk for both layers. (e) Wavefunction components of the edge tail in the TI layer, showing particle spin- $\uparrow$ ($u_{r\uparrow}^{\text{TI}}$, solid lines) and spin- $\downarrow$ ($u_{r\downarrow}^{\text{TI}}$, faded lines) components. Amplitudes are rescaled by a decaying envelope to emphasize the oscillatory behavior. (f) Oscillation frequency (ν) of the CEM tail as a function of interlayer coupling $t_{\perp}$. The white line shows the $[k_x, 0]_{\text{min}}$ values from Fig. 3(c) ($\lambda = 2m$).

a redistribution of the edge mode's weight from the TI layer at small $t_{\perp}$ to the SC layer at larger $t_{\perp}$.

Moreover, the spatial profile in the SC layer at the edge evolves from Lorentzian-like at low $t_{\perp}$ to Gaussian-like at higher $t_{\perp}$, closely following the differences in the PrI gap transition from a minimum at the Γ point to a finite-momentum contour [see panels (e) and (f) in Fig. 3]. This evolution demonstrates that the SC-layer edge profile encodes key features of the underlying band structure and the nature of the induced gap.

To quantify the spatial decay of the edge mode, panel (d) plots $\ln n(r)$ for both layers over a range of $t_{\perp}$ values, where $n(r) = [n_{\text{TI}}(r) + n_{\text{SC}}(r)]$ denotes the spatially resolved edge-state density. Solid and dashed lines represent results for the TI and SC layers, respectively. The tails are modeled as exponential decays of the form $n(r) = Ae^{-r/\lambda_{\text{CEM}}}$, where λ_{CEM} is the localization length. This leads to the following relation:

$$\ln n(r) = -\frac{r}{\lambda_{\text{CEM}}} + \ln A. \quad (12)$$

The linear trends in $\ln(n(r))$ confirm this exponential behavior (slope $\propto 1/\lambda_{\text{CEM}}$). With increasing $t_{\perp}$, the slope becomes

steeper, corresponding to the strong localization near the edge. At large $t_{\perp}$, such as $t_{\perp} = 2\Delta_0$, the plots also display an oscillatory modulation superimposed on the decay, indicative of interference effects in the edge-state envelope. Interestingly, the oscillations in the SC and TI layers are shifted, consistent with the spatial shift in the density maxima seen in panel (c).

We further investigate the spatial structure of CEM in strong interlayer coupling regime by analyzing the wavefunction components in the TI layer, for a representative edge state near $E = 0$, as shown in panels (e) and (f). Panel (e) displays the rescaled tails of the wavefunction for several values of $t_{\perp}$, annotated above the panel. These are rescaled by an exponential factor given by $e^{+0.1r}$ to amplify the decay tail. Solid and faded lines correspond to the spin- $\uparrow$ ($u_{r\uparrow}^{\text{TI}}$) and spin- $\downarrow$ ($u_{r\downarrow}^{\text{TI}}$) components, respectively. The wavefunction is rotated by a phase such that the $u_{r\uparrow}^{\text{TI}}$ has only real part and $u_{r\downarrow}^{\text{TI}}$ has only imaginary part; the magnitude of these is shown in the panel. A clear oscillatory pattern emerges in the spatial structure of the wavefunction of these edge-localized states, particularly pronounced in the strong-coupling regime.

To quantify the oscillation behavior, we perform a fast Fourier transform on the spatial profiles and extract the

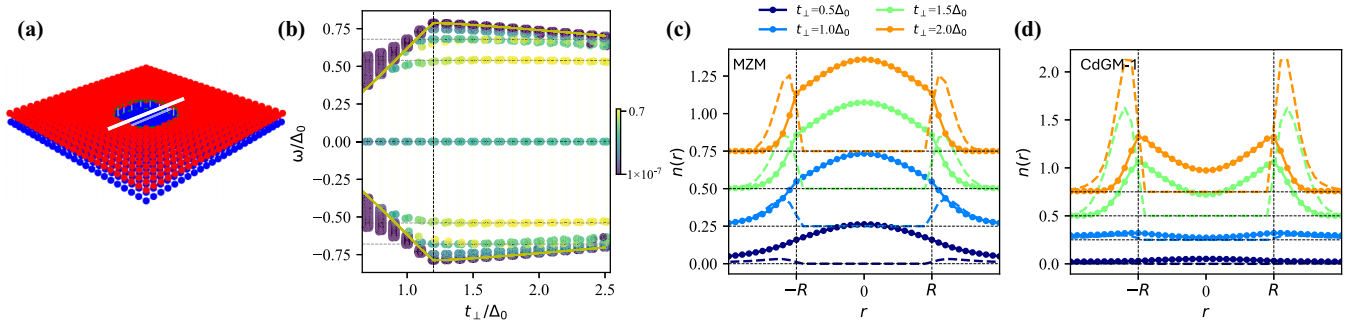


FIG. 5. Nature of Majorana zero mode and Caroli-de Gennes–Matricon states in the bilayer model. (a) Schematic of the bilayer lattice with an antidot created in the superconducting layer, realized by removing the SC layer locally and applying a magnetic field through the antidot region. (b) In-gap vortex-bound states for a set of interlayer couplings $t_\perp$. The color scale indicates the degree of localization in the vortex. Yellow lines show overlay of the proximity-induced gap from Fig. 3(c) ($\lambda = 2m$). (c) Spatial profile of the probability density $n(r)$ for the vortex-localized MZM, shown along a linear cut through the vortex core in the 2D lattice illustrated in panel (a). Solid and dashed lines correspond to the topological insulator and superconductor layers, respectively. (d) Same as panel (c), but for the first excited CdGM state.

dominant frequencies. Panel (f) plots these oscillation frequencies as a function of $t_\perp$ in the regime where PrI gap minimum shifts away from Γ point in the BZ. We observe a monotonic increase in the dominant oscillation frequency with $t_\perp$, consistent with the growing Fermi wave vector k_F shown as the green line in Fig. 3(c). This behavior further confirms that the spatial oscillations of the edge state are directly tied to the underlying momentum-space structure of the hybridized bands. Broadening in frequency trend can be attributed to multiple PrI gap minima across the BZ, leading to interference effects in the real-space profiles. These edge features can be observed as the local density of states by the STM/STS measurements.

The oscillatory decay of the CEMs bears resemblance to the edge-state behavior in the Bernevig-Hughes-Zhang model of a 2DTI, where oscillations in the edge wavefunction emerge when the bulk band structure features a ring of extrema in k space [57]. However, in our case, the presence of multiple bands near the Fermi level introduces additional complexity, leading to richer interference patterns and more intricate spatial structure.

C. In-gap states bound to the antidot

Majorana zero modes can emerge in the core of a vortex that traps a single flux quantum in a topological p -wave superconductor. To model this scenario, we introduce an antidot of radius $R = 10$, where the SC lattice sites are removed within the antidot and trapping a single flux quantum. Details of this construction are provided above in Sec. II A, and the geometry is illustrated in Fig. 5(a). Inside the antidot, only the lattice sites of the 3DTI SS remain, and the flux is confined entirely within this region.

Figure 5 presents the in-gap states localized in the antidot. Two distinct classes of bound states are observed: (1) the Majorana zero mode and (2) the Caroli-de Gennes–Matricon states.

Panel (b) shows the eigenvalue spectrum of in-gap states bound to vortex as a function of the interlayer coupling $t_\perp$. The color bar indicates the degree of localization within the vortex

region: Bright yellow corresponds to states strongly confined to the vortex core, while darker blue denotes more delocalized states. For clarity, edge-localized states have been removed from the plot. Yellow curve represents the bulk gap estimated from the momentum-space model, with the shaded region indicating the corresponding energy window. As expected, the eigenspectrum has a particle-hole symmetry across the zero-energy mode.

We observe two zero-energy states for all $t_\perp$ shown here, exhibiting strong and increasing localization in the antidot, as $t_\perp$ increases, reflected by the shift from blue to yellow. These states are identified as MZMs. Their internal structure, including spin and spatial profiles, is analyzed in detail in subsequent sections.

Within the bulk gap, we find several discrete states that are strongly localized in the vortex core. These states are identified as CdGM modes [58]. The CdGM “number” is assigned according to the energy separation from the MZM. Although they are topologically trivial, they differ qualitatively from CdGM states in a conventional s -wave vortex; the contrasts are examined in detail in the wavefunction analysis section.

The first and second CdGM levels emerge at $t_\perp \simeq 0.8\Delta_0$. The localization in vortex increases with $t_\perp$ characterized by increasing yellow color, and the two levels remain nearly degenerate. Notably, these modes separation from MZM increases with $t_\perp$ while the PrI gap grows, but remain essentially flat once the PrI gap begins to shrink. A third CdGM branch appears at $t_\perp \simeq 0.9\Delta_0$, and their separation from the MZM appears to closely track the PrI gap. Further, this mode localization is strongest when the PrI gap is largest, and diminishes as the PrI gap decreases. Beyond these, additional CdGM states are observed whose energies track evolution of the PrI gap even more closely.

Panel (c) shows probability density $n(r)$ of the MZM in TI $n_{\text{TI}}(r)$ and SC $n_{\text{SC}}(r)$ layers, plotted using solid and dashed lines, respectively, along a spatial cut through the vortex core as indicated in panel (a). In the TI layer, the MZM is sharply localized at center of the antidot, with a pronounced maximum at its core. In contrast, the SC-layer probability density peaks near the antidot boundary. Interestingly, spectral weight in the

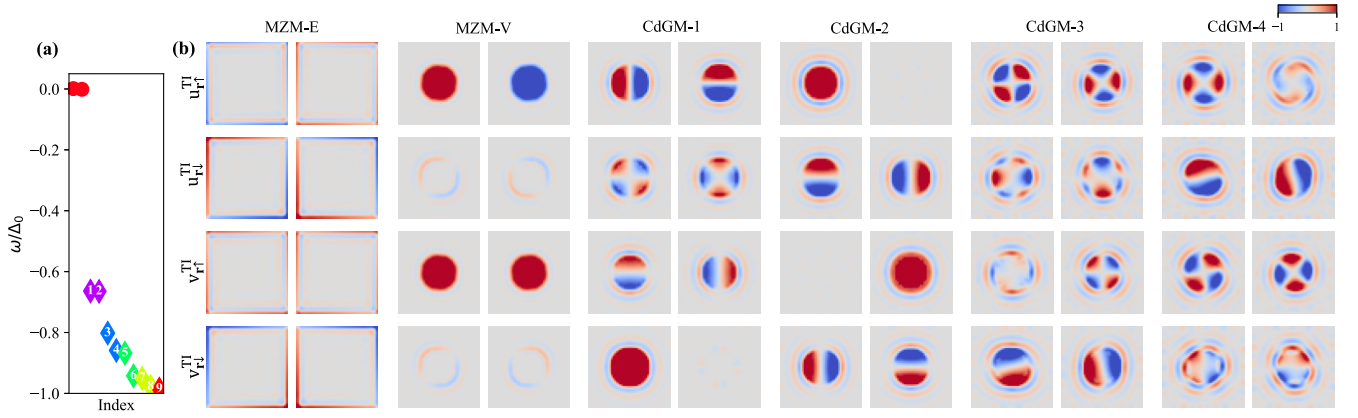


FIG. 6. Wavefunction components of vortex-bound states in the TI layer. (a) Energy spectrum of vortex-bound states near the Fermi level. (b) Spatial profiles of the Bogoliubov-de Gennes wavefunction components ($u_{r\uparrow}^{\text{TI}}, u_{r\downarrow}^{\text{TI}}, v_{r\uparrow}^{\text{TI}}, v_{r\downarrow}^{\text{TI}}$) in the TI layer for the Majorana zero mode and the four lowest-energy states adjacent to it. Each pair of columns corresponds to one eigenstate, with the left and right columns showing the real and imaginary parts of the wavefunction components, respectively. The color scale indicates the spatial amplitude of each component. Results are shown for interlayer coupling $t_{\perp} = 1.5\Delta_0$.

SC layer increases more rapidly with $t_{\perp}$ than the TI layer, consistent with the trend observed in the CEMs, a feature of the enhanced hybridization with increasing $t_{\perp}$.

Panel (d) displays probability density $n(r)$ of first CdGM state for the same spatial cut, again distinguishing between the TI (solid line) and SC (dashed line) layers. In the case of $t_{\perp} = 0.5\Delta_0$, CdGM states are not stabilized within the PrI gap; therefore, the leading state can be understood as a bulk state as can be seen in panel (b). This bulk state has maxima near the antidot center. However, as $t_{\perp}$ increases the CdGM states appear within the PrI gap. The first CdGM (CdGM-1), shown in the panel, is localized at the antidot boundary in both the TI and SC layers.

The distinct spatial profiles of the MZM and first CdGM provide an important signature to distinguish between these two modes realized in the hybrid structure and should be accessible in the local density of states measurement using STM/STS. We further delve into the precise nature of the wavefunction realized in the hybrid system below.

Wavefunction. We now investigate wavefunctions of the in-gap states near zero energy. These are primarily localized in the TI layer, and therefore, we focus on the TI part of the wavefunction, given by $|\Psi_n(\mathbf{r})\rangle \approx (u_{r\uparrow}^{\text{TI}}c_{r\uparrow}^{\dagger} + u_{r\downarrow}^{\text{TI}}c_{r\downarrow}^{\dagger} + v_{r\uparrow}^{\text{TI}}c_{r\uparrow} + v_{r\downarrow}^{\text{TI}}c_{r\downarrow})|0\rangle$, where $\mathbf{r}$ denotes the lattice site index within the TI layer. Numerically, $\Psi_n(\mathbf{r}) = U^{\dagger}\phi_{\mathbf{r}}^{\dagger}$, where $U^{\dagger}$ is the eigenvector of the real-space Hamiltonian [Eq. (4)]. Since the wavefunction is defined up to an arbitrary global phase, we apply a phase rotation to improve visualization.

Figure 6 presents the energy spectrum and the corresponding site-resolved wavefunction components, computed for $t_{\perp} = 1.5\Delta_0$ and using an $L = 51$ lattice size as it allows for better visualization of the wavefunction. For this large $t_{\perp}$, finite-size effects are minimal.

Panel (a) shows the eigenenergies, and panel (b) shows the spatial wavefunction profiles of the two MZMs and selected CdGM states as indexed. In each panel, the first and second columns correspond to the real and imaginary parts of the wavefunction, respectively. Note that the spectrum here shows minor energy differences compared to Fig. 5(b), due to a

reduced system size used here for better visualization, but does not affect the results otherwise.

In the presence of a single flux quantum, the system hosts two degenerate MZMs. These modes can be reorthogonalized into two spatially distinct solutions: (1) an edge MZM (MZM-E) and (2) a vortex MZM (MZM-V), as shown in panel (b). The edge MZM is entirely localized at the lattice's boundary, whereas the vortex MZM is confined within the antidot.

Using the structure of the wavefunctions shown in panel (b), the two Majorana modes localized in the antidot and lattice edge can be expressed as

$$\gamma_V = \sum_{\mathbf{r}} [\chi_V^{\uparrow}(\mathbf{r})(e^{-i\frac{\pi}{4}}c_{r\uparrow}^{\dagger} + e^{+i\frac{\pi}{4}}c_{r\uparrow}) + \chi_V^{\downarrow}(\mathbf{r})(-iY_1^{+}c_{r\downarrow}^{\dagger} + iY_1^{-}c_{r\downarrow})], \quad (13a)$$

$$\gamma_E = \sum_{\mathbf{r}} [\chi_E^{\uparrow}(\mathbf{r})(-ie^{-i\frac{\pi}{4}}c_{r\uparrow}^{\dagger} + ie^{+i\frac{\pi}{4}}c_{r\uparrow}) + \chi_E^{\downarrow}(\mathbf{r})(Y_1^{+}c_{r\downarrow}^{\dagger} + Y_1^{-}c_{r\downarrow})], \quad (13b)$$

where $\chi_V^{\sigma}(\mathbf{r})$ and $\chi_E^{\sigma}(\mathbf{r})$ denote the spin-resolved spatial envelopes for the vortex (V) and edge (E) Majorana zero modes, which are taken to be real. The functions $Y_1^{\pm} = x \pm iy$ represent angular-momentum-based symmetry factors associated with the orbital structure of the states. The gauge choice for γ_V is fixed to satisfy the Majorana condition, and γ_E carries a relative $e^{i\frac{\pi}{2}}$ phase compared to the fermionic part shown in MZM-E wavefunction. In this form, both Majoranas satisfy $\gamma_{E(V)}^{\dagger} = \gamma_{E(V)}$ and the anticommutation relation $\{\gamma_E, \gamma_V\} = 0$.

The vortex MZM has $|\chi_V^{\uparrow}| \gg |\chi_V^{\downarrow}|$, indicating that it is almost fully spin polarized along the direction of the magnetic field. The spin- $\downarrow$ component is negligible in magnitude and exhibits an angular nodal structure, in contrast to the nearly nodeless spin- $\uparrow$ profile. In contrast, the edge Majorana has $|\chi_E^{\uparrow}| < |\chi_E^{\downarrow}|$, indicating a relative spin flip in the edge mode. The identification of the spin-up form of MZM-V offers opportunities to isolate the vortex mode using spin-polarized STM/STS [59].

TABLE I. Angular momentum quantum number l associated with the wavefunctions of in-gap states in the 3DTI SS/SC hybrid vortex system, as illustrated in Fig. 6(b).

	m_J	$u_{\uparrow}^{\text{TI}}$	$u_{\downarrow}^{\text{TI}}$	$v_{\uparrow}^{\text{TI}}$	$v_{\downarrow}^{\text{TI}}$
MZM-V	0	0	1	0	-1
CdGM-1	1	1	2	1	0
CdGM-2	0	0	1	0	-1
CdGM-3	2	2	3	2	1
CdGM-4	-2	-2	-1	-2	-3

Panel (a) displays additional in-gap states, distinct from the MZM, numbered by increasing energy relative to the MZM. Their corresponding wavefunctions are shown in the remaining columns of panel (b), up to the fourth CdGM state (CdGM-4). Because these states lie below the Fermi level, their wavefunctions exhibit a dominant particle component ($|u_n| > |v_n|$), and a clear particle-hole asymmetry is evident in their spatial structure. Notably, all these CdGM states are localized within the vortex core and lack any corresponding edge state, indicating their topologically trivial nature. As a result, they can be fully described by the boundary conditions imposed by the vortex geometry. Importantly, here the first CdGM has a large gap in contrast to the gap between CdGM states, isolating the MZMs. This can be attributed to the missing SC layer within the vortex, and makes it distinct from the topological vortex modes reported in the bulk Fe-based superconductor [24].

The vortex setup considered here possesses rotational symmetry in two dimensions, implying that the total angular momentum operator J_z commutes with Hamiltonian in continuum limit of the lattice. As a result, J_z is a conserved quantity and can be used to label the eigenstates via a good quantum number, denoted by m_J . A variety of angular momentum symmetries consistent with the spatial structure of the numerically computed wavefunctions is summarized in Table I. We find that the wavefunctions shown in panel (b) are consistent with the ansatz:

$$\Psi_{m_J}(r, \varphi) = e^{i(m_J + \frac{1}{2}(\sigma_z - N)\tau_z)\varphi} \Psi_{m_J}(r). \quad (14)$$

Here, σ_z term accounts for the spin-momentum locking in the two spin channels and $N \in \mathbb{Z}$ denotes the vortex number [see Eq. (10)], while τ_z is the third Pauli matrix in particle-hole (Nambu) space. Furthermore, $m_J + (N/2)$ must be half-integer in order to ensure continuity of the wavefunction. The J_z matrix in the TI subspace can be written as $\text{diag}[m_J + (\frac{1}{2} - \frac{N}{2}), m_J + (-\frac{1}{2} - \frac{N}{2}), m_J - (\frac{1}{2} - \frac{N}{2}), m_J - (-\frac{1}{2} - \frac{N}{2})]$. For $N = 1$, $J_z = \text{diag}[m_J, m_J - 1, m_J, m_J + 1]$, with $m_J \in \mathbb{Z}$, is consistent with the results tabulated in Table I. This ansatz is also consistent with the wavefunction reported for an antidot in a simpler model with the proximity-included implicitly in the TI SS Hamiltonian [15,16] and induced topological superconductor in a superconducting nanowire shell [60]. From the ansatz, it is clear that the four TI components in the wavefunction have a well-defined angular symmetry, where $l_{u_{\sigma}}$ and $l_{v_{\sigma}}$ characterize the particle and hole sectors, respectively, in both the spin sectors.

In addition to the distinct angular momentum symmetries, the CdGM states exhibit several features that set them apart from the MZMs.

In particular, CdGM-2 shares the same angular quantum number as the MZM, with $m_J = 0$ in both cases. However, the CdGM-2 mode shows a significantly larger weight in the spin- $\downarrow$ sector, unlike the MZM. Additionally, a mild particle-hole asymmetry is observed, reflected in the unequal amplitudes of the particle (u_n) and hole (v_n) components.

CdGM-1 and CdGM-2, also identified in Fig. 5(b), appear nearly degenerate in energy. This quasidegeneracy persists across all the values of $t_{\perp}$ considered here, indicating that it is intrinsic rather than parameter specific. These two modes are distinguished by their angular quantum numbers: $m_J = 1$ for CdGM-1 and $m_J = 0$ for CdGM-2, confirming their distinct character.

Interestingly, higher-energy modes such as CdGM-1, CdGM-3, and CdGM-4 correspond to increasing $|m_J|$, consistent with their interpretation as higher-order vortex excitations with $m_J = 1, 2$ and 3 , respectively. A defining feature of all these modes is a difference in the angular nodes between the particle-hole sector for the spin- $\downarrow$ components, i.e., $|l_{u_{\downarrow}} - l_{v_{\downarrow}}| = 2$.

In all CdGM modes, there is an angular momentum shift between the spin- $\uparrow$ and spin- $\downarrow$ wavefunctions in both the particle and hole sectors, attributable to spin-momentum locking in the vortex ($|l_{u_{\uparrow}(v_{\uparrow})} - l_{u_{\downarrow}(v_{\downarrow})}| = 1$).

The intricate structure of the CdGM states stands in stark contrast to the in-gap states found in vortices of conventional s -wave superconductors, as will be further elucidated in the discussion on the s -wave case below. This richness arises from the spin-momentum locking inherent to the 3DTI surface, which plays a pivotal role in shaping the vortex-bound states. In particular, it is essential to the ansatz in Eq. (14) for capturing the symmetry structure of the wavefunctions.

Additionally, in-gap states display Friedel-like oscillations outside the antidot boundary, reminiscent of the oscillatory features observed in the CEMs discussed in Fig. 4. These oscillations become increasingly pronounced for in-gap states with energies approaching the bulk continuum, suggesting enhanced interference effects as the quasiparticle wavefunctions become less localized.

Vortex in s -wave superconductor. To better understand the nature of in-gap states in the TI/SC hybrid system and contrast them with those in a conventional s -wave superconductor, we analyze a simplified model consisting solely of the SC lattice described by Eq. (2), incorporating an antidot as illustrated in Fig. 7(a). Unlike the TI/SC hybrid system, in this case, the lattice sites are explicitly included inside the antidot region. Pairing potential is defined by Eq. (10), with $\Delta = 0$ within the antidot, this discontinuity is the defining characteristic that distinguishes the antidot from the surrounding superconducting region.

We explore two cases for the model: (1) without a flux quantum ($\Phi = 0$) and (2) with a flux quantum ($\Phi = \Phi_0$) trapped in the antidot marked by the green line in Fig. 7(a). These setups allow us to explore the spatial dependence and structure of vortex-bound states. Figure 7 presents the results for this analysis. Experimentally, several works have investigated vortex- and impurity-bound states in s -wave

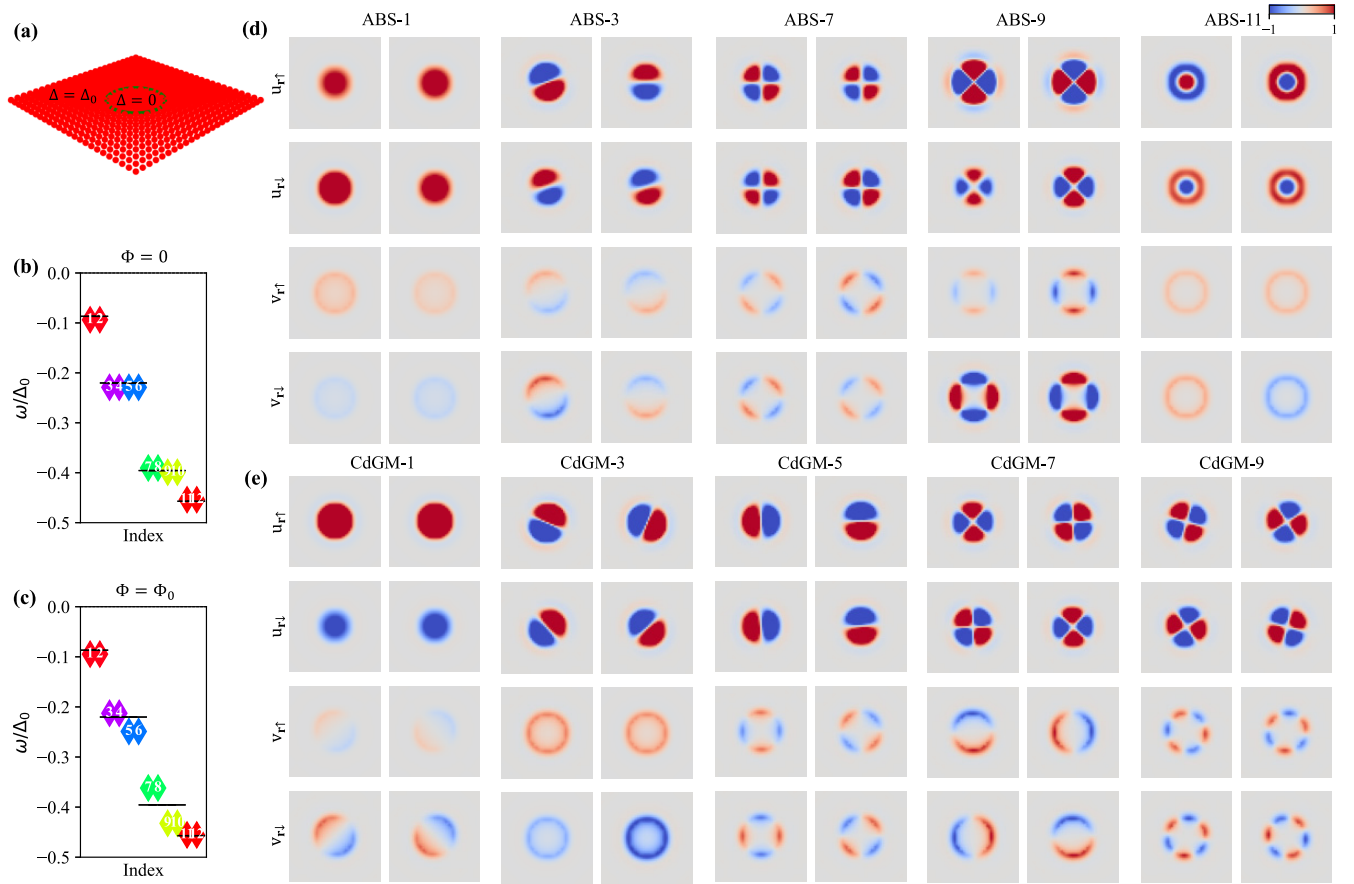


FIG. 7. Vortex in an s -wave superconductor. (a) Schematic of the lattice model with a vortex. (b), (c) In-gap energy spectra of the superconducting layer without magnetic flux ($\Phi = 0$) and with a single flux quantum ($\Phi = \Phi_0$). Black lines denote eigenenergies of free particles confined in a disk-shaped infinite potential well given by Eq. (15). (d), (e) Real (left) and imaginary (right) parts of the Bogoliubov-de Gennes wavefunction components ($u_{r\uparrow}$, $u_{r\downarrow}$, $v_{r\uparrow}$, $v_{r\downarrow}$) for representative vortex-bound states from panels (b) and (c). The color scale indicates the spatial amplitude of each component.

superconductors [61,62], though a detailed comparison of the vortex state structure remains limited in the literature. Theoretical works comparing the vortex-bound states in the TI/SC hybrid to such states in a 2D SC layer have focused on Abrikosov vortices [15] and on antidot-based vortices in the regime of $k_F \gg R^{-1}$ [16], distinct from the $k_F \approx 0$ regime considered here.

Panel (b) shows the energy spectrum of antidot-bound states in the lattice model for the zero-flux case ($\Phi = 0$), with eigenstates marked by diamond symbols and indexed by increasing energy relative to the Fermi level.

The spectrum exhibits clear signatures of quantization consistent with rotational symmetry. These states can be understood using an approximate continuum model describing a free particle of effective mass m_b confined within a disk of radius R , where the confinement is provided by the superconducting gap Δ_0 , under the condition that the normal-state bands [see Fig. 2(a)] lie entirely within the superconducting gap, i.e., $\omega_{SC}(\mathbf{k} \rightarrow \Gamma) = |\mu - \varepsilon_{SC} - 4t_{SC}| \ll |\Delta_0|$. Under this condition, the particle and hole branches in the Nambu picture do not overlap and we can effectively describe the wavefunction by a single component.

The quasiparticle states in this geometry satisfy a second-order differential equation, with solutions of the form

$\Psi_b(r, \varphi) = \mathcal{R}(r) e^{il\varphi}$, where l is the angular momentum quantum number. Solutions of the equation for radial wavefunction $\mathcal{R}(r)$ are Bessel functions $\mathcal{J}_l(kr)$. Imposing the boundary condition $\mathcal{J}_l(kR) = 0$ at the disk edge leads to a discrete set of allowed energy modes given by

$$E_b^{nl} = \frac{\hbar^2}{2m_b} \frac{x_{nl}^2}{R^2}, \quad (15)$$

where x_{nl} is the n th zero of the Bessel function $\mathcal{J}_l(kr)$. The levels given by Eq. (15), shown as short black lines in panel (b), agree well with the lattice results using a fitted prefactor $\frac{\hbar^2}{(2m_b R^2)} = 0.015\Delta_0$ (see Appendix B for details). In our lattice model in the limit $\mathbf{k} \rightarrow \Gamma$, the particle trapped in the antidot has the dispersion given by $|\omega_{SC}(\mathbf{k}, \Delta_0 = 0)| \approx t_{SC}|\mathbf{k}|^2$. Using the relation $\hbar|\mathbf{k}|^2/(2m_b) = t_{SC}|\mathbf{k}|^2$ leads to $\hbar^2/(2m_b R^2) = t_{SC}/R^2 \approx 0.02\Delta_0$, very close to the prefactor value used above. The minor difference can be attributed to the finite SC gap used in the lattice model.

The solutions presented in panel (b) correspond to x_{10} (states 1 and 2), x_{11} (3, 4, 5, and 6), x_{12} (7, 8, 9, and 10), and x_{20} (11 and 12). The red, magenta/blue, and green points correspond to angular momentum quantum numbers $l = 0, \pm 1, \pm 2$ for the first radial mode ($n = 1$). The $l = 0$

TABLE II. Angular momentum quantum number l associated with the wavefunctions of in-gap states in a vortex hosted by an s -wave superconductor, shown for the cases with zero flux ($\Phi = 0$) and finite flux ($\Phi = \Phi_0$), as illustrated in Figs. 7(d) and 7(e).

ABS	m_J	$u_\uparrow$	$u_\downarrow$	$v_\uparrow$	$v_\downarrow$	CdGM	m_J	$u_\uparrow$	$u_\downarrow$	$v_\uparrow$	$v_\downarrow$
ABS-1	1/2	0	0	0	0	CdGM-1	0	0	0	-1	-1
ABS-3	3/2	1	1	1	1	CdGM-3	1	1	1	0	0
ABS-7	5/2	2	2	2	2	CdGM-5	-1	-1	-1	-2	-2
ABS-9	5/2	2	2	2	2	CdGM-7	2	2	2	1	1
ABS-11	1/2	0	0	0	0	CdGM-7	-2	-2	-2	-3	-3

states are twofold degenerate due to spin, while $l \neq 0$ states are fourfold degenerate due to combined spin and orbital symmetries. Higher radial modes, such as the $n = 2$ states, also appear, with the subsequent red points representing $n = 2$, $l = 0$.

Panel (c) shows the energy spectrum of the vortex-bound states in the lattice model with finite magnetic flux ($\Phi = \Phi_0$), indicated by diamond symbols. For reference, the eigen-spectrum of the corresponding particle in a disk continuum model is overlaid. In the presence of flux, the previously fourfold-degenerate states split into twofold-degenerate pairs. The $l = 0$ states retain their twofold degeneracy due to spin, while states with nonzero angular momentum ($l \neq 0$) exhibit reduced degeneracy, twofold marking a clear departure from the fourfold degeneracy observed in the zero-flux case. This lifting of degeneracy originates from flux-induced splitting of the orbital angular momentum sectors: the magnetic field breaks time-reversal symmetry and couples directly to orbital, but not spin, degrees of freedom. The physical origin and implications of this behavior are further elaborated below.

Panels (d) and (e) show the corresponding wavefunctions from the lattice model for the vortex configurations with zero flux ($\Phi = 0$) and finite flux ($\Phi = \Phi_0$), respectively. Each column is labeled by the associated state number. As in previous figures, the left and right columns display the real and imaginary parts of the wavefunctions, respectively. The rich angular symmetries evident in these panels and tabulated in Table II are consistent with the ansatz for the vortex-bound wavefunctions [15,16,58]. Incorporating the conserved total angular momentum quantum number m_J , the wavefunction can be expressed as

$$\Psi_{m_J}(r, \varphi) = e^{i(m_J + \frac{1}{2}(-\mathbb{I} - N)\tau_z)\varphi} \Psi_{m_J}(r), \quad (16)$$

where φ is the polar angle, τ_z acts on the particle-hole space, and N encodes the flux number. Similar to the TI/SC case, $m_J + (N/2)$ is half of an odd integer. This form captures the angular behavior consistent with the observed numerical solutions. Importantly in this case, spin symmetry is preserved ($|l_{u_\uparrow(v_\uparrow)} - l_{u_\downarrow(v_\downarrow)}| = 0$) in contrast to the spin locking in the TI/SC interface case.

In the zero-flux case, the in-gap states can be interpreted as Andreev bound states confined within the normal region by the surrounding superconducting gap. These bound states are discrete solutions of a confined geometry, with wavefunctions shaped by the antidot boundary conditions.

Panel (d) shows the spatial profiles of these wavefunctions, with each column labeled by the ABS index corresponding to its energy level. One representative state from each

degenerate multiplet below the Fermi level is shown. The angular structure of these states is fully captured by the ansatz in Eq. (16), which reflects the disk geometry and associated angular momentum classification.

Interestingly, the radial profiles reveal an asymmetry between particle and hole components: The particle sector resembles a Bessel function $\mathcal{J}_l(kR)$, while the hole sector appears shifted and resembles $\mathcal{J}_{l+1/2}(kR)$. This subtle difference results in radial phase shifts between u_n and v_n . Nevertheless, no angular asymmetry is observed between the two sectors, consistent with preserved spin degeneracy in the absence of spin-orbit coupling. Additionally, the hole amplitude remains suppressed relative to the particle component, as expected from the bound-state condition $|u_n| > |v_n|$ for states below the Fermi level.

We next examine how the vortex-bound states change upon introducing a single magnetic flux quantum ($\Phi = \Phi_0$), where the in-gap states can be understood as CdGM states, for which the spectrum is shown in panel (c). The corresponding energy wavefunctions are shown in panel (e) with the label for the CdGM indexed on each column. Again, Eq. (16) fully captures the angular symmetry realized in the continuum limit of the lattice. The particle and hole sector radial dependence show the behavior akin to zero-flux case. However, a key difference emerges in the angular behavior: A mismatch of $\Delta l = 1$ is observed between the particle and hole sectors, reflecting the phase winding introduced by the magnetic field in the vortex. The spin-resolved wavefunctions remain aligned ($\Delta l = 0$), preserving the spin symmetry, as the spin does not directly couple to the flux. Here too, states below the Fermi level continue to exhibit dominant particle components ($|u_n| > |v_n|$).

These results highlight the qualitatively distinct nature of in-gap states in conventional s -wave superconductors compared to systems exhibiting emergent p -wave pairing. Our spatial and spectral analysis underscores the unique fingerprints of topological superconductivity in engineered heterostructures, providing a robust framework for interpreting future experiments on vortex-bound states and unconventional pairing mechanisms.

D. Single-layer model: SC layer integrated out

Here, we discuss routes to use an effective single-layer model [50,51], in which the SC layer is integrated out. The Hamiltonian is given by

$$H_{\text{eff}} = H_{\text{TI}} + \sum_{\mathbf{r}} (\Delta_{\text{eff},\mathbf{r}} \psi_{\mathbf{r}}^\dagger \sigma_y \psi_{\mathbf{r}}^\dagger + \text{H.c.}). \quad (17)$$

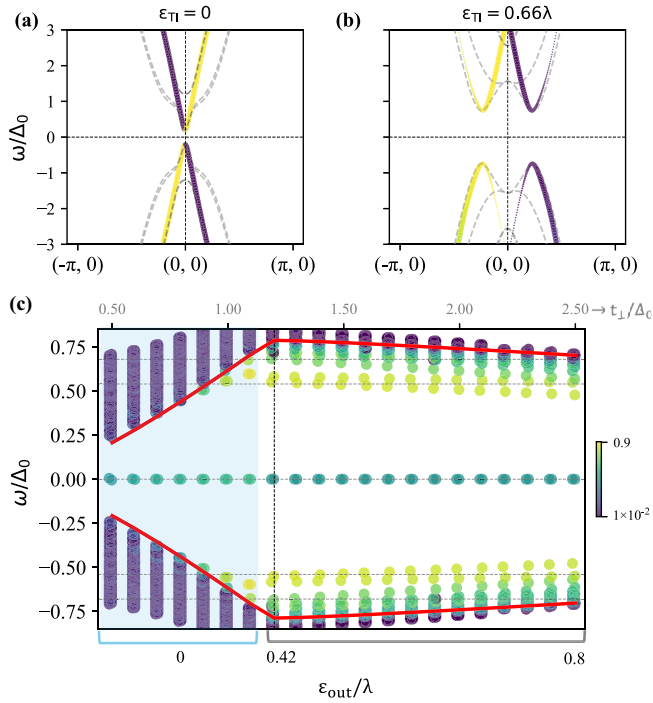


FIG. 8. Single-layer model. (a), (b) Band structures for $\varepsilon_{\text{TI}} = 0$ and 0.66λ for $\Delta_{\text{eff}} = 0.2\Delta_0$ and $0.74\Delta_0$. Yellow (blue) color denotes the spin polarization parallel (antiparallel) to y direction. Dashed black lines are overlays from the respective bilayer model. (c) Spectrum for the in-gap states evaluated using a single-layer model with an antidot trapping a single magnetic flux quantum, for comparison with Fig. 5(b). The chiral edge states are removed. Red lines indicate the PrI gap (Δ_{PrI}) and values on the top of panel are the corresponding $t_{\perp}/\Delta_0$ values from the bilayer model. Shaded blue region marks states when the band minima are at Γ point; the remaining data show states for the minima away from Γ , simulated by changing ε_{TI} outside the vortex (ε_{out}), as indicated below the panel.

Here, H_{TI} is the 3DTI SS Hamiltonian given by Eq. (1) and $\Delta_{\text{eff},r} = \Delta_{\text{eff}}$ is the effective pairing used in the model. Same as in the bilayer model, we use $\Delta_{\text{eff}} = 0$ inside the antidot and a finite Δ_{eff} outside the vortex, given by Eq. (10). $\Delta_{\text{eff}} = \Delta_{\text{PrI}}$ is used to reproduce the characteristics of the bilayer model discussed above. The results of the effective single-layer model are shown in Fig. 8. Depending on the location of the band extrema in the bilayer model, a different corresponding parametrization scheme of the single-layer model is necessary. To achieve the agreement between the two models, ε_{TI} may attain different values inside the antidot (ε_{in}) and outside of it (ε_{out}).

(1) *Minimum at Γ .* In the single-layer model, setting $\varepsilon_{\text{in/out}} = 0$ ensures that the band minimum remains fixed at the Γ point. This behavior mimics the bilayer model in the regime of low interlayer tunneling strength ($t_{\perp}$), where the PrI gap also exhibits its minimum at Γ , as shown in Fig. 3(c). Since the PrI gap in the bilayer model depends on $t_{\perp}$, we incorporate this effect into the single-layer model by replacing the intrinsic pairing potential with an effective value, $\Delta_{\text{eff}} \equiv \Delta_{\text{PrI}}$. Panel (a) compares the band structure obtained from the single-layer model (thick lines) using $\Delta_{\text{eff}} = 0.2\Delta_0$ to the bilayer result (black dashed line) at $t_{\perp} = 0.5\Delta_0$, which yields

$\Delta_{\text{PrI}} = 0.2\Delta_0$. The good agreement confirms the validity of this effective model approximation.

Panel (c) presents the spectrum of in-gap states in the single-layer model with an antidot trapping a magnetic flux. The shaded blue region highlights results where the band minimum is constrained to the Γ point by setting $\varepsilon_{\text{in/out}} = 0$, while the effective pairing Δ_{eff} is matched to the PrI gap extracted from the bilayer model. Red line indicates the PrI gap as a function of $t_{\perp}$ from the bilayer calculation. Horizontal axis corresponds to different values of $t_{\perp}/\Delta_0$ ranging from 0.5 to 1.1. This simplified model reproduces the MZM-CdGM energy gap observed in the full bilayer calculation [see Fig. 5(b)] with remarkable accuracy.

(b) *Minima at finite $\mathbf{k}$.* A band structure with minima at finite $\mathbf{k}$ in the BZ can be realized in the single-layer model by tuning the on-site energy ε and adjusting it to match the finite- $\mathbf{k}$ minimum observed in the bilayer model, as shown in Fig. 3(c). To reproduce the PrI gap, we again set $\Delta_{\text{eff}} = \Delta_{\text{PrI}}$. Panel (b) displays the resulting band structure from the single-layer model (thick lines), using $\Delta_{\text{eff}} = \Delta_{\text{PrI}} = 0.74\Delta_0$ and $\varepsilon_{\text{TI}} = 0.66\lambda$, chosen to simulate the bilayer model with $t_{\perp} = 2\Delta_0$ (black dashed line). The excellent agreement at low energies confirms the efficacy of this mapping.

Panel (c) outside the blue-shaded region shows the in-gap states in the single-layer model for a vortex trapping a magnetic flux. These states are computed using $\varepsilon_{\text{in}} = 0$ and ε_{out} varied from 0.42λ to 0.8λ , as labeled along the horizontal axis. This choice reflects the physical setting of the bilayer model, where the 3DTI SS layer inside the antidot remains unaffected due to the absence of the superconducting layer in that region. This mapping captures the bilayer behavior for $t_{\perp}/\Delta_0$ ranging from 1.2 to 2.5.

Overall, the single-layer model reproduces the in-gap spectra of the bilayer system with good fidelity, though some differences emerge. In particular, for $t_{\perp} = 1.2\Delta_0$, a mild discontinuity is observed compared to the bilayer case. Additionally, the lowest CdGM mode shifts toward the MZM as ε_{out} increases (i.e., as the PrI gap decreases), in contrast to the bilayer case where this mode remains nearly constant.

IV. CONCLUSIONS

To summarize, we have introduced a bilayer model for exploring the interface between of a 3DTI SS and 2D s -wave superconductor motivated by the recent Fe(Te, Se)/Bi₂Te₃ heterostructure [45]. By systematically varying the interlayer tunneling ($t_{\perp}$), we investigated evolution of the PrI gap, the formation of CEMs, and the emergence of in-gap states, including MZMs and CdGM states.

Our results demonstrate that interlayer hybridization fundamentally reshapes the low-energy spectrum. Explicit inclusion of the superconducting layer, beyond the Fu-Kane model [2], contributes nontrivially to edge-state localization and spin texture, particularly in the strong-coupling regime. Increasing $t_{\perp}$ shifts the PrI gap away from the Γ point, leading to a Mexican-hat dispersion in the vicinity of the gap in contrast to a dispersion with a single minimum for the case of Γ point. At the edge, this leads to a finite Fermi momentum and Friedel-like oscillations in the spatial profiles of the in-gap chiral edge states. These findings open opportunities for

experimental exploration for the two cases via STM/STS in both the interior of the proximitized TI surface and the boundaries between superconducting and magnetic regions of the 3DTI surface.

By introducing an antidot to emulate a vortex, we examined the resulting in-gap spectrum and identified robust MZMs localized at both the system boundary and vortex core. The energy spacing between MZMs and CdGM states is significantly enhanced at large $t_{\perp}$, driven by suppressed density of states in the SC layer near the antidot. Spin-resolved wavefunction analysis further reveals angular momentum shifts in the CdGM states absent in conventional s -wave systems, highlighting the emergent p -wave character of the bilayer system. A direct comparison with a standalone s -wave superconductor confirms that in-gap states in the bilayer exhibit qualitatively distinct spatial and spectral signatures due to the interplay of topology and proximity effects. These results provide practical criteria for discriminating MZMs from CdGM excitations via spin-resolved STM/STS and for distinguishing the heterostructure response from that of a conventional s -wave superconductor. Notably, the removal of the SC layer within the antidot produces a much larger MZM-CdGM separation than in bulk Fe-based superconductors [24], providing practical routes for isolating MZMs in spectroscopic measurements.

We further introduced an effective single-layer mapping that captures key features of the bilayer system, including the vortex spectrum and gap evolution, while reducing computational complexity and providing a useful framework for qualitative exploration of vortex physics beyond the Fu-Kane picture.

Together, these findings offer a microscopic understanding of the role of interlayer coupling in topological SC-3DTI heterostructures and provide experimentally relevant predictions for tuning and identifying Majorana modes. This work establishes a foundation for future explorations of topological superconductivity in engineered interfaces, including investigations of disorder effects, braiding protocols, and the impact of additional symmetry-breaking perturbations.

Our work is also relevant to further investigate the role of a “topological proximity effect,” as reported in Bi/TiBiS₂ heterostructures [63]; the surface bands of a 3DTI can migrate to an attached metallic layer. This effect could also lead to the topological superconductivity when the attached metal undergoes a superconducting transition. In principle, both the superconducting proximity effect and the topological proximity effect should exist in any hybrid structures consisting of a topological insulator and a superconductor, and the relative strength between the two proximity effects is controlled by the hybridization strength between the two constituent systems.

Finally, our work motivates future first-principles investigations of Fe(Te, Se)/Bi₂Te₃ and related heterostructures. Incorporating realistic materials parameters will enable material-specific predictions for the nature of PrI gap, the stability of in-gap vortex states, and ultimately the conditions for robust MZMs.

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DATA AVAILABILITY

The data that support the findings of this article are not publicly available. The data are available from the authors upon reasonable request.

APPENDIX A: PHASE FACTORS

In the presence of a vector potential, both electron hopping and the SC pairing potential acquire phase factors. Since different notations have been used in the literature, here we summarize our choice of phase factors based on the gauge transformation.

To incorporate the effect of magnetic flux, the vector potential $\mathbf{A}$ must satisfy the constraint $\oint \mathbf{A} \cdot d\mathbf{l} = \frac{\hbar}{e} \Phi$, where Φ is the enclosed flux. Here, we have set speed of light $c = 1$. This result introduces a Peierls phase in the hopping term, such that $c_{\mathbf{r}}^{\dagger} c_{\mathbf{r}'} \rightarrow e^{i\Phi_{\mathbf{r}\mathbf{r}'}} c_{\mathbf{r}}^{\dagger} c_{\mathbf{r}'}$, where $\Phi_{\mathbf{r}\mathbf{r}'} = -\frac{e}{\hbar} \int_{\mathbf{r}}^{\mathbf{r}'} \mathbf{A}(\mathbf{s}) \cdot d\mathbf{s}$.

Under a local U(1) gauge transformation characterized by a scalar field $\chi(\mathbf{r})$, the vector potential transforms as $\mathbf{A}'(\mathbf{r}) = \mathbf{A}(\mathbf{r}) + \nabla\chi(\mathbf{r})$. Correspondingly, the fermionic and pairing fields transform as

$$c_{\mathbf{r}} \rightarrow e^{i\chi(\mathbf{r})} c_{\mathbf{r}}, \quad (\text{A1})$$

$$\Delta_{\mathbf{r}} \rightarrow e^{2i\chi(\mathbf{r})} \Delta_{\mathbf{r}}. \quad (\text{A2})$$

Under these transformations, the BdG Hamiltonian remains gauge invariant.

Importantly, the net magnetic flux must vanish outside the vortex region [64]. This condition requires that the transformed vector potential satisfies $\oint \mathbf{A}'(\mathbf{r}) \cdot d\mathbf{l} = 0$ when integrated around the entire system. Applying this to the gauge-transformed vector potential leads to

$$\oint \nabla\chi(\mathbf{r}) \cdot d\mathbf{l} = -\oint \mathbf{A} \cdot d\mathbf{l}. \quad (\text{A3})$$

This implies a specific structure for the scalar field:

$$\chi(r, \varphi) = -N\varphi + \chi_0, \quad (\text{A4})$$

where $\chi(r, \varphi)$ depends only on the polar angle φ . The integer winding number N corresponds to the number of flux quanta trapped in the vortex, and its sign reflects the direction of the magnetic field.

APPENDIX B: SOLUTION FOR A PARTICLE BOUND TO THE VORTEX

We now analyze the wavefunction under disk-shaped boundary conditions. The surrounding superconductor induces a finite gap in the system, allowing the central nonsuperconducting region to be treated as an antidot that hosts bound states.

In our model, the energy scale of the normal-state dispersion in the antidot region, given by $\omega_{\text{SC}}(\mathbf{k} \rightarrow \Gamma, \Delta = 0)$, satisfies $|\omega_{\text{SC}}| \ll |\Delta_0|$, where Δ_0 denotes the superconducting gap. This condition ensures that the particle and hole branches in Nambu space have small overlap and we can effectively describe the wavefunction by a single component. At the same time, the normal region acts as an effective potential well for quasiparticle confinement, supporting discrete in-gap states localized within the antidot.

In the presence of a magnetic field in the antidot, the momentum operator is given by $\mathbf{p} \rightarrow -i\hbar\nabla + |e|\mathbf{A}(\mathbf{r})$, and the Schrödinger equation with the particle mass m_b is given by

$$\left[\frac{1}{2m_b} (-i\hbar\nabla + |e|\mathbf{A}(\mathbf{r}))^2 + V(\mathbf{r}) \right] \psi(\mathbf{r}) = E_b \psi(\mathbf{r}). \quad (\text{B1})$$

In polar coordinates, $\mathbf{A}(\mathbf{r}) = A_r \hat{\phi}$, and the above equation simplifies to

$$\left[-\frac{\hbar^2}{2m_b} \frac{1}{r^2} \left\{ r \frac{\partial}{\partial r} \left(r \frac{\partial}{\partial r} \right) + \frac{\partial^2}{\partial \varphi^2} \right\} + \frac{1}{2m_b} e^2 A_r^2 - 2i\hbar |e| A_r \frac{1}{2m_b} \frac{1}{r} \frac{\partial}{\partial \varphi} \right] \psi(r, \varphi) = E_b \psi(r, \varphi). \quad (\text{B2})$$

We assume a separable solution $\psi(r, \varphi) = \mathcal{R}(r)e^{il\varphi}$ and use the form of vector potential inside the vortex. Substituting this in the Schrödinger equation leads to the radial part given by

$$r^2 \frac{\partial^2 \mathcal{R}(r)}{\partial r^2} + r \frac{\partial \mathcal{R}(r)}{\partial r} + \left\{ r^2 k^2 - \left(l + \frac{|e|A_r r}{\hbar} \right)^2 \right\} \mathcal{R}(r) = 0. \quad (\text{B3})$$

Here, $k = \frac{1}{\hbar} \sqrt{2m_b E_b}$ and l is the orbital angular momentum of the bound particle, as the system has the rotational symmetry.

The vector potential in polar coordinate for magnetic field along z is

$$A_r = \begin{cases} \frac{r}{2\pi R^2} \Phi, & \text{for } r \leq R, \\ \frac{1}{2\pi r} \Phi, & \text{for } r > R. \end{cases} \quad (\text{B4})$$

As in the main text, we consider $\Phi = N\Phi_0$. Using the form of the vector potential, the solution for the radial part is given by

$$l' = \begin{cases} l + \frac{|e|}{2\pi\hbar} \left(\frac{r}{R} \right)^2 \Phi, & \text{for } r \leq R, \\ l + \frac{|e|}{2\pi\hbar} \Phi, & \text{for } r > R. \end{cases} \quad (\text{B5})$$

In the absence of a magnetic field ($N = 0$, i.e., $\Phi = 0$), the solutions to the radial Schrödinger equation correspond to the roots of the Bessel function, $\mathcal{J}_l(kr)$, since $l' = l$ in this case. To satisfy the boundary condition that the wavefunction vanishes at the vortex edge ($r = R$), the allowed wave vectors are quantized as $kR = x_{nl}$, where x_{nl} is the n th zero of $\mathcal{J}_l(kr)$. The corresponding bound-state energies are given by

$$E_b^{nl} = \frac{\hbar^2}{2m_b} \frac{x_{nl}^2}{R^2}. \quad (\text{B6})$$

For zero flux, the $l = 0$ state yields a nondegenerate energy level, while states with $l > 0$ exhibit twofold degeneracy due to rotational symmetry.

Figure 7(b) compares these analytic energy levels from Eq. (B6) with numerical results obtained from a lattice model of the SC layer hosting an antidot with radius $R = 10$. To match the continuum results with the lattice data, we use $\hbar^2/(2m_b R^2) = 0.015\Delta_0$ as a fitting parameter.

This bound-state picture accurately captures the in-gap states of the lattice model, with the exception of an additional twofold spin degeneracy that is explicitly included in the lattice formulation but is absent in the scalar continuum model considered here.

As a result, all the lattice model eigenenergies show at least twofold degeneracy due to spin. For $l \neq 0$, a further twofold degeneracy appears, consistent with the Bessel-function solutions in the zero-flux ($\Phi = 0$) limit.

For the finite-flux case ($N = 1$), the analysis becomes more subtle due to the modified differential equation governing the system, as can be seen from Eq. (B5). Outside the vortex core, the solutions remain Bessel functions but with a shifted angular momentum index, reflecting the presence of magnetic flux. Inside the vortex, however, the solutions deviate from standard Bessel functions. Nonetheless, inside the antidot $r < R$, and limiting the $l < l' < l + 1$, with larger contribution from the antidot boundary. For simplicity assuming the mean radial distance $\langle r \rangle \rightarrow R$, the solutions in that region can therefore be approximately described by Bessel functions. Importantly, the degeneracy associated with the angular momentum quantum number l is lifted for $l \neq 0$, consistent with the breaking of time-reversal symmetry by the magnetic field threading the vortex.

Figure 7(c) compares these analytical predictions with the eigenenergies obtained from the lattice simulation of the SC layer containing an antidot with radius $R = 10$ and a magnetic flux quantum Φ . The results clearly demonstrate the lifting of degeneracy for finite l values, as expected from the theoretical considerations above.

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