

Time-reversal symmetric topological superconductivity in Machida-Shibata lattices

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Recent experiments engineered special spin-degenerate Andreev bound states in atomic cages of adatoms on superconductors, the Machida-Shibata states, a promising building block for quantum matter. Here, we investigate the formation of time-reversal symmetric bands by hybridizing multiple such states and analyzing their electronic topological properties assuming small on-site electron repulsion. The low-energy theory shows that competing emerging singlet and triplet superconducting pairings drive the formation of topologically nontrivial phases in symmetry class DIII. Therefore, we predict that Kramers pairs of Majorana zero modes will appear at the ends of Machida-Shibata chains, while two-dimensional lattices will host helical Majorana edge modes. Additionally, we discover extended regions in the Brillouin zone with vanishing superconducting pairings, which are lifted by the repulsive electron interactions. Our findings offer new perspectives for manipulating topological superconductivity and pairings in nonmagnetic adatom systems.

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I. INTRODUCTION

Topological superconductivity has been a subject of an immense amount of research motivated by the potential technological impact of topological protection and non-Abelian effects [1,2], particularly in platforms that potentially host Majorana modes [3–7]. The initial momentum of the field was generated by the observation of zero-bias peaks in nanowires proximitized by superconductors [8,9], a path that recently faced challenges due to impurities leading to ambiguities [10,11]. On the other hand, adatoms deposited on clean superconducting surfaces provide unprecedented control over system purity and hints for a plethora of time-reversal symmetry-breaking phases, including quantum spin systems [12,13], topological nodal point superconductivity [14], localized Majorana zero modes in one-dimensional (1D) artificial magnetic chains [15,16], and propagating chiral Majorana modes in 2D magnet-superconductor hybrids [17,18].

A central objective of this study is to propose a platform for realizing topological superconductivity in symmetry class DIII [19–21]. Atoms with magnetic anisotropy, when deposited on superconductors, induce spin-polarized electronic Yu-Shiba-Rusinov (YSR) states [22–24], which serve as building blocks for constructing topological superconductors. Yet, the realization of nontrivial topological phases in time-reversal-symmetric adatom systems remains experimentally elusive. For adatom species with negligible magnetic polarization, the predicted electronic spin-degenerate in-gap states [25] are typically energetically close to the coherence peaks, and thus can typically be neglected [26].

However, recent experiments have emphasized the significance of such bound states, the so-called Machida-Shibata states (MSSs), by assembling adatoms in spatially tunable atomic cages and controlling their energy as particle-in-a-box states [27–29], first demonstrated in Ag quantum corrals deposited on thin Ag(111) islands grown on superconducting Nb(110) [27]. In principle, MSSs can be realized in all superconductor-metal or -alloy composites with a Shockley state extending over their surfaces [30–32]. Additionally, manifestations of MSSs are reported in transmon qubit Josephson junctions [33,34], and similar hybridized states have been realized in Andreev molecule setups [35,36]. The MSS, albeit spatially extended, constitutes a tunable nonmagnetic analog to the YSR state and opens possibilities for engineering distinct time-reversal-symmetric topological phases.

In this manuscript, we investigate the topological electronic phases of MS bands formed by coupling multiple MSSs via indirect tunneling processes to a common bulk. To this end, we adapt the Green's function techniques developed for magnetic adatom systems [37–39]. Since time-reversal symmetry is naturally preserved, the MS bands belong to symmetry class DIII, in contrast to Shiba bands, which belong to symmetry class D due to the magnetic impurities [40]. Achieving topologically nontrivial phases in class DIII by proximity-induced superconductivity from the *s*-wave parent superconductor alone is impossible to achieve due to the no-go theorem of Ref. [41]. Yet, in the presence of small repulsive electron interactions inside the corrals that break this prerequisite, we demonstrate that the MS bands can intersect the Fermi energy, leading to topologically nontrivial phenomenology. Regarding experimental signatures, the MS bands show no sensitivity to the spin-polarization of differential conductance STM measurements, in contrast to Shiba bands, and they accommodate distinct Kramers' protected double Majorana features in 1D and helical propagating

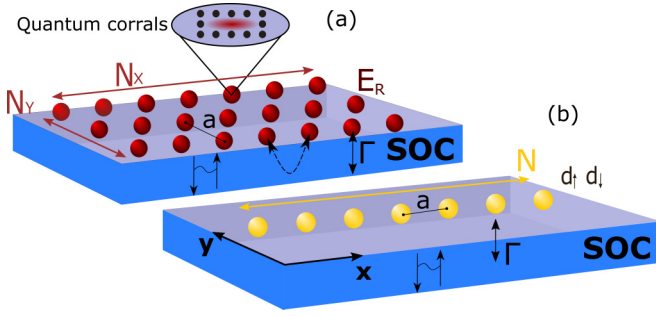


FIG. 1. Setup: Adatom manipulation on the surface of a superconductor (blue) with Rashba spin-orbit coupling (SOC) constructs arrays of quantum corrals and induces Machida-Shibata states. Each state is described by localized spinful electronic levels (here called d-levels) with energy E_R (red and yellow spheres), which are coupled via a common bulk. Geometries: (a) square lattice with lattice constant a ($N_x \times N_y$ sites) and (b) one-dimensional N -site chain.

Majorana modes in 2D. Nontrivial phases in this class require unconventional superconducting correlations and a $SU(2)$ -spin symmetry-breaking mechanism [41–44], which in our case is achieved by nonvanishing Rashba spin-orbit coupling (SOC) in the superconducting bulk. Physically, the Rashba SOC is motivated by the crystal inversion symmetry breaking in the direction perpendicular to the host material's surface in combination with spin-orbit coupling in the atomic levels [45]. For more complex materials, such as Bi/Ag(111) surface alloys, structural anisotropies on the confinement surface lead to additional unconventional Rashba bands and an emerging singlet-triplet superconducting order parameter competition [46–48].

We describe the microscopic theory and derive the effective low-energy four-band Hamiltonian to demonstrate a competition between the emergent singlet and triplet superconducting couplings, which dictates the spectral gap closings and, thus, the topological phases of the system. Subsequently, we consider one- and two-dimensional lattices of MSSs, see Fig. 1, and picture the boundary modes and their spatial profiles. By tuning physical parameters such as the on-site MS energy and SOC strength, we construct phase diagrams that accommodate trivial and nontrivial phases. We investigate the effect of repulsive Coulomb interactions using a mean-field theory, and we demonstrate that they are the essential element for making the induced singlet parameter non-semi-definite and allowing nontrivial phases to appear when all couplings are considered. Additionally, we find extended regions in the Brillouin zone where both the singlet and triplet superconducting order parameters become flat and vanish in 1D chains of MSSs when a 2D superconductor plays the role of the substrate. Notably, we observe cusplike features in the effective pairing amplitudes, akin to those predicted in YSR systems [40]. Thereby, our work draws attention to the topological properties and applications of nonmagnetic adatom lattices on superconductors.

II. MICROSCOPIC DESCRIPTION

We describe the MSSs by a superconducting Anderson model for localized electrons. This neglects the spatial structure of the MSS inside the corrals but faithfully captures

their essential characteristics, namely their energetic position and particle-hole asymmetry [27,29]. We extend this approximation to multiple coupled quantum corrals on a lattice described by electron annihilation operators $\hat{d}_{j,\sigma}$ localized at positions $\mathbf{R}_j$, which we refer to as d-levels, in the presence of superconductivity, see Fig. 1. To this end, we consider the following Hamiltonian in second quantization:

$$\begin{aligned} \hat{H} &= \hat{H}_{MS} + \hat{H}_{SC} + \hat{H}_T, \\ \text{with } \hat{H}_{MS} &= E_R \sum_{\sigma,j} d_{\sigma,j}^\dagger d_{\sigma,j} + U \sum_j d_{\uparrow,j}^\dagger d_{\uparrow,j} d_{\downarrow,j}^\dagger d_{\downarrow,j}, \\ \hat{H}_{SC} &= \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} c_{\mathbf{k},\sigma}^\dagger c_{\mathbf{k},\sigma} + \lambda \sum_{\mathbf{k}} |\mathbf{k}| (ie^{-i\theta(\mathbf{k})} c_{\mathbf{k},\uparrow}^\dagger c_{\mathbf{k},\downarrow} + \text{H.c.}) \\ &\quad - \Delta \sum_{\mathbf{k}} (c_{\mathbf{k},\uparrow}^\dagger c_{-\mathbf{k},\downarrow}^\dagger + \text{H.c.}), \\ \hat{H}_T &= V \sum_{\mathbf{k},\sigma,j} (e^{i\mathbf{k}\mathbf{R}_j} c_{\mathbf{k},\sigma}^\dagger d_{\sigma,j} + \text{H.c.}), \end{aligned} \quad (1)$$

where $\hat{H}_{MS}$, $\hat{H}_{SC}$, $\hat{H}_T$ describe the corral levels, substrate, and the tunneling between them, respectively. Here, $\epsilon_{\mathbf{k}} = \mathbf{k}^2/2m - E_F$ is the dispersion relation of the continuum bulk superconductor with Fermi energy E_F , effective electron mass m , and SOC strength λ . We set $\hbar = 1$. Throughout, a denotes the lattice constant of the chain or square lattice of d-levels, as illustrated in Fig. 1. The dimensionality of the superconducting bulk in Eq. (1) is not constrained. To obtain analytical results for finite SOC, we focus on a 2D bulk superconductor [49]. E_R is the spin-independent energy of the d-levels while $\theta(\mathbf{k})$ refers to the azimuthal angle of the wave vector $\mathbf{k}$ in the plane parallel to the surface. Additionally, we consider local scattering at the MSS sites with potential $V_j(\mathbf{r}) = V\delta(\mathbf{r} - \mathbf{R}_j)$, where $\mathbf{r}$ refers to the position of the bulk electrons. The on-site repulsive interaction, U , is qualitatively included to account for Coulomb repulsions that originate from the real-space confinement of the d-levels. This interaction is neglected first, i.e., $U = 0$, until specified. In the case of a single pair of d-levels in Eq. (1), a pair of MSSs appears in the superconducting gap [25]. The broadening of the d-levels is determined by the hybridization strength $\Gamma = \pi\nu|V|^2$, where ν is the normal state density of states of the bulk at the Fermi energy. A similar model has been studied in the context of dense magnetic adatom chains [37]. In contrast, the model in Eq. (1) preserves time-reversal symmetry, and both spin-species need to be considered. To study the topological phases of the system, it suffices to focus on the low-energy limit $E/\Delta \rightarrow 0$ [50], because topological phases can only change upon closure of the spectral gap. In this limit, we integrate out the bulk modes and derive an effective BdG Hamiltonian (see Appendix A for details)

$$\begin{aligned} H_{\text{eff}} &= \begin{pmatrix} h_{i,j} & \Delta_{i,j} \\ \Delta_{i,j}^\dagger & -\sigma_z h_{i,j} \sigma_z \end{pmatrix}, \\ h_{i,j} &= \begin{pmatrix} h_{i,j}^N & h_{i,j}^F \\ h_{i,j}^{F\dagger} & h_{i,j}^N \end{pmatrix}, \quad \Delta_{i,j} = \begin{pmatrix} \Delta_{i,j}^S & \Delta_{i,j}^T \\ \Delta_{i,j}^{T*} & -\Delta_{i,j}^S \end{pmatrix}, \end{aligned} \quad (2)$$

defined in the basis $(d_{\uparrow,j}^\dagger \ d_{\downarrow,j}^\dagger \ d_{\downarrow,j} \ d_{\uparrow,j})^\dagger$, which describes a system of coupled MSSs and the corresponding

bands. The matrix elements $h_{i,j}^N$ include the on-site energy of the d-levels and long-range hoppings mediated by the bulk. The $h_{i,j}^F$ matrix elements describe long-range spin-flips between d-levels. The $\Delta_{i,j}^S$ and $\Delta_{i,j}^T$ matrix elements are the induced singlet (on-site and long-range) and triplet superconducting pairings, respectively. The induced matrix elements are proportional to the scattering strength Γ . Importantly, $h_{i,j}^F$ and $\Delta_{i,j}^T$ vanish for zero SOC $\lambda = 0$; see Appendix A.

For periodic boundary conditions, we transform the Hamiltonian in Eq. (2) to momentum space

$$H_{\text{eff}}(\mathbf{p}) = \begin{pmatrix} h^N(\mathbf{p}) & h^F(\mathbf{p}) & \Delta^S(\mathbf{p}) & \Delta^T(\mathbf{p}) \\ h^{F*}(\mathbf{p}) & h^N(\mathbf{p}) & -\Delta^{T*}(\mathbf{p}) & -\Delta^S(\mathbf{p}) \\ \Delta^{S*}(\mathbf{p}) & -\Delta^T(\mathbf{p}) & -h^N(\mathbf{p}) & h^F(\mathbf{p}) \\ \Delta^{T*}(\mathbf{p}) & -\Delta^{S*}(\mathbf{p}) & h^{F*}(\mathbf{p}) & -h^N(\mathbf{p}) \end{pmatrix}, \quad (3)$$

defined in the basis $\Psi_{\mathbf{p}} = (d_{\uparrow,\mathbf{p}}^\dagger \quad d_{\downarrow,\mathbf{p}}^\dagger \quad d_{\downarrow,-\mathbf{p}} \quad d_{\uparrow,-\mathbf{p}})^\dagger$ and $h^N(\mathbf{p}) = \sum_{\mathbf{x}} e^{i\mathbf{p}\cdot\mathbf{x}} h_{\mathbf{x}}^N$, where $\mathbf{x}$ runs over the entire lattice and similarly for $h^F(\mathbf{p})$, $\Delta^S(\mathbf{p})$, $\Delta^T(\mathbf{p})$. Importantly, $h^N(\mathbf{p})$ and $\Delta^S(\mathbf{p})$ are even but $h^F(\mathbf{p})$ and $\Delta^T(\mathbf{p})$ are odd functions in momentum $\mathbf{p}$. In the following, we systematically classify the topological phases associated with Eq. (3) by studying its symmetry class and topological invariant [19–21]. The effective Hamiltonian in Eq. (3) is generally gapped due to the induced on-site singlet pairing, and a nonvanishing SOC breaks the spin-SU(2) symmetry. Inheriting from the original Hamiltonian in Eq. (1), H_{eff} belongs to symmetry class DIII, respecting the particle-hole symmetry $\mathcal{C} = \tau_x \sigma_x K$ with $\mathcal{C}^2 = 1$ and time-reversal symmetry $\mathcal{T} = i\tau_z \sigma_y K$ with $\mathcal{T}^2 = -1$, where σ , τ are Pauli matrices in spin and particle-hole space, respectively. We conclude that the eigenmodes of Eq. (3) appear in Kramers pairs. Without SOC, the system reduces to two spinless subsystems in class BDI. For strictly translational invariant one-dimensional systems, the long-range spin-flip parameter $h^F(p)$ is purely real and the triplet pairing $\Delta^T(p)$ is purely imaginary (see Appendix B). As a consequence, the unitary operator $\mathcal{U} = \tau_z \sigma_y$ commutes with $H_{\text{eff}}(p)$. The system block-diagonalizes into two blocks, each with chiral symmetry and characterized by an integer topological invariant. The two invariants are identical because a time-reversal (or particle-hole) symmetry anticommutes with $\mathcal{U}$ and hence maps one block onto the other, connecting them. For the sake of generality, we keep our analysis at the level of the single DIII system. To calculate the single-particle eigenvalues, we write Eq. (3) as a tensor product of Pauli matrices and square it twice; see Appendix B for the derivation. Interestingly, for 1D lattices, the condition for a zero-energy crossing, i.e., $E_{\pm} = 0$, is equivalent to finding a momentum p_0 , such that

$$\begin{aligned} \Delta^S(p_0) &= \pm \text{Im} \Delta^T(p_0), \\ h^N(p_0) &= \mp \text{Im} h^F(p_0), \end{aligned} \quad (4)$$

see Appendix B for details. Once the first condition in Eq. (4) is satisfied, the second one can be fulfilled by an appropriate choice of the on-site energy E_R , which can be freely tuned by the size of the corrals. Qualitatively, the competition between the singlet, Δ^S , and triplet, Δ^T , pairings determines the zero-energy crossings and, thus, the topological phases [42].

III. RESULTS

Next, we demonstrate concrete examples by considering a 2D bulk superconductor with a linearized dispersion $\epsilon_{\mathbf{k}\pm} = \tilde{v}_F(k_{\pm} - k_{F\pm})$ around the Fermi level, where $\pm$ corresponds to the two helicity bands in the presence of SOC. The bands are characterized by the Fermi wave vectors $k_{F\pm}$, SOC renormalized Fermi velocity, $\tilde{v}_F$, and the modified normal state density of states $\nu_{\pm}$ at the Fermi energy, see Appendix C. In this case, the matrix elements are

$$\begin{aligned} h_{n,m}^N &= E_R \delta_{n,m} + (1 - \delta_{n,m}) \text{Im}(w_{n,m}^e), \\ h_{n,m}^F &= (1 - \delta_{n,m}) e^{-i\phi_{n,m}} \text{Re}(w_{n,m}^o), \\ \Delta_{n,m}^S &= -\Gamma \delta_{n,m} - (1 - \delta_{n,m}) \text{Re}(w_{n,m}^e), \\ \Delta_{n,m}^T &= -(1 - \delta_{n,m}) e^{-i\phi_{n,m}} \text{Im}(w_{n,m}^o), \end{aligned}$$

with $w_{n,m}^e = \sum_{\mu=\pm} \frac{\Gamma_{\mu}}{2} (J_0[x_{n,m}^{\mu}] + iH_0[x_{n,m}^{\mu}])$,

$$w_{n,m}^o = \sum_{\mu=\pm} \frac{\mu\Gamma_{\mu}}{2} (iJ_1[x_{n,m}^{\mu}] + H_{-1}[x_{n,m}^{\mu}]), \quad (5)$$

where J_n, H_n are the n th Bessel and Struve functions, respectively, which are holomorphic in the whole complex plane for integer n . Also, $\phi_{n,m}$ is the azimuthal angle of the vector $\mathbf{R}_n - \mathbf{R}_m$ and $x_{n,m}^{\pm} = (k_{F\pm} + i\xi^{-1})|\mathbf{R}_n - \mathbf{R}_m|$, where ξ is the superconducting coherence length. Here, the renormalized scattering strength, $\Gamma_{\pm} = \pi \nu_{\pm} |V|^2$, is proportional to Γ . Importantly, all matrix elements in Eq. (5), except for the on-site energy E_R , scale with the scattering strength Γ . Any modification in Γ can be compensated by an appropriate adjustment to E_R , guaranteeing that the value of Γ (or V) is not critical for satisfying the condition $E_{\pm} = 0$ and thus realizing nontrivial phases. In the case of a 1D lattice, this statement can be inferred from the matrix elements in Eq. (5) since both Δ^S and Δ^T are proportional to Γ , and thus the first condition in Eq. (4) does not depend on Γ . Similarly, the effective mass m rescales the renormalized SOC strength $\tilde{\lambda} = m\lambda/k_F$ and $\nu_{\pm}$, and thus Γ as well; see Eq. (C1) in Appendix C. Therefore, the only critical parameters for realizing nontrivial phases are the Fermi wave vector, the SOC strength, and the on-site energy. In the following, we fix the lattice positions, $\{\mathbf{R}_j\}$, of the d-levels and study the cases of one-dimensional chains and two-dimensional square lattices separately while varying the aforementioned critical parameters. For the plots that follow, we fix the effective mass to be of the order of the electron mass, $m \sim m_e$, and consider the scattering strength $|V| = 5\Delta$, which leads to $\Gamma \sim 0.1\Delta$, such that the energy bands remain deep inside the gap and the low-energy approximation holds. The Fermi wave vector determines the coupling strength between corrals. Within the approximation scheme of the low-energy model, which neglects the geometry of the quantum corrals, we expect the Fermi wave vector to be only indirectly associated to the value of the bulk material, and we therefore set $k_F a \sim 1$. This guarantees a sufficiently strong corral hybridization for achieving nontrivial phases. Also, we choose finite and small values for the renormalized SOC strength, $\tilde{\lambda}$, throughout the plots to demonstrate nontrivial phases. The coherence length calculated at the middle of

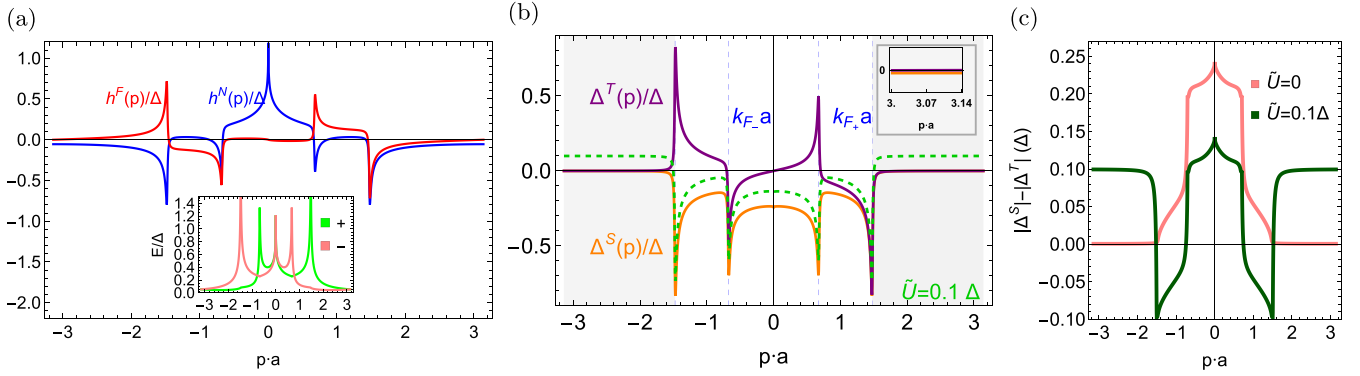


FIG. 2. Flattening of effective couplings in the low-energy theory for one-dimensional chains. (a) Long-range hoppings, $h^N(p)$, and spin-flip parameters, $h^F(p)$, in the first Brillouin zone for $E_R = 0$. The inset shows the two helicity bands of the dispersion relation. (b) Singlet, $\Delta^S(p)$ (orange for $\tilde{U} = 0$ and dashed green for $\tilde{U} = 0.1\Delta$), and triplet, $\Delta^T(p)$, superconducting order parameters. The inset zooms in the flat region (gray shading). (c) Difference $|\Delta^S| - |\Delta^T|$ of the singlet and triplet parameters in the presence ($\tilde{U} = 0.1\Delta$) and absence ($\tilde{U} = 0$) of interactions [adopted parameter values: $k_F a = 1.2$, $\tilde{\lambda} = \lambda/u_F = 0.4$, $m = 10^{-2}(a^2\Delta)^{-1}$, $|V| = 5\Delta$, and $N_{\text{cutoff}} = 1000$].

the energy gap, $\xi = \sqrt{\lambda^2 + u_F^2}/\Delta$, where $u_F = k_F/m$ is the bare Fermi velocity, physically determines an effective cutoff length N_{cutoff} for the couplings in Eq. (5) and distinguishes between the dilute and dense lattice limits, depending on the material/parameter choice.

First, we place N d-levels in a chain geometry, separated by a lattice constant a , see Fig. 1(b). We consider periodic boundary conditions and the long chain limit $N \gg 1$ to plot the elements in Eq. (5) in Fourier space, see Fig. 2(b). We resolve the long-range hopping and spin-flip parameters, assuming a vanishing on-site energy $E_R = 0$, see Fig. 2(a). Yet, $h^N(p)$ can be shifted by a nonvanishing E_R . Additionally, we demonstrate the effective singlet, $\Delta^S(p)$, and triplet, $\Delta^T(p)$, superconducting order parameters, see Fig. 2(b). We notice the flattening of $\Delta^{S,T}(p)$ for momenta greater than the maximum of the Fermi wave vectors of the two helicity bands, i.e., $p > \max(k_{F+}, k_{F-})$. This flattening is not numerically exact due to the finite Fourier transform cutoff N_{cutoff} , see the inset in Fig. 2(b). Furthermore, we observe characteristic cusps in the Brillouin zone that form around the momenta $p = k_{F\pm}$. We explain these effects by analytically computing the continuous Fourier transform of the singlet and triplet order parameters in the dense chain limit, both of which approach infinity at $p = k_{F\pm}$, due to the $1/\sqrt{k_F^2 - p^2}$ factor, and vanish for $p > \max(k_{F+}, k_{F-})$ due to the combination of Heaviside Θ functions that enter the exact expressions, see Appendix G. The finite cusps and flattenings transcend the dense limit and survive for finite values of $k_F a$. The singlet parameter includes both on-site and long-range elements. The observed cancellation of $\Delta^S(p)$ is lifted as $k_F a$ increases. This is because in the ultradilute limit $k_F a \gg 1$, the on-site singlet superconducting pairing dominates and the system thus becomes topologically trivial. As shown in Fig. 2(b), the singlet pairing is larger than the triplet pairing in the Brillouin zone (apart from the small oscillations due to the finite cutoff). The dominance of the singlet parameter places our system in the regime where the no-go theorem of Ref. [41] applies. The theorem states that any noninteracting electronic system proximity-coupled to a parent superconductor is locked in the trivial phase of class DIII whenever the matrix product

$\Delta(\mathbf{p}) \mathcal{T}_{\text{sc}}$ is positive-semidefinite (PSD) at every momentum, where $\Delta(\mathbf{p})$ is the parent's superconducting pairing matrix and $\mathcal{T}_{\text{sc}}$ is the unitary representation of time-reversal acting on the same internal indices. For the four-band effective Hamiltonian in Eq. (3), the PSD condition reduces to the inequality $|\Delta^S(p)| \geq |\Delta^T(p)|$ for every momentum p (see Appendix D), since the eigenvalues of $\Delta(p) \mathcal{T}_{\text{sc}}$ are $|\Delta^S(p)| \pm |\Delta^T(p)|$. Inspection of Fig. 2(c) shows that at $U = 0$ this inequality is satisfied throughout the Brillouin zone, so the system is rigorously locked in the trivial phase. Circumventing this trivial fate requires a mechanism that drives some momentum out of the PSD region, which we now show is provided by the on-site repulsion.

In experimental setups [27–29], the confinement of the surface state in quantum corrals induces, in principle, weak repulsive particle-particle interactions, which we have so far neglected. Such interactions, effectively described by the term $U d_{\uparrow,j}^\dagger d_{\uparrow,j} d_{\downarrow,j}^\dagger d_{\downarrow,j}$ with $U > 0$ in Eq. (1), influence the singlet-triplet pairing competition. To quantify this, we consider a mean-field decoupling of the interaction term in the superconductivity channel and the mean-field parameter $\delta := \langle d_{\uparrow,j}^\dagger d_{\downarrow,j} \rangle$, see Appendix E. We find that the on-site singlet order parameter gets renormalized, $\Delta_{i,i}^{S,R} = -\Gamma + \tilde{U}$ with $\tilde{U} = -U\delta$, while the long-range singlet and all triplet pairings remain unaffected. By numerical evaluation of the mean-field parameter δ_R which minimizes the free-energy, $\partial \mathcal{F} / \partial \delta|_{\delta=\delta_R} = 0$, in the first iteration of the self-consistency equation, we find that the singlet order parameter is suppressed, i.e., $\delta_R < 0$ or $\tilde{U} > 0$, in the presence of repulsive interactions, see Appendix E for details. Qualitatively, this suppression favors nontrivial topological phases, since the condition in Eq. (4) is more readily satisfied. As a consequence, $|\Delta^S(p)| < |\Delta^T(p)|$ in a finite momentum interval [see Fig. 2(c)], so the PSD prerequisite of the no-go theorem fails and a nontrivial DIII phase becomes possible—one of the key ideas of the present manuscript. We emphasize, however, that violating the PSD condition is necessary but not sufficient for nontrivial topology: it lifts the trivial-phase lock without guaranteeing that the system is topologically nontrivial. Determining whether a nontrivial DIII phase is realized requires explicit

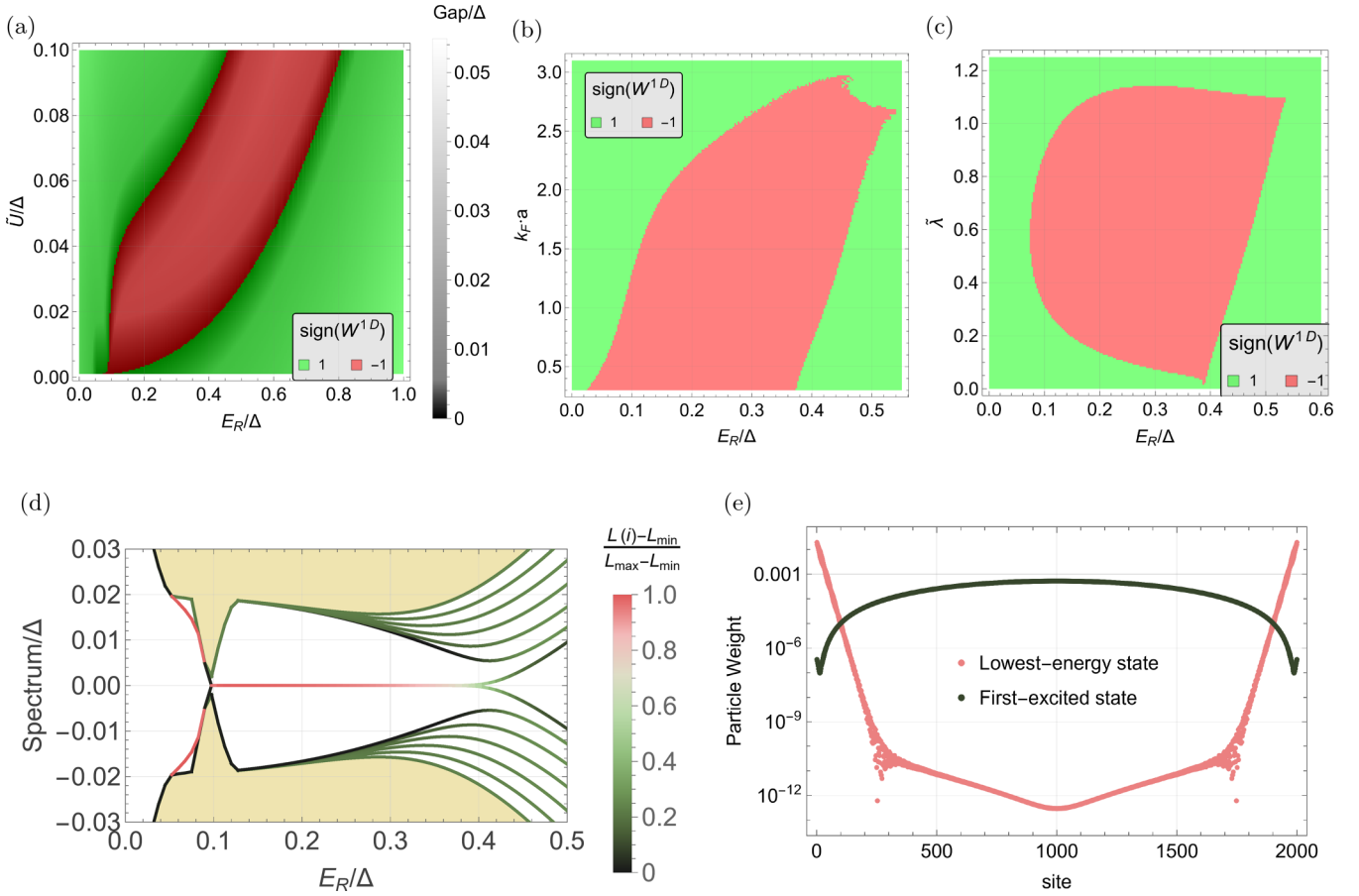


FIG. 3. Nontrivial topological phases and Majorana Kramers pairs in a one-dimensional chain with a finite repulsive interaction $\tilde{U}$. The $\mathbb{Z}_2$ topological invariant, W^{1D} , identifies trivial (1) and nontrivial (-1) phases, (a) depending on the repulsion interaction $\tilde{U}/\Delta$ and the on-site energy E_R/Δ , (b) depending on the on-site energy E_R/Δ and the Fermi wave vector $k_F a$, (c) depending on the on-site energy E_R/Δ and the SOC $\tilde{\lambda}$. (d) Real-space spectrum (lowest energy eigenvalues) as a function of the bare energy E_R for a chain-length of $N = 2000$. The yellow shading indicates higher energy states that we neglect. The color code uses the localization measure $L(i)$, see Eq. (6), that demonstrates the real-space edge localization of each state with $L_{\min}$, $L_{\max}$ being the minimum and maximum values, respectively, for all data. (e) Real-space mapping of the particle component of the wave function of the lowest energy (pink) and first excited (green) eigenstates along the chain at $E_R = 0.2\Delta$ (white dot in (a)), demonstrated in logarithmic scale. Common parameter values: $m = 10^{-2}(a^2\Delta)^{-1}$, $|V| = 5\Delta$. Panel (a) $k_F a = 1.2$, $\tilde{\lambda} \equiv \lambda/u_F = 1/3$. Panel (b): $\tilde{\lambda} = 1/3$, $\tilde{U} = 0.02\Delta$. Panel (c): $k_F a = 1.2$, $\tilde{U} = 0.02\Delta$. Panels (d) and (e): $k_F a = 1.2$, $\tilde{\lambda} = 1/3$, $\tilde{U} = 0.02\Delta$.

computation of the $\mathbb{Z}_2$ invariant W^{1D} , which we perform below.

We demonstrate the real-space spectrum for a chain of N sites as a function of the on-site energy E_R , see Fig. 3(d). Notably, there is a parameter region with the lowest eigenenergy being almost zero signifying the topologically nontrivial phase which hosts a Kramers pair of Majorana zero modes in each chain end. The zero-energy eigenvalues are lifted when the spectral gap closes, leading to a topological phase transition to the trivial phase. We highlight that all eigenvalues are doubly degenerate due to time-reversal-symmetry. To quantify the real-space localization of the eigenmodes we employ the localization measure [color scale in Fig. 3(d)]

$$L(i) = \sum_{j=1}^{j=N} |\psi_j^i|^2 [j - (N+1)/2]^2 / [(N+1)/2 - 1]^2, \quad (6)$$

where ψ_j^i is the wave function of the i th eigenstate at site j . This localization measure approaches $L \approx 1/3$ for a uniformly distributed state and $L \approx 1$ for an edge localized state

in the large- N limit. Additionally, we resolve the particle part of the wave function of the zero-energy mode in logarithmic scale and compare it to the one of the first excited state, see Fig. 3(e). Evidently, the wave function of the zero-energy mode is exponentially localized near the boundaries of the chain by the induced coherence length, ξ , that enters in the matrix elements in Eq. (5), while the wave function of the first excited state is spread along the chain.

To confirm the topological origin of the zero-energy modes, we calculate the topological invariant for the effective Hamiltonian in momentum space in Eq. (3). For the construction of the topological invariant, we follow the approach of [42] and numerically compute the determinant of the projection of the Kato propagator K , along the path p from $p = 0$ to $p = \pi$, on an arbitrary choice of Bloch eigenfunctions $\det(K)$. For the construction of the topological invariant W^{1D} , we use $W^{1D} = \det(K) \frac{\text{Pf}(\theta_0)}{\text{Pf}(\theta_\pi)}$, where θ_p is the matrix representation of the time-reversal operator on the occupied Bloch eigenvectors at the time-reversal-invariant momenta, $p \in \{0, \pi\}$, and Pf denotes the Pfaffian. The determinant can

take two values $\det(K) = \pm 1$ in the limit of taking infinite steps in the partition of the path p from $0 \rightarrow \pi$. Therefore, the topological invariant is $W^{1D} = 1$ for a trivial and $W^{1D} = -1$ for a nontrivial phase. For practical purposes, we compute the $\text{sgn}(W^{1D})$, see Fig. 3, to avoid nonquantized values that numerically emerge due to the finite discretization of the momentum interval for the Kato propagator. We show that a small repulsive interaction, $\tilde{U} > 0$, is essential for opening nontrivial topological phases whose boundaries coincide with the band-gap closings, see Fig. 3(a). Note that we restrict the range of our computation to small values of the repulsive interaction, $0 < \tilde{U} < 0.1\Delta$, where the mean-field treatment of Eq. (1) is justifiable. We demonstrate the dependence of the topological invariant on the Fermi wave vector, k_F , and the on-site energy E_R/Δ , see Fig. 3(b). The nontrivial phase disappears above a critical value of the Fermi wave vector. Indeed, in the ultradilute limit $k_F a \gg 1$, the on-site singlet superconductivity dominates and the chain is topologically trivial since the conditions in Eq. (4) cannot be satisfied. Note that the boundary of the phase diagram for $k_F a = 1.2$ in Fig. 3(b) agrees with the zero-energy crossings, shown in the finite system in Fig. 3(d). Moreover, we study the dependence of the topological invariant, W^{1D} , on the renormalized SOC strength $\tilde{\lambda}$ and on-site energy E_R , see Fig. 3(c). Even in the limit of weak SOC, $\tilde{\lambda} \rightarrow 0$, the system becomes nontrivial with a fine-tuning of E_R . The case $\tilde{\lambda} = 0$ is always trivial because the triplet order parameter vanishes. In the opposite limit of large SOC, $\tilde{\lambda} = \lambda m/k_F \gg 1$, the system becomes trivial. In this limit, the coupling strength Γ_- of one of the helicity bands becomes very small, see Eq. (C1). In such cases, the band is pushed away from zero energy, making it impossible to experience a topological phase transition for any value of the on-site energy E_R . Thus, we find only trivial phases for large values of $\tilde{\lambda}$ in Fig. 3(c). This is in contrast to typical topological phase diagrams of YSR bands [51], which demonstrate alternations between trivial and nontrivial phases when the SOC strength is increased to larger values. Last, as discussed previously in the text, we note that the other parameters of the system may change the phase boundaries in the topological phase diagrams [shown in Figs. 3(b) and 3(c)] but do not let the nontrivial phases completely disappear.

We next extend our study to two-dimensional square lattices with N_x, N_y lattice sites in the x, y directions, respectively, see Fig. 1(a). In this geometry, we find helical Majorana edge modes, in contrast to the end states that appear in one-dimensional chains. To demonstrate boundary modes, we consider a cylindrical geometry by taking periodic boundary conditions in the y -direction, in which case the momentum p_y is a good quantum number, and the limit $N_y \rightarrow \infty$. In this setup, in the topologically nontrivial phase, we find time-reversal-symmetric pairs of dispersive edge modes which are localized near the open boundaries and higher energy modes which are extended throughout the bulk, see Fig. 4. A broader study of the topological phases in 2D lattices requires the calculation of the relevant topological invariant in the symmetry class DIII by taking two 1D cuts (for $p_y = 0$ and $p_y = \pi$) in the Brillouin zone and multiplying the calculated 1D invariants in these cuts, $W^{2D} = W_{p_y=0}^{1D} \times W_{p_y=\pi}^{1D}$ [41]. In general, we find that the 2D topological phase diagrams differ from the 1D. Specifically, the 2D equivalents of the diagrams in

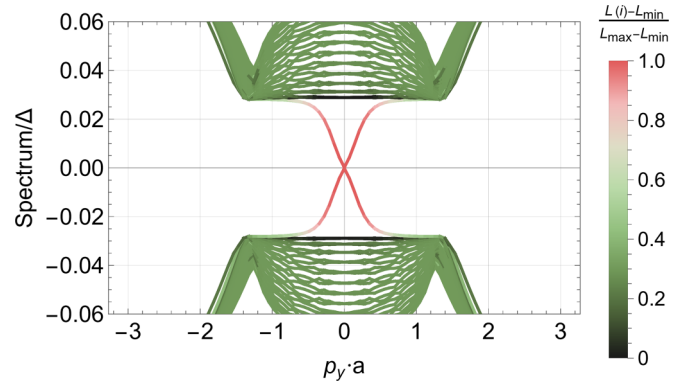


FIG. 4. Localization of edge modes in two-dimensional lattices in a cylindrical geometry with finite repulsive interaction $\tilde{U} = 0.05\Delta$. States are colored according to their edge localization, using the localization measure, $L(i)$, in Eq. (6). [Adopted parameter values: $m = 10^{-2}(a^2\Delta)^{-1}$, $|V| = 5\Delta$, $\tilde{\lambda} = 1/3$, $k_F a = 0.1$, $E_R = 0.1\Delta$, $N_x = 90$].

Figs. 3(b) and 3(c) demonstrate extended nontrivial phases, see Appendix F for details. Notably, the main characteristic features for triviality for large $k_F a$ and the nontrivial region vanishing at $\tilde{\lambda} = 0$ remain. For topological phase diagrams shown in Fig. 6, a nearest-neighbor cutoff was considered due to computation limitations. Once the physical long-range couplings are restored, small-repulsive interactions $\tilde{U} > 0$ are still required for generating nontrivial phases, similarly to the one-dimensional chains, and lead to quantitatively different topological phase diagrams. For fully periodic boundary conditions, the triplet superconducting pairing in Eq. (3) can be simplified in the continuum limit, i.e., $|\mathbf{p}|a \ll 1$,

$$\hat{\Delta}^T = \vec{d}(\mathbf{p})\vec{\sigma}, \vec{d}(\mathbf{p}) = ig(p)(p_x, p_y, 0), \text{ where} \quad (7)$$

$$g(p) = - \sum_{R \neq 0} J_1(pR) \text{Im}(w^o(R))/p,$$

where J_1 is the Bessel function, $g(p) \in \mathbb{R}$, and the superconducting pairing is helical [52]. This is in contrast to the chiral triplet pairing that governs Shiba systems due to time-reversal-symmetry breaking [39].

IV. CONCLUSIONS

On a superconducting substrate, MS bands can be engineered by constructing arrays of adatom quantum corrals. We find that in the presence of small repulsive interactions inside the corrals, the triplet pairing can dominate over the singlet pairing leading to nontrivial topological phases in class DIII. We emphasize that such type of effective superconducting correlations is fundamentally different to the case of Shiba bands, where only effective chiral triplet pairings are present. This leads to distinct helical Majorana boundary modes in two-dimensional MS lattices and Kramers degenerate Majorana zero modes in one-dimensional chains. Interestingly, we find that the superconducting pairings become flat for a finite momenta range when long-range couplings between MSSs are not negligible. Let us address the experimental relevance of the parameters used in the model. While the effective electron mass, m and spin-orbit coupling $\tilde{\lambda}$ correspond to the

experimental range [27,28], we chose hybridization strengths Γ and effective corral distances $k_F a$ that are up to an order of magnitude smaller. First, we chose a $\Gamma \sim 0.1\Delta$ to remain within the validity regime of the low-energy theory. Larger values of Γ do not change the qualitative behavior of our model, but would merely distort the dispersion relation further away from the Fermi level. Topological phase transitions would still be captured faithfully because they happen at the Fermi level. Second, in an experiment, the parameter $k_F a$ mostly describes the hybridization strength between corral modes instead of the actual Fermi momentum. An estimate of this parameter requires material-specific first-principle calculations that consider the corrals' specific geometry, which exceeds the scope of our current study and links the effective parameters in our model to the ones of the experimental configuration. A promising setup for increasing the nearest-neighbor MSSs hybridization would entail removing adatoms from the boundaries of neighboring corrals, allowing the respective MS states to hybridize sufficiently, which has been realized in elliptical and square Cu(111) corrals in the normal state [53,54]. In the absence of superconductivity, multiple-corral setups have shown long-range hybridization patterns when placed in one and two-dimensional geometries, forming artificial molecular structures [55]. From the typical candidate materials (Ag, Cu, Au) that host Shockley surface states on their (111) surface, Au is most promising due to the large spin-orbit coupling at its atomic levels [32]. For Au, we consider $u_F = 1.4 \times 10^6$ m/s [56] and $\lambda = 0.33$ eV Å [57], leading to $\tilde{\lambda} = \lambda/(\hbar u_F) = 0.04$, which is sufficiently strong to achieve nontrivial phases without exhaustive precision for tuning the chemical potential E_R/Δ . It is worth mentioning that metals with more complex electronic structures than noble metals, such as Bi and its (111) surface, are promising for experimenting with our proposal due to the possibility for epitaxial growth and large Fermi wavelength [58], despite not having a clear Shockley type of surface state.

Our results inspire future experiments for constructing lattices of quantum corrals and varying their mutual couplings. The construction of quantum corrals with tunable sizes offers experimental control on the corrals' on-site energies which control the topological invariant of the setup. Such lattices can host nontrivial phases and boundary modes in class DIII beyond the recently studied magnetic adatom lattices in class D. The MSSs and thus the boundary modes are spread within corrals of dozens of nm² surface area [27–29], which enables experimental detection due to their extended real-space signal. Fabricating corral lattices would involve the lateral manipulation of potentially thousands of adatoms. Yet, this could be achieved using state-of-the-art STM manipulation techniques [16,53,59], or developing machine-learning-supported construction. Despite the distinct microscopic modeling of alternative platforms that host MSSs, e.g., the transmon qubit Josephson junctions [33,34], our study inspires research adapted to these systems. Additionally, we envision tunable control of the edges modes hybridization by introducing weak violations of time-reversal-symmetry, e.g., with an introduction of small magnetic fields. We propose synthesizing extended lattices of magnetic adatom-quantum corral composites [29] where Kramers degeneracy is broken and topological phases beyond class DIII can be generated.

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DATA AVAILABILITY

There are no publicly available research data or software supporting this manuscript. Requests for further information or data should be sent to the authors.

APPENDIX A: DERIVATION OF THE EFFECTIVE HAMILTONIAN

To deal with the SOC term in Eq. (1), we transform our bulk Hamiltonian H_{SC} to the helicity basis

$$\begin{aligned} c_{\mathbf{k}+} &= \frac{1}{\sqrt{2}}(ie^{-i\theta(\mathbf{k})}c_{\mathbf{k}\downarrow} + c_{\mathbf{k}\uparrow}), \\ c_{\mathbf{k}-} &= \frac{1}{\sqrt{2}}(c_{\mathbf{k}\downarrow} + ie^{i\theta(\mathbf{k})}c_{\mathbf{k}\uparrow}), \end{aligned} \quad (\text{A1})$$

where $\theta(\mathbf{k})$ is the azimuthal angle for the momentum of the c electrons. The bulk Hamiltonian is rewritten

$$\begin{aligned} H_{\pm} &= \sum_{\mathbf{k}, \pm} \epsilon_{\mathbf{k}\pm} c_{\mathbf{k}\pm}^{\dagger} c_{\mathbf{k}\pm} \\ &\quad - \sum_{\mathbf{k}, \pm} \Delta_{\mathbf{k}\pm}^* c_{\mathbf{k}\pm}^{\dagger} c_{-\mathbf{k}\pm}^{\dagger} + \Delta_{\mathbf{k}\pm} c_{-\mathbf{k}\pm} c_{\mathbf{k}\pm}, \end{aligned} \quad (\text{A2})$$

where $\epsilon_{\mathbf{k}\pm} = \frac{\mathbf{k}^2}{2m} - \epsilon_F \pm \lambda|\mathbf{k}|$ and $\Delta_{\mathbf{k}\pm} = \Delta e^{\pm i[\theta(\mathbf{k}) + \frac{\pi}{2}]}$. The tunneling in Eq. (1) in the basis (A1) is

$$\begin{aligned} H_T &= \frac{V}{\sqrt{2}} \sum_{\mathbf{k}, \sigma, j} e^{i\mathbf{k}\mathbf{R}_j} ((ie^{i\theta(\mathbf{k})}c_{\mathbf{k}-}^{\dagger} + c_{\mathbf{k}+}^{\dagger})d_{\uparrow, j} \\ &\quad + (c_{\mathbf{k}-}^{\dagger} + ie^{-i\theta(\mathbf{k})}c_{\mathbf{k}+}^{\dagger})d_{\downarrow, j}) + \text{H.c.} \end{aligned} \quad (\text{A3})$$

We next use the Green's function equations of motion to integrate out the bulk modes and derive the effective Hamiltonian in Eq. (3). We define the matrix Green's function in Zubarev's notation [60] of the d-levels

$$\check{G} = \ll \begin{pmatrix} d_{\uparrow, i} \\ d_{\downarrow, i} \\ d_{\uparrow, i}^{\dagger} \\ d_{\downarrow, i}^{\dagger} \end{pmatrix}; \begin{pmatrix} d_{\uparrow, j}^{\dagger} & d_{\downarrow, j}^{\dagger} & d_{\downarrow, j} & d_{\uparrow, j} \end{pmatrix} \gg. \quad (\text{A4})$$

In general, we can write

$$[E - \hat{H}_{\text{eff}}(E)]\check{G} = \hat{1}, \quad (\text{A5})$$

where the matrix $\hat{H}_{\text{eff}}(E)$ is derived in the following by the Green's function equations of motion [61]. The Green's

functions of the d-levels are

$$\begin{aligned}(E - E_R)G_{d_{\uparrow,m}d_{\uparrow,m}^\dagger} &= 1 + \frac{V^*}{\sqrt{2}} \sum_{\mathbf{k}} (-ie^{-i\theta} G_{\mathbf{k}_-d_{\uparrow,m}^\dagger}) + \frac{V^*}{\sqrt{2}} \sum_{\mathbf{k}} G_{\mathbf{k}_+d_{\uparrow,m}^\dagger}, \\ (E - E_R)G_{d_{\downarrow,m}d_{\downarrow,m}^\dagger} &= 1 + \frac{V^*}{\sqrt{2}} \sum_{\mathbf{k}} G_{\mathbf{k}_-d_{\downarrow,m}^\dagger} + \frac{V^*}{\sqrt{2}} \sum_{\mathbf{k}} (-ie^{i\theta} G_{\mathbf{k}_+d_{\downarrow,m}^\dagger}).\end{aligned}\quad (\text{A6})$$

We then substitute the sums of the Green's function that involve bulk modes and find

$$\begin{aligned}(E - \epsilon_{\mathbf{k}_+})G_{\mathbf{k}_+d_{\uparrow,m}^\dagger} &= \sum_i \left(\frac{V_i}{\sqrt{2}} G_{d_{\uparrow,i}d_{\uparrow,m}^\dagger} + \frac{iV_i e^{-i\theta}}{\sqrt{2}} G_{d_{\downarrow,i}d_{\uparrow,m}^\dagger} \right) - \Delta_+^* G_{-\mathbf{k}_+d_{\uparrow,m}^\dagger}, \\ (E + \epsilon_{\mathbf{k}_+})G_{-\mathbf{k}_+d_{\uparrow,m}^\dagger} &= \sum_i \left(-\frac{iV_{i,-\mathbf{k}}^* e^{i\theta}}{\sqrt{2}} G_{d_{\downarrow,i}d_{\uparrow,m}^\dagger} - \frac{V_{i,-\mathbf{k}}}{\sqrt{2}} G_{d_{\uparrow,i}d_{\uparrow,m}^\dagger} \right) - \Delta_+ G_{\mathbf{k}_+d_{\uparrow,m}^\dagger}, \\ (E - \epsilon_{\mathbf{k}_-})G_{\mathbf{k}_-d_{\uparrow,m}^\dagger} &= \sum_i \left(\frac{iV_i e^{i\theta}}{\sqrt{2}} G_{d_{\uparrow,i}d_{\uparrow,m}^\dagger} + \frac{V_i}{\sqrt{2}} G_{d_{\downarrow,i}d_{\uparrow,m}^\dagger} \right) - \Delta_-^* G_{-\mathbf{k}_-d_{\uparrow,m}^\dagger}, \\ (E + \epsilon_{\mathbf{k}_-})G_{-\mathbf{k}_-d_{\uparrow,m}^\dagger} &= \sum_i \left(-\frac{V_{i,-\mathbf{k}}^*}{\sqrt{2}} G_{d_{\downarrow,i}d_{\uparrow,m}^\dagger} - \frac{iV_{i,-\mathbf{k}} e^{-i\theta}}{\sqrt{2}} G_{d_{\uparrow,i}d_{\uparrow,m}^\dagger} \right) - \Delta_- G_{\mathbf{k}_-d_{\uparrow,m}^\dagger}.\end{aligned}\quad (\text{A7})$$

By solving Eq. (A7) and substituting in the first Eq. (A6), we obtain

$$\begin{aligned}\left(E - E_R + \frac{E\Gamma}{\sqrt{\Delta^2 - E^2}}\right)G_{d_{\uparrow,m}d_{\uparrow,m}^\dagger} &= 1 - \frac{\Delta\Gamma}{\sqrt{\Delta^2 - E^2}} G_{d_{\downarrow,m}d_{\uparrow,m}^\dagger} + \sum_j G_{d_{\uparrow,j}d_{\uparrow,m}^\dagger} (S_{3,j,m} + S_{4,j,m}) \\ &\quad + \sum_j G_{d_{\downarrow,j}d_{\uparrow,m}^\dagger} (S_{5,j,m} + S_{6,j,m}) + \sum_j G_{d_{\downarrow,j}d_{\uparrow,m}^\dagger} S_{7,j,m} - \sum_j G_{d_{\uparrow,j}d_{\uparrow,m}^\dagger} S_{8,j,m},\end{aligned}\quad (\text{A8})$$

and, similarly, for the opposite spin species

$$\begin{aligned}\left(E - E_R + \frac{E\Gamma}{\sqrt{\Delta^2 - E^2}}\right)G_{d_{\downarrow,m}d_{\downarrow,m}^\dagger} &= 1 + \frac{\Delta\Gamma}{\sqrt{\Delta^2 - E^2}} G_{d_{\uparrow,m}d_{\downarrow,m}^\dagger} + \sum_j G_{d_{\downarrow,j}d_{\downarrow,m}^\dagger} (S_{3,j,m} + S_{4,j,m}) \\ &\quad - \sum_j G_{d_{\uparrow,j}d_{\downarrow,m}^\dagger} (S_{5,j,m} + S_{6,j,m})^* - \sum_j G_{d_{\uparrow,j}d_{\downarrow,m}^\dagger} S_{7,j,m} - \sum_j G_{d_{\downarrow,j}d_{\downarrow,m}^\dagger} S_{8,j,m}^*,\end{aligned}\quad (\text{A9})$$

with the definitions

$$\begin{aligned}S_{3,j,m} &= \frac{|V|^2}{2} \sum_{\mathbf{k}, \mu=\pm} \frac{e^{i\mathbf{k}(\mathbf{R}_j - \mathbf{R}_m)} E}{E^2 - \epsilon_{\mathbf{k}_\mu}^2 - \Delta^2}, & S_{4,j,m} &= \frac{|V|^2}{2} \sum_{\mathbf{k}, \mu=\pm} \frac{e^{i\mathbf{k}(\mathbf{R}_j - \mathbf{R}_m)} \epsilon_{\mathbf{k}_\mu}}{E^2 - \epsilon_{\mathbf{k}_\mu}^2 - \Delta^2}, \\ S_{5,j,m} &= \frac{|V|^2}{2} \sum_{\mathbf{k}, \mu=\pm} \frac{i\mu e^{-i\theta} e^{i\mathbf{k}(\mathbf{R}_j - \mathbf{R}_m)} E}{E^2 - \epsilon_{\mathbf{k}_\mu}^2 - \Delta^2}, & S_{6,j,m} &= \frac{|V|^2}{2} \sum_{\mathbf{k}, \mu=\pm} \frac{i\mu e^{-i\theta} e^{i\mathbf{k}(\mathbf{R}_j - \mathbf{R}_m)} \epsilon_{\mathbf{k}_\mu}}{E^2 - \epsilon_{\mathbf{k}_\mu}^2 - \Delta^2}, \\ S_{7,j,m} &= \frac{|V|^2}{2} \sum_{\mathbf{k}, \mu=\pm} \frac{e^{i\mathbf{k}(\mathbf{R}_j - \mathbf{R}_m)} \Delta}{E^2 - \epsilon_{\mathbf{k}_\mu}^2 - \Delta^2}, & S_{8,j,m} &= \frac{|V|^2}{2} \sum_{\mathbf{k}, \mu=\pm} \frac{i\mu e^{-i\theta} e^{i\mathbf{k}(\mathbf{R}_j - \mathbf{R}_m)} \Delta}{E^2 - \epsilon_{\mathbf{k}_\mu}^2 - \Delta^2}.\end{aligned}\quad (\text{A10})$$

Note that S_3, S_4, S_7 are even and S_5, S_6, S_8 are odd under the exchange $i \leftrightarrow j$. Also, S_3, S_4, S_7 are real. Importantly, the elements S_5, S_6, S_8 vanish for vanishing SOC in the bulk. In the low-energy limit, $E/\Delta \rightarrow 0$, S_3, S_5 vanish, and Eq. (A5) becomes an eigenvalue equation with the effective Hamiltonian in Eq. (2). We find

$$\begin{aligned}h_{i,j}^N &= E_R \delta_{i,j} + (1 - \delta_{i,j}) \lim_{\frac{E}{\Delta} \rightarrow 0} S_{4,i,j}, \\ h_{i,j}^F &= (1 - \delta_{i,j}) \lim_{\frac{E}{\Delta} \rightarrow 0} S_{6,i,j},\end{aligned}$$

$$\begin{aligned}\Delta_{i,j}^S &= -\Gamma \delta_{i,j} + (1 - \delta_{i,j}) \lim_{\frac{E}{\Delta} \rightarrow 0} S_{7,i,j}, \\ \Delta_{i,j}^T &= -(1 - \delta_{i,j}) \lim_{\frac{E}{\Delta} \rightarrow 0} S_{8,i,j},\end{aligned}\quad (\text{A11})$$

where specific formulas for these matrix elements are demonstrated in Sec. III in the main text and Appendix C, after appropriate specifications and approximations specified there.

APPENDIX B: EIGENVALUE CALCULATION

To calculate the eigenvalues for the general problem, we Fourier transform the real space functions S_i ,

$F_i(\mathbf{p}) = \sum_j e^{i\mathbf{p}\mathbf{R}_j} S_{i,0,j}$, and rewrite the complex functions $F_6 = \text{Re}F_6 + i\text{Im}F_6$ and $F_8 = \text{Re}F_8 + i\text{Im}F_8$. In the following, we work with the momentum space functions. We write

$$H(\mathbf{p}) = \tau_z \sigma_0 (F_4 + E_R) - \tau_0 \sigma_y \text{Im}F_6 + \tau_0 \sigma_x \text{Re}F_6 \\ + \tau_x \sigma_z (-\Gamma + F_7) + \tau_y \sigma_x \text{Im}F_8 + \tau_y \sigma_y \text{Re}F_8. \quad (\text{B1})$$

We square the Hamiltonian and obtain

$$H^2 - (F_4 + E_R)^2 - (F_7 - \Gamma)^2 - |F_6|^2 - |F_8|^2 \\ = -2\tau_z \sigma_y [(F_4 + E_R)\text{Im}F_6 + (F_7 - \Gamma)\text{Im}F_8] \\ + 2\tau_z \sigma_x [(F_4 + E_R)\text{Re}(F_6) + (F_7 - \Gamma)\text{Re}F_8] \\ + 2\tau_y \sigma_0 (\text{Re}F_6 \text{Im}F_8 - \text{Im}F_6 \text{Re}F_8). \quad (\text{B2})$$

The above is further simplified by considering the identity $\text{Re}F_6 \text{Im}F_8 - \text{Im}F_6 \text{Re}F_8 = \text{Im}F_6^* F_8$. Equation (B2) is squared again and projected to the energy eigenstates to give an eigenvalue equation

$$\frac{1}{4}(E^2 - (F_4 + E_R)^2 - (F_7 - \Gamma)^2 - |F_6|^2 - |F_8|^2)^2 \\ = |F_4 + E_R|^2 |F_6|^2 + |F_7 - \Gamma|^2 |F_8|^2 + \text{Im}F_6 F_8^* \\ + 2(F_4 + E_R)(F_7 - \Gamma)\text{Re}F_6 F_8^*. \quad (\text{B3})$$

In the 1D case, $\text{Re}F_6 = \text{Re}F_8 = 0$, and Eq. (B3) simplifies to

$$E_{\pm,\pm} = \pm \sqrt{(F_4 + E_R \pm \text{Im}F_6)^2 + (-\Gamma + F_7 \pm \text{Im}F_8)^2} \\ = \pm \sqrt{[h^N(p) \pm \text{Im}h^F(p)]^2 + [\Delta^S(p) \mp \text{Im}\Delta^T(p)]^2}, \quad (\text{B4})$$

where we use the relations in Eq. (A11) in momentum space for the second equality.

APPENDIX C: 2D BULK SYSTEM

The sums in Eq. (A10) are solved in a 2D bulk system. We linearize the dispersion of the bulk $\epsilon_{\mathbf{k}\pm} = (\mathbf{k}^2 - k_F^2)/2m \pm \lambda|\mathbf{k}|$ to get the renormalized parameters

$$k_{\pm} = k_{F\pm} + \epsilon_{\mathbf{k}\pm}/\tilde{v}_F, \quad k_{F\pm} = k_F(\sqrt{\tilde{\lambda}^2 + 1} \mp \tilde{\lambda}), \\ \tilde{v}_F = u_F \sqrt{\tilde{\lambda}^2 + 1}, \quad \tilde{\lambda} = \lambda m/k_F, \quad \xi = \tilde{v}_F/\sqrt{\Delta^2 - E^2}, \\ v_{\pm} = \frac{m}{2\pi} \left(1 \mp \frac{\tilde{\lambda}}{\sqrt{\tilde{\lambda}^2 + 1}} \right). \quad (\text{C1})$$

We also consider a 2D lattice of MS impurities at positions $\mathbf{R}_j = |\mathbf{R}_j|(\cos(\phi_j), \sin(\phi_j))$. Using the above, we write the relevant integrals

$$S_{4,j,m}^{2D} = \frac{|V|^2}{2} \sum_{\mathbf{k}, \mu=\pm} \frac{e^{i|\mathbf{k}||\mathbf{R}_j - \mathbf{R}_m| \cos(\theta - \phi_{j,m})} \epsilon_{\mathbf{k}\mu}}{E^2 - \epsilon_{\mathbf{k}\mu}^2 - \Delta^2}, \\ S_{6,j,m}^{2D} = \frac{|V|^2}{2} \sum_{\mathbf{k}, \mu=\pm} \frac{i\mu e^{-i\theta} e^{i|\mathbf{k}||\mathbf{R}_j - \mathbf{R}_m| \cos(\theta - \phi_{j,m})} \epsilon_{\mathbf{k}\mu}}{E^2 - \epsilon_{\mathbf{k}\mu}^2 - \Delta^2},$$

$$S_{7,j,m}^{2D} = \frac{\Delta|V|^2}{2} \sum_{\mathbf{k}, \mu=\pm} \frac{e^{i|\mathbf{k}||\mathbf{R}_j - \mathbf{R}_m| \cos(\theta - \phi_{j,m})}}{E^2 - \epsilon_{\mathbf{k}\mu}^2 - \Delta^2}, \\ S_{8,j,m}^{2D} = \frac{\Delta|V|^2}{2} \sum_{\mathbf{k}, \mu=\pm} \frac{i\mu e^{-i\theta} e^{i|\mathbf{k}||\mathbf{R}_j - \mathbf{R}_m| \cos(\theta - \phi_{j,m})}}{E^2 - \epsilon_{\mathbf{k}\mu}^2 - \Delta^2}. \quad (\text{C2})$$

We define $x_{j,m}^{\pm} = (k_{F\pm} + i\xi^{-1})|\mathbf{R}_j - \mathbf{R}_m|$. In the limit $\lim_{\frac{E}{\Delta} \rightarrow 0}$, we find [39,49,51]

$$\lim_{\frac{E}{\Delta} \rightarrow 0} S_{4,j,m}^{2D} = \sum_{\mu=\pm} \frac{\Gamma_{\mu}}{2} \text{Im}J_0[x_{j,m}^{\mu}] + iH_0[x_{j,m}^{\mu}], \\ \lim_{\frac{E}{\Delta} \rightarrow 0} S_{6,j,m}^{2D} = e^{-i\phi_{j,m}} \sum_{\mu=\pm} \frac{\mu\Gamma_{\mu}}{2} \text{Re}iJ_1[x_{j,m}^{\mu}] + H_{-1}[x_{j,m}^{\mu}], \\ \lim_{\frac{E}{\Delta} \rightarrow 0} S_{7,j,m}^{2D} = - \sum_{\mu=\pm} \frac{\Gamma_{\mu}}{2} \text{Re}J_0[x_{j,m}^{\mu}] + iH_0[x_{j,m}^{\mu}], \\ \lim_{\frac{E}{\Delta} \rightarrow 0} S_{8,j,m}^{2D} = e^{-i\phi_{j,m}} \sum_{\mu=\pm} \frac{\mu\Gamma_{\mu}}{2} \text{Im}iJ_1[x_{j,m}^{\mu}] + H_{-1}[x_{j,m}^{\mu}], \quad (\text{C3})$$

where $\Gamma_{\pm} = \pi v_{\pm}|V|^2$ and J_n and H_n are the n th Bessel and Struve functions, respectively.

APPENDIX D: POSITIVE-SEMIDEFINITE CONDITION FOR THE SUPERCONDUCTING PAIRING

In this appendix, we derive the inequality $|\Delta^S(\mathbf{p})| \geq |\Delta^T(\mathbf{p})|$, which the no-go theorem of Ref. [41] imposes on the four-band effective Hamiltonian in Eq. (3) as a condition for being locked in the trivial phase of class DIII. In the standard Nambu basis defined below Eq. (3), the pairing of spinors $d^{\dagger}d^{\dagger}$ enter the bilinear $\frac{1}{2}\Psi^{\dagger}H_{\text{eff}}\Psi$ through the upper right 2×2 block of $H_{\text{eff}}(\mathbf{p})$,

$$\begin{pmatrix} \Delta^S(\mathbf{p}) & \Delta^T(\mathbf{p}) \\ -\Delta^{T*}(\mathbf{p}) & -\Delta^S(\mathbf{p}) \end{pmatrix}, \quad (\text{D1})$$

where the time-reversal symmetry of H_{eff} enforces $\Delta^S(\mathbf{p}) \in \mathbb{R}$. Because the hole sector of the basis lists spin in the order $(\downarrow, \uparrow)$ rather than $(\uparrow, \downarrow)$, a σ_x permutation of the columns relates Eq. (D1) to the canonical pairing matrix $\Delta(\mathbf{p})$ entering $\frac{1}{2} \sum_{\mathbf{p}, \alpha\beta} \Delta_{\alpha\beta}(\mathbf{p}) d_{\alpha,\mathbf{p}}^{\dagger} d_{\beta,-\mathbf{p}}^{\dagger}$:

$$\Delta(\mathbf{p}) = \begin{pmatrix} \Delta^T(\mathbf{p}) & \Delta^S(\mathbf{p}) \\ -\Delta^S(\mathbf{p}) & -\Delta^{T*}(\mathbf{p}) \end{pmatrix}. \quad (\text{D2})$$

The required antisymmetry $\Delta(-\mathbf{p})^{\top} = -\Delta(\mathbf{p})$ follows from the parities $\Delta^S(-\mathbf{p}) = \Delta^S(\mathbf{p})$ and $\Delta^T(-\mathbf{p}) = -\Delta^T(\mathbf{p})$. The antiunitary time-reversal operator $\mathcal{T} = \mathcal{U}_{\mathcal{T}}K$ is invariant under $\mathcal{U}_{\mathcal{T}} \rightarrow e^{i\phi}\mathcal{U}_{\mathcal{T}}$ for any $\phi \in \mathbb{R}$; the unitary representation $\mathcal{T}_{\text{sc}}$ acting on the parent superconductor's spin index therefore carries one free overall phase. Following Ref. [41], we exercise this freedom to render $\Delta(\mathbf{p})\mathcal{T}_{\text{sc}}$ positive-semidefinite. Writing

$$\Delta^S(\mathbf{p}) = |\Delta^S(\mathbf{p})| e^{i\theta}, \quad (\text{D3})$$

with $\theta \in \{0, \pi\}$ a constant phase across the Brillouin zone [and $\theta = \pi$ in our regime, since $\Delta^S(\mathbf{p}) < 0$ throughout, see

Fig. 2(b)], we choose

$$\mathcal{T}_{\text{sc}} = -i e^{-i\theta} \sigma_y, \quad (\text{D4})$$

which reduces to the standard $\mathcal{T}_{\text{sc}} = i\sigma_y$ when $\theta = \pi$. Substituting Eqs. (D3) and (D4) into Eq. (D2) and computing the matrix product entry by entry yields

$$\Delta(\mathbf{p}) \mathcal{T}_{\text{sc}} = \begin{pmatrix} |\Delta^S(\mathbf{p})| & -e^{-i\theta} \Delta^T(\mathbf{p}) \\ -e^{-i\theta} \Delta^{T*}(\mathbf{p}) & |\Delta^S(\mathbf{p})| \end{pmatrix}, \quad (\text{D5})$$

which is Hermitian for $\theta \in \{0, \pi\}$. The structure in Eq. (D5) yields the spectrum

$$\text{eig}[\Delta(\mathbf{p}) \mathcal{T}_{\text{sc}}] = |\Delta^S(\mathbf{p})| \pm |\Delta^T(\mathbf{p})|, \quad (\text{D6})$$

since the phase $e^{-i\theta}$ rotates the in-plane $\mathbf{d}$ -vector but does not alter its magnitude. Both eigenvalues are non-negative if and only if

$$\Delta(\mathbf{p}) \mathcal{T}_{\text{sc}} \geq 0 \iff |\Delta^S(\mathbf{p})| \geq |\Delta^T(\mathbf{p})| \quad \text{for every } \mathbf{p}, \quad (\text{D7})$$

which is the inequality cited in the main text.

APPENDIX E: EFFECTS OF COULOMB INTERACTION

We consider small repulsive interactions $U \ll \Gamma$ and $U > 0$, introduced in Eq. (1). In this limit, a mean-field approximation of the interaction term is considered [62],

$$\begin{aligned} U d_{\uparrow,j}^\dagger d_{\uparrow,j} d_{\downarrow,j}^\dagger d_{\downarrow,j} &\rightarrow -U \langle d_{\uparrow,j}^\dagger d_{\downarrow,j}^\dagger \rangle d_{\uparrow,j} d_{\downarrow,j} \\ &\quad - U \langle d_{\uparrow,j} d_{\downarrow,j} \rangle d_{\uparrow,j}^\dagger d_{\downarrow,j}^\dagger \\ &\quad + U \langle d_{\uparrow,j} d_{\downarrow,j} \rangle \langle d_{\uparrow,j}^\dagger d_{\downarrow,j}^\dagger \rangle. \end{aligned} \quad (\text{E1})$$

We define $\delta := \langle d_{\uparrow,j} d_{\downarrow,j} \rangle$, which needs to be treated self-consistently and assumed to be real. Since the interaction term does not involve bulk modes, the terms can be directly

transferred to the effective Hamiltonian,

$$\begin{aligned} H_U = \sum_{i,j} & (h_{i,j}^N d_{\uparrow,j}^\dagger d_{\uparrow,i} + h_{i,j}^N d_{\downarrow,j}^\dagger d_{\downarrow,i} + h_{i,j}^F d_{\uparrow,j}^\dagger d_{\downarrow,i} \\ & + \Delta_{i,j}^{S,R} d_{\uparrow,j}^\dagger d_{\downarrow,i}^\dagger + \Delta_{i,j}^T d_{\uparrow,j}^\dagger d_{\uparrow,i}^\dagger \\ & + \Delta_{i,j}^{T*} d_{\downarrow,j}^\dagger d_{\downarrow,i}^\dagger) + U\delta^2 + \text{H.c.}, \end{aligned} \quad (\text{E2})$$

where the renormalized singlet superconductivity term reads $\Delta_{i,j}^{S,R} = \Delta_{i,j}^S - U\delta\delta_{i,j}^K$, where $\delta_{i,j}^K$ is the Kronecker delta function. The mean-field parameter δ needs to be treated self-consistently. We write the partition function of the free theory

$$\mathcal{Z} = e^{-\beta U \delta^2} \prod_{\mathbf{k},m} (1 + e^{-\beta E_m(\mathbf{k})}), \quad (\text{E3})$$

where the product is over the occupied bands. The free energy is

$$\mathcal{F} = -k_B T \int d\mathbf{k} \sum_m \ln(1 + e^{-\beta E_m(\mathbf{k})}) + U\delta^2. \quad (\text{E4})$$

The minimization of the free energy reads

$$\left. \frac{\partial \mathcal{F}}{\partial \delta} \right|_{\delta=\delta_R} = 2U\delta_R + \sum_m \int d\mathbf{k} n_F(E_m) \left. \frac{\partial E_m}{\partial \delta} \right|_{\delta=\delta_R} = 0, \quad (\text{E5})$$

where n_F is the Fermi distribution. In our case, the index m takes distinct values for the two helicity bands of our system. In Fig. 5(a), we show the derivative of the free energy with respect to the order parameter $\partial \mathcal{F} / \partial \delta$ for different values of E_R / Δ . The sign of the root of this derivative, δ_R , determines the qualitative influence of the Coulomb interaction on the on-site superconductivity strength. The mean-field Eq. (E5) is approximated in the first iteration of self-consistency. If $\delta_R > 0$ it is enhanced, while for $\delta_R < 0$ it is suppressed. To this end, we show in Fig. 5(b) that δ_R is typically negative for a wide range of parameters when considering a large real-space cutoff. Thus, we conclude that repulsive Coulomb interactions

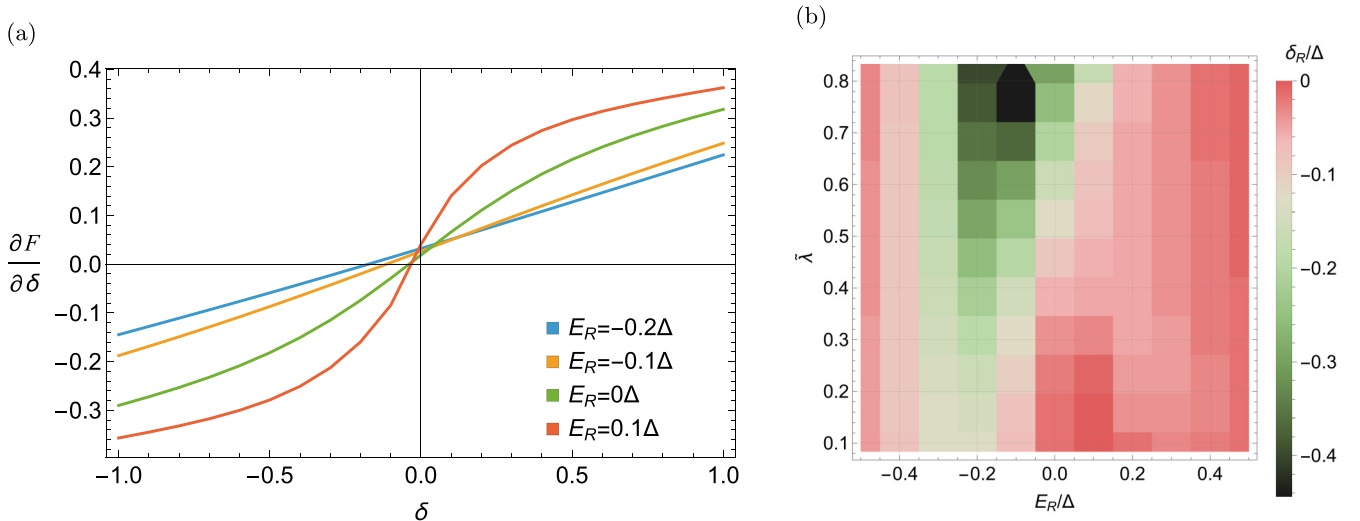


FIG. 5. Suppression of singlet superconductivity in the presence of repulsive on-site interactions, U . (a) Free-energy derivative with respect to the mean-field parameter, $\partial \mathcal{F} / \partial \delta$, as a function of δ for various E_R / Δ around the Fermi level. (b) Mean-field parameter, δ_R , that minimizes the free energy as a function of the renormalized spin-orbit coupling strength $\tilde{\lambda}$ and E_R / Δ . [Parameters: $U = 0.1\Delta$, $\beta = 10$, $k_F a = 1.2$, $m = 10^{-2}(a^2 \Delta)^{-1}$, $|V| = 5\Delta$, a cutoff $N = 300$, and $\tilde{\lambda} = 0.25$ for (a)].

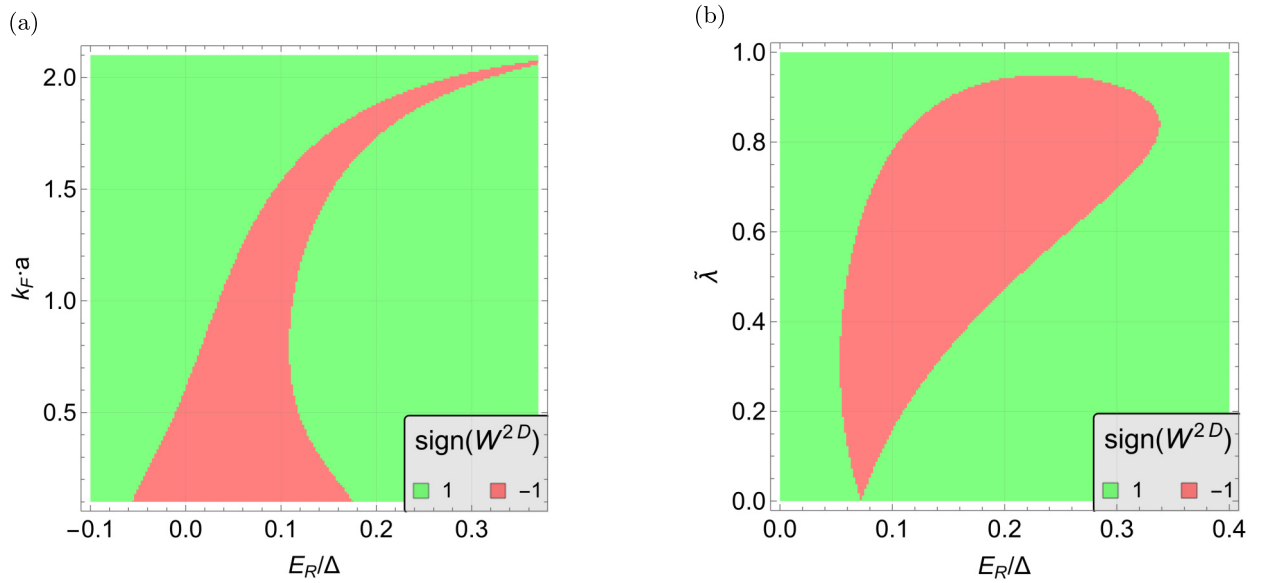


FIG. 6. Topological phase diagram for two-dimensional lattices with periodic boundary conditions with a nearest-neighbor cutoff and a small repulsive on-site interaction $\tilde{U}$. Topological invariant, $\text{sgn}(W^{2D})$, depending (a) on the on-site energy E_R/Δ and the Fermi wave vector $k_F a$ for a fixed renormalized spin-orbit coupling strength $\tilde{\lambda} = 0.25$, and (b) on the on-site energy E_R/Δ and $\tilde{\lambda}$ for $k_F a = 1.2$. [Parameters: $m = 10^{-2}(a^2\Delta)^{-1}$, $|V| = 5\Delta$, and $\tilde{U} = 0.05\Delta$].

suppress the singlet superconductivity, allowing the triplet part to dominate in parts of the Brillouin zone and, eventually, enabling the possibilities for realizing nontrivial topological phases.

APPENDIX F: TOPOLOGICAL INVARIANT IN 2D LATTICES

Here, we demonstrate the topological phases in 2D lattices by numerical computation of the topological invariant W^{2D} . A possible zero-energy crossing in one of the time-reversal inversion symmetric lines of the Brillouin zone $p_y = 0$ or $p_y = \pi$ induces changes in the topological invariant W^{2D} . The topological phase diagram, see Fig. 6, can be directly compared to the 1D case of Fig. 3 in the main text, that has been plotted for the same parameter set. Such a comparison indicates that the 2D geometry can support a nontrivial phase for a broader range of parameters.

APPENDIX G: FOURIER TRANSFORMATION OF MATRIX ELEMENTS IN DENSE 1D CHAINS

Here we focus on some qualitative characteristics of the plots in Fig. 2 and explain them by analyzing the continuous Fourier transform of the singlet, $\Delta_{i,j}^S$, and triplet, $\Delta_{i,j}^T$, superconducting matrix elements in Eq. (5). The continuous

and discrete Fourier transforms are expected to match in the dense limit $k_F a \ll 1$. The argument of the special functions of Eq. (5) is approximately $(k_{F\pm} + i/\xi)a \approx k_{F\pm}a$, in the realistic limit $\xi \gg k_{F\pm}$. For the above, we write the Fourier transforms of the relevant Bessel functions

$$\begin{aligned}\mathcal{F}_{0\pm} &:= \mathcal{F}[J_0(k_{F\pm}|j|)] = \frac{\Lambda_{\pm}(p)}{\sqrt{k_{F\pm}^2 - p^2}}, \\ \mathcal{F}_{1\pm} &:= \mathcal{F}[\text{sgn}(j)J_1(k_{F\pm}|j|)] = \frac{ip\Lambda_{\pm}(p)}{k_{F\pm}\sqrt{k_{F\pm}^2 - p^2}}, \\ \Lambda_{\pm}(p) &= \Theta(p + k_{F\pm}) - \Theta(p - k_{F\pm}),\end{aligned}\quad (\text{G1})$$

where Θ is the Heaviside step function. Despite the considered approximations, the analytical expressions for the superconducting singlet $\Delta^S(p) \sim \Gamma_+ F_{0+} + \Gamma_- F_{0-}$ and triplet $\Delta^T(p) \sim \Gamma_+ F_{1+} - \Gamma_- F_{1-}$ pairings reveal the essential characteristics of Fig. 2 in the main text. In specific, Eq. (G1) predicts divergences at $p = k_{F\pm}$ and a vanishing of the pairings for $|p| > \max(k_{F+}, k_{F-})$ due to the $\Lambda_{\pm}$ factor. These characteristics transcend to the discrete Fourier transform of the singlet and triplet order parameters that we analyze in the main text. Indeed, Fig. 2 reveals finite cusps at momenta $p = k_{F\pm}$ and approximately flat regions, due to the finite cutoff considered, for momenta $|p| > \max(k_{F+}, k_{F-})$.

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