Helical Majorana surface states of strongly disordered topological superconductors with time-reversal symmetry

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Noncentrosymmetric superconductors with strong spin-orbit coupling and the B phase of $^3$He are possible realizations of topological superconductors with time-reversal symmetry. The nontrivial topology of these time-reversal invariant superconductors manifests itself at the material surface in terms of helical Majorana modes. In this paper, using extensive numerical simulations, we investigate the stability and properties of these Majorana states under strong surface disorder, which influences both bulk and surface states. To characterize the effects of strong disorder, we compute the level spacing statistics and the local density of states of both two- and three-dimensional topological superconductors. The Majorana surface states, which are located in the outermost layer of the superconductor, are protected against weak disorder, due to their topological characteristic. Sufficiently strong disorder, on the other hand, partially localizes the surface layer, but leads to the appearance of new extended states in the second and third inward layers. At the crossover from weak to strong disorder the surface state wave functions and the local density of states show signs of critical delocalization. We find that at this crossover the edge density of states of two-dimensional topological superconductors exhibits a zero-energy divergence, reminiscent of the Dyson singularity of quasi-one-dimensional dirty superconductors. Interestingly, we observe that for all disorder strengths and configurations there always exist two extended states at zero-energy that can carry thermal current.

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I. INTRODUCTION

Topological superconductors are attracting a growing interest, due to fundamental considerations as well as potential use for applications in quantum information and device fabrication. As a consequence of the bulk-boundary correspondence, topological superconductors host chiral or helical Majorana states at the material surface. Noncentrosymmetric superconductors (NCSs) with strong spin-orbit coupling have been proposed as candidate materials for time-reversal invariant topological superconductivity, and the B phase of superfluid $^3$He is believed to be an experimental realization of a topological superconductor with time-reversal symmetry. The Majorana states of these systems are protected by time-reversal and particle-hole symmetry and exhibit a helical spin texture. That is, the spin orientation of the surface states is coupled to their momentum.

While due to charge neutrality the helical Majorana mode does not couple to electromagnetic fields, it can be detected by applying an effective gravitational field, i.e., a temperature gradient or rotations of the superconductor. At zero Fermi energy one helical Majorana surface mode carries a quantized thermal conductance, which is given by $\kappa/T = \pi k_B^2 / (6\hbar)$ Since there is no relevant or marginal time-reversal symmetric perturbation that can be added to the surface Dirac Hamiltonian, the helical Majorana state is robust against the influence of weak disorder and interactions.

Only variations of the Fermi velocity are allowed as a symmetry preserving deformation of the effective Dirac equation describing the surface state, and hence an energy gap cannot be opened in the surface spectrum. However, this argument is based on an effective description of the surface state, which breaks down for perturbations with a strength $\gamma$ larger than the bulk superconducting gap $\Delta$. In order to study the effects of disorder with $\gamma \geq \Delta$, the disorder induced coupling between the surface and bulk states needs to be taken into account. While the effects of disorder on topological superconductor surface states have been investigated extensively in terms of low-energy effective Dirac theories, the study of disordered Majorana states at the surface of bulk lattice models has remained an open problem.

In this paper, we examine the effects of strong disorder on the helical Majorana surface modes of two- and three-dimensional topological superconductors in symmetry class DIII using bulk lattice Hamiltonians. This is of relevance for experiments, since surfaces of unconventional superconductors are often intrinsically disordered, or can be disordered on purpose by depositing impurity atoms using, e.g., sputtering techniques. To investigate the effects of strong surface impurities on the surface and bulk quasiparticle wave functions, we employ large-scale numerical simulations of two- and three-dimensional Bogoliubov-de Gennes (BdG) lattice Hamiltonians and compute the local density of states and the level spacing statistics of the wave functions. As a prototypical example of a time-reversal invariant topological superconductor, we consider a noncentrosymmetric superconductor with $(s + p)$-wave pairing symmetry. We find that weak nonmagnetic impurities with $\gamma \ll \Delta$ do not affect the helical Majorana state in any way [Fig. 1(b)], in agreement with the fact that there does not exist any marginal or relevant perturbation of the surface Dirac Hamiltonian. For moderate nonmagnetic impurities with $\gamma \sim \Delta$, the disorder induces a strong coupling between the bulk and surface states. With increasing disorder strength $\gamma$ the wave functions in the surface layer become less and less delocalized and eventually show a probability density that is reminiscent of critical delocalization [Fig. 1(c)]. Strong disorder with $\gamma \gg \Delta$, on the other hand, induces localization in the surface layer and leads to the emer-
gence of new extended states in the second and third inward layers. Interestingly, we find that for all disorder strengths extended zero-energy states exist, which indicates that a diffusive thermal metal phase cannot be realized at the surface of a class DIII topological superconductor. Finally, we also consider magnetic surface disorder, which removes the time-reversal symmetry protection of the surface states. We find that whether the Majorana surface state is gapped out, sensitively depends on the direction in which the impurity spins are polarized (Fig. 7).

This paper is organized as follows. In Sec. II we introduce the BdG Hamiltonian describing a noncentrosymmetric superconductor with nontrivial topology, discuss its symmetry properties, and derive the surface Dirac Hamiltonian. Using exact diagonalization we investigate in Sec. II A and Sec. II B the influence of nonmagnetic impurities on the surface states of three-dimensional and two-dimensional topological superconductors, respectively. To this end, we compute the local surface density of states, the momentum-resolved spectral function, and the level spacing statistics. This is followed by a brief discussion of the effects of magnetic surface disorder in Sec. IV. We conclude in Sec. V with a summary and an outlook on future work.

II. SURFACE STATES OF TIME-REVERSAL INVARIANT TOPOLOGICAL SUPERCONDUCTORS

As a prototypical example of a time-reversal invariant topological superconductor in class DIII we study two- and three-dimensional noncentrosymmetric superconductors. Fully gapped noncentrosymmetric superconductors with dominant triplet pairing have been shown to be topologically nontrivial both in two and three dimensions.

A. Model definition

At a phenomenological level noncentrosymmetric superconductors can be described by a $4 \times 4$ BdG Hamiltonian
\[
\mathcal{H} = \frac{1}{2} \sum_k \Phi_k^\dagger H_k \Phi_k,
\]
with
\[
H_k = \begin{pmatrix}
\Delta_k^\dagger & -h^T_{-k} \\
-h_k & \Delta_k
\end{pmatrix},
\]
and the Nambu spinor $\Phi_k = (c_{k \uparrow}, c_{k \downarrow}, c_{-k \uparrow}, c_{-k \downarrow})^T$, where $c_{k \sigma}$ represents the electron annihilation operator with momentum $k$ and spin $\sigma$. The normal part of the Hamiltonian $h_k = \varepsilon_k \sigma_0 + \lambda \sigma_k$ describes electrons on a square or cubic lattice with kinetic term $\varepsilon_k = \sum_{i=1}^{d} t \cos(k_i) - \mu$. Here, $t$ denotes the nearest-neighbor hopping amplitude, $\mu$ is the chemical potential, $\sigma$ is the vector of Pauli matrices, $\lambda \sigma_k$ represents a Rashba-type spin-orbit coupling with strength $\lambda$, and $d \in \{2,3\}$ is the spatial dimension. The antisymmetric spin-orbit coupling vector $I_k$ is restricted by the symmetries of the noncentrosymmetric crystal. In the following we consider a three-dimensional NCS with cubic point group $O$ as well as a two-dimensional NCS with tetragonal point group $C_{4v}$. Within a tight-binding expansion, the lowest order term for the cubic point group $O$ is written as
\[
I_k = \sin k_x \hat{x} + \sin k_y \hat{y} + \sin k_z \hat{z}.
\]

Examples of $O$ point-group NCSs include Mo$_3$Al$_2$C, Li$_2$Pd$_4$Pt$_3$-P, La$_3$Rh$_4$Sn$_3$, and La$_3$Rh$_4$Sn$_3$. For the $C_{4v}$ point group, which is relevant for thin films of CePt$_3$Si, we have
\[
I_k = \sin k_y \hat{x} - \sin k_x \hat{y}.
\]

In passing we note that two-dimensional topological superconductors with SOC given by Eq. (1c) can also be engineered in heterostructures, for example, by depositing a material with strong SOC on a conventional $s$-wave superconductor.

In the absence of inversion symmetry the superconducting gap function $\Delta_k$ contains both spin-singlet and spin-triplet pairing components
\[
\Delta_k = (\Delta_s \sigma_0 + \Delta_t \mathbf{d}_k \cdot \sigma)(i\sigma_2),
\]
where $\Delta_s$ and $\Delta_t$ denote the spin-singlet and spin-triplet pairing amplitudes, respectively. The triplet pairing vector $\mathbf{d}_k$ is assumed to be aligned with the spin-orbit pseudovector $I_k$, since this choice maximizes the superconducting transition temperature. Moreover, we take the pairing amplitudes $\Delta_s$ and $\Delta_t$ to be real and positive. For our numerical calculations, we set the model parameters to $t = 4.0$, $\lambda = -2.0$, $\Delta_s = 0.5$, and $\Delta_t = 2.0$. For the three-dimensional NCS with SOC (1d) we set the chemical potential to $\mu = 8.0$, whereas for the two-dimensional NCS with SOC (1c) we set $\mu = 4.0$. We have checked that our results do not depend on the particular choice of the model parameters as long as the triplet pairing component is dominant, i.e., $\Delta_t > \Delta_s$.

Hamiltonian (1) is invariant under all the symmetries of symmetry class DIII. That is, $H_k$ satisfies time-reversal symmetry $T^{-1} H_{-k} T = H_k$, with $T^2 = -1$, and particle-hole symmetry $C^{-1} H_{-k} C = -H_k$, with $C^2 = +1$. The time-reversal and particle-hole symmetry operators are given by $T = \sigma_0 \otimes i\sigma_2 \mathcal{K}$ and $C = \sigma_1 \otimes \sigma_0 \mathcal{K}$, respectively, where $\mathcal{K}$ denotes the complex conjugation operator. For dominant triplet pairing $\Delta_t > \Delta_s$, Hamiltonian (1) is topologically nontrivial both in two and three dimensions. In three dimensions, the topological characteristics are described by a three-dimensional winding number ($Z_2$-type invariant), while in two dimensions the topology is characterized by a $Z_2$ index.

B. Effective low energy Hamiltonian

Before studying the effects of surface disorder, let us first derive a low-energy effective Dirac Hamiltonian describing the helical Majorana surface states both for the three-dimensional and two-dimensional topological NCS.

1. Surface states of three-dimensional topological NCS

In the long-wave-length limit, we can disregard the momentum dependence of the normal part of the Hamiltonian
and replace \( h_k \) by a position-dependent mass term \( m(z) \), with \( m(z) \rightarrow +m_0 \) for \( z \rightarrow +\infty \) and \( m(z) \rightarrow -m_0 \) for \( z \rightarrow -\infty \), which describes a domain wall centered at \( z = 0 \). The domain-wall bound states can be written as
\[
e^{i(k_l x + k_y y)}\psi_{1(2)}^{2D}(z),
\]
with
\[
\psi_{1(2)}^{2D}(z) = \exp \left[ \int_0^z \frac{m(z')}{\Delta} \right] \psi_{1(2)}^{2D},
\]
\[
\psi_{1(2)}^{2D} = \frac{1}{\sqrt{2}}(i, 0, 0, 1)^T, \quad \text{and} \quad \psi_{2(2)}^{2D} = \frac{1}{\sqrt{2}}(0, i, 1, 0)^T,
\]
where we have neglected the influence of a finite spin-singlet pairing amplitude. The low-energy effective Hamiltonian \( \tilde{H}_k \) for the surface state is obtained by projecting the Hamiltonian onto the subspace \( \Psi^{2D} = \{ \psi_{1(2)}^{2D}, \psi_{2(2)}^{2D} \} \) spanned by the two bound-state wavefunctions \( \psi_{1(2)}^{2D} \) and \( \psi_{2(2)}^{2D} \), i.e.,
\[
\tilde{H}_k^{2D} = \langle \psi^{2D} | H_k | \psi^{2D} \rangle = \Delta_1(k_x \sigma_1 - k_y \sigma_2).
\]
Time-reversal and particle-hole symmetry operators in the subspace formed by the surface modes are given by \( T_{2D} = -i \sigma_3 K \) and \( C_{2D} = -i \sigma_1 K \), respectively. These two symmetries severely restrict the possible perturbations that can be added to the surface Hamiltonian \( \Gamma \). We find that the mass term \( m \sigma_0 \) is prohibited by time-reversal symmetry, whereas the chemical potential \( \mu \sigma_0 \) is forbidden by particle-hole symmetry. Moreover the \( U(1) \) gauge potentials \( A_x \sigma_2 \) and \( A_y \sigma_1 \) are disallowed since they break both time-reversal and particle-hole symmetry. The only symmetry-allowed perturbations are variations of the spin-triplet amplitude \( \Delta_1 \) which are odd in momentum \( k \). These momentum-dependent perturbations can be neglected in the long-wave-length approximation.

However, the effective description \( \Gamma \) does not capture perturbations with a magnitude larger than the gap energy \( \Delta_1 \). Hence, the helical Majorana states could potentially become unstable in the presence of surface disorder with a strength \( \gamma > \Delta_1 \). We will study this question in detail in Sec. III using exact diagonalization of the bulk Hamiltonian \( \mathcal{H} \).

2. Edge states of two-dimensional topological NCS

Repeating similar steps as above, we find that the low-energy Hamiltonian describing the edge states of a two-dimensional topological superconductor in class DIII is given by
\[
\tilde{H}_k^{1D} = \langle \psi^{1D} | H_k | \psi^{1D} \rangle = -\Delta_1 k_x \sigma_3,
\]
where \( \psi^{1D} \) is the space formed by the edge modes, which is spanned by \( \psi_1^{1D} = \frac{1}{\sqrt{2}}(0, i, 0, 1)^T \) and \( \psi_2^{1D} = \frac{1}{\sqrt{2}}(-i, 0, 1, 0)^T \). Time-reversal and particle-hole symmetry

![Graph](image-url)
in the edge-mode subspace read $\tilde{T}_{1D} = -i\sigma_2 K$ and $\tilde{C}_{1D} = -i\sigma_3 K$, respectively. As before, we find that there is no symmetry-allowed mass term that can be added to the edge Hamiltonian (3), indicating that the helical Majorana edge modes are robust against disorder with strength $\gamma < \Delta_1$. To demonstrate that the two-dimensional topological NCS, as opposed to the three-dimensional one, has a $\mathbb{Z}_2$-type topological characteristic, let us consider a doubled version of the edge Hamiltonian (3), i.e., $\Delta_1 k_x \sigma_3 \otimes \sigma_0$. In contrast to Hamiltonian (4) the doubled Hamiltonian $\Delta_1 k_x \sigma_3 \otimes \sigma_0$, can be fully gapped out by the symmetry preserving mass term $m \sigma_2 \otimes \sigma_2$. That is, two-dimensional topological NCS are characterized by an odd number of Kramer’s pairs of Majorana edge states.

### C. Surface disorder

To study the stability of the helical Majorana states under strong surface disorder, we consider uncorrelated random on-site potentials given by

$$\mathcal{H}_{\text{imp}} = \sum_{k,q} \Phi_k^{\dagger} V_q^{\beta} \Phi_{k+q},$$

where $V_q^{\beta} = (1/\sqrt{N}) \sum_n v(n) S^{\beta} e^{-i q \cdot r_n}$ denotes the Fourier transform of the on-site potentials $v(n) S^z$ at the surface sites $r_n$ with strength $v(n)$. We investigate the effects of both nonmagnetic impurities ($\beta = 0$) and magnetic scatterers ($\beta = \{x, y, z\}$) described by $v(n) S^{\beta} = v(n) \sigma_3 \otimes \sigma_0$ and $v(n) S^{\beta = \{x, y, z\}} = v(n) \sigma_3 \otimes \sigma_1, \sigma_0 \otimes \sigma_2, \sigma_2 \otimes \sigma_3$, respectively. The disorder distribution is assumed to be Gaussian like, i.e., for each lattice site on the surface the local potential $v(n)$ is drawn from a box distribution with $p[v(n)] = 1/\gamma$ for $v(n) \in [-\gamma/2, +\gamma/2]$. As discussed above, nonmagnetic disorder with $\gamma < \Delta_1$ does not couple to the surface states. Impurity spins, on the other hand, lift the time-reversal protection of the helical Majorana modes and can therefore strongly modify the surface states even for $\gamma < \Delta_1$. Within the low-energy theory of Sec. II B, we find that impurity spins give rise to the following additional term in the low-energy Hamiltonian (3) describing the helical Majorana modes of the three-dimensional topological NCS

$$\langle \psi^{2D} \mid V_{q}^{\beta} \mid \psi^{2D} \rangle = \begin{cases} v_q \sigma_3 & \text{if } \beta = z \\ 0 & \text{otherwise} \end{cases}.$$  

That is, only the out-of-plane spin component of magnetic impurities couples to the surface states. Similarly, the edge states of the two-dimensional topological NCSs only couple to the $x$ spin component of impurity spins, since

$$\langle \psi^{1D} \mid V_{q}^{\beta} \mid \psi^{1D} \rangle = \begin{cases} -v_q \sigma_1 & \text{if } \beta = x \\ 0 & \text{otherwise} \end{cases}.$$  

### III. NUMERICAL RESULTS

Using exact diagonalization algorithms we compute the eigenenergies $E_m$ and eigenstates $\varphi_m$ of $H_k$, Eq. (1), in the presence of surface disorder described by Eq. (5). The effects of surface impurities are best revealed in the local surface density of states

$$\rho_l(\omega, r_n) = \frac{\hbar}{4\pi} \Im \sum_{j=1}^{4} \sum_m \frac{\left| \varphi_m(l, r_n, j) \right|^2}{\omega - E_m + i\eta},$$

and the momentum-resolved spectral function

$$A_l(\omega, k \parallel j) = \frac{\hbar}{4\pi} \Im \sum_{j=1}^{4} \sum_m \frac{\left| \varphi_m(l, k \parallel j) \right|^2}{\omega - E_m + i\eta},$$

with $\varphi_m(l, r_n, j) = (1/\sqrt{N}) \sum_n \varphi_m(l, r_n, j) e^{-ik \parallel j \cdot r_n}$. Here, $k \parallel j$ denotes the surface momentum, $r_n$ are the surface
sites, \( l \) represents the layer index, and \( j \) is the combined spin and particle-hole index. The expressions \( \langle \Phi_m(l, r) \rangle^2 \) are evaluated with an intrinsic broadening \( \gamma = 0.05 \) for finite lattices of size up to \( 50 \times 20 \times 30 \) in three dimensions and \( 1000 \times 40 \) in two dimensions.

To obtain further insight into the localization or delocalization properties of the surface states we also compute the level spacing distribution function \( P(s) \), where \( s = |E_m - E_{m+1}|/\delta(E_m) \) is the normalized spacing between two nearest levels \( E_m \) and \( E_{m+1} \) with \( \delta(E_m) \) the mean level spacing near \( E_m \). We note that for systems with a density of states that changes rapidly with energy [see, e.g., Fig. 3(a)], the normalization of the level spacing intervals by the mean level spacing \( \delta(E_m) \) is particularly important. As usual, the probability distribution \( P(s) \) is normalized such that \( \int_0^\infty P(s)ds = 1 \) and \( \int_0^\infty sP(s)ds = 1 \). In a disordered quantum system the energy level distribution reflects the localization properties of the system.\(^{22,63} \) In a delocalized phase nearby energy levels repel each other leading to a Wigner-Dyson-like level statistics. In a localized phase, on the other hand, different levels can be arbitrarily close to each other, which gives rise to Poissonian statistics.

### A. Three-dimensional topological NCS

We start by discussing the effects of nonmagnetic disorder on the helical Majorana states of three-dimensional topological NCSs. Figures 1(a)-(e) show the spectral function \( A(\omega, k_x) \) integrated over the three outermost layers, which is of the order of the decay length of the subgap surface states. In the clean case, \( \gamma = 0 \), surface states exist at energies smaller than the bulk energy gap \( \Delta = \Delta_x = \Delta_y = 1.5 \) and form a helical Majorana cone, which is centered at the \( \Gamma \) point of the surface Brillouin zone [Fig. 1(a)]. In accordance with the discussion of Sec. II B, we find that weak and even moderately strong disorder leaves the spectral function almost unchanged, apart from small broadening effects [Figs. 1(b) and 1(c)]. That is, the surface states are mostly located in the outermost layer \( l = 1 \) and remain unaffected by nonmagnetic impurities of strength \( \gamma \sim \Delta \). Conversely, strong surface disorder with strength of the order of the band width, \( \gamma \simeq 5t \), completely destroys the momentum-space structure of the subgap surface states. For this disorder strength, the wave function probability densities \( |\Phi_m(l, r)|^2 \) exhibit sharp peaks, see Figs. 1(f) and 1(g). The real-space structures of \( |\Phi_m(l, r)|^2 \) for different wave functions with nearby energies appear to be correlated, forming clusters of differently colored peaks. In other words, the surface state wave functions show signs of critical delocalization. Finally, for extremely strong impurity scatterers \( \gamma \gg t \), almost fully localized impurity states are formed in the surface layer, while in the second and third outermost layers extended states reemerge, forming helical Majorana bands with a well-defined linear dispersion [Figs. 1(e), 1(h) and 1(i)]\(^{22,63} \).

To obtain further insight into the localization and delocalization properties of the surface states, it is instructive to examine the probability distribution of the local density of states \( P[\tilde{\rho}_l(\omega)] \), where

\[
\tilde{\rho}_l(\omega) = \rho_l(\omega)/\langle \rho_l(\omega) \rangle
\]

represents the local density of states normalized to its mean value \( \langle \rho_l(\omega) \rangle \) on the \( l \)-th layer. Figure 2 displays the layer-resolved probability distribution of \( \tilde{\rho}_l(\omega) \) for energies within the interval \( |\omega| < \Delta/3 \). In the weakly disordered case [Fig. 2(a)], \( P[\tilde{\rho}_l] \) exhibits a narrow peak at \( \tilde{\rho}_l = 1 \), indicating that the surface states are unperturbed by the impurities and hence completely delocalized. For very strong surface scatterers [Fig. 2(c)], on the other hand, the probability distribution \( P[\tilde{\rho}_l(\omega)] \) for the surface layer \( l = 1 \) is peaked at \( \tilde{\rho}_1 = 0 \), which signals localization\(^{22} \) whereas \( P[\tilde{\rho}_l(\omega)] \) for the next three inward layers \( l = 2, 3, 4 \) has a maximum at \( \tilde{\rho}_l = 0 \). Together with the results of Fig. 1 this demonstrates that for strong disorder with \( \gamma \gg t \), helical Majorana states with well-defined momenta reemerge in the second and third inward layers, while the outermost layer becomes (almost) localized. At the crossover from the weak to the strong disorder regime, which occurs at \( \gamma \simeq 5t \), \( P[\tilde{\rho}_l(\omega)] \) in all four layers shows a broad peak. The disorder-averaged total density of states \( \rho_{tot}(\omega) = \sum_l \sum_{r_n} \rho_l(\omega, r_n) \) in Fig. 3(a) reveals that for \( \gamma = 5t \) there exists a large number of ingap states, which completely fill up the superconducting gap. For even larger disorder strength, \( \gamma \gg t \), on the other hand, the num-
The effects of disorder on the superconductor and its surface states effectively become weaker. Importantly, we find that for all disorder strengths and disorder configurations there exist two extended zero-energy Majorana surface states [see red traces in Fig. 1(i)-(i)]. These zero-energy modes appear in the total density of states of Fig. 2(a) as a narrow peak at $\omega = 0$.

Finally, we present in Fig. 2(b) the level spacing distribution function $P(s)$ for ingap states with energies within the interval $|\omega| < \Delta/3$ in the presence of surface disorder with strength $\gamma = 5t$ and $\gamma = 30t$. Interestingly, we find that for $\gamma = 5t$ the level statistics $P(s)$ fits the generalized Wigner surmise (see Ref. 25). This indicates that the ingap states remain delocalized with significant overlap, giving rise to level repulsion. For $\gamma = 30t$, however, there are deviations from the generalized Wigner surmise, which we attribute to (almost) localized states in the strongly disordered surface layer $l = 1$. These localized states do not exhibit level repulsion and hence lead to Poissonian level spacing statistics, which is superimposed on the class DIII level statistics of the extended states in the second and third layers.

### B. Two-dimensional topological NCS

Next, we examine the helical Majorana states at the edge of a two-dimensional topological NCS with nonmagnetic edge disorder. In Fig. 4 we present the spectral function $A(\omega, k_x)$, Eq. (8), summed over the three outermost layers. As for the three-dimensional NCS, we find that in the clean case, $\gamma = 0$, edge states appear at energies smaller than the bulk gap $\Delta$, forming two Majorana bands that cross at $k_x = 0$ of the surface Brillouin zone [Fig. 4(a)]. As a consequence of time-reversal symmetry, ingap states with opposite edge momenta have opposite spin polarization. This completely prohibits backscattering among the edge states by nonmagnetic impurities. Moreover, as discussed in Sec. 1B, the only symmetry allowed perturbation of the edge Hamiltonian is $\gamma = 0$, which is a variation of the superconducting gap $\Delta$, i.e., changes in the Fermi velocity of the Majorana bands. Hence, one expects that nonmagnetic disorder with strength $\gamma \leq \Delta$ does not affect the surface states, which is confirmed by our numerical results in Fig. 4(b). Indeed, for $\gamma \leq \Delta$ the probability distribution $P(\ln(\omega))$ of the ingap states shows a sharp peak at $\gamma = 30t$ [Fig. 5(a)], indicating that the edge states are completely delocalized.

For stronger edge disorder with $\gamma$ of the order of the band width $5t$, the spectral function $A(\omega, k_x)$ becomes smeared out, but a clear momentum-space dispersion is still visible. We find that for this disorder strength extended edge states, which form Majorana bands with well-defined dispersions, strongly interact with more localized ingap states. Moreover, comparing Figs. 4(a) and 4(b), we observe that edge disorder significantly modifies the Fermi velocity of the Majorana modes, particularly around zero energy. Interestingly, at $\gamma = 5t$ the probability distribution $P(\ln(\omega))$ is strongly broadened [Fig. 5(b)] and the disorder-averaged total density of states $\rho_{\text{tot}}(\omega)$ exhibits a pronounced peak at $\omega = 0$ (blue trace in Fig. 6). The latter is reminiscent of the Dyson singularity at zero-energy which occurs in (quasi-)one dimensional dirty superconductors belonging to symmetry class DIII [60-63]. That is, the spectral function of Fig. 3(d) and the total density of states of Fig. 6 indicate that the edge states near zero energy have different (de)localization properties than the ones further away from the band center. Further increasing the disorder strength to $\gamma = 30t$, we observe that the number of ingap states decreases, the height of the zero-energy peak in $\rho_{\text{tot}}$ is reduced significantly, and the Majorana bands recover a perfectly linear dispersion (Fig. 4(e) and red trace in Fig. 6). This shows that the effects of the edge disorder on the bulk superconductor and its Majorana ingap states effectively decreases for $\gamma \gg t$. In fact, just as for the three-dimensional topological superconductor, very strong impurity scatterers give rise to almost fully localized edges states in the surface layer, while the extended states that form the Majorana bands are now located in the second and third outermost layers [Fig. 5(c)]. Overall, we find that disorder affects the Majorana modes of two-dimensional topological NCSs less strongly than those of three-dimensional topological NCSs. In part, this is due to the helical spin texture of the Majorana modes, which completely prohibits backscattering at the one-dimensional NCS edge, whereas it only partially suppresses scattering across the
Majorana cone of a three-dimensional topological NCS.

IV. MAGNETIC SURFACE DISORDER

Magnetic surface disorder lifts the time-reversal symmetry protection of the helical Majorana cone and therefore can induce a full gap in the surface spectrum. In Figs. 7(a)-(b) we show the spectral function $A(\omega, k_z)$ integrated over the three outermost layers at the (001) surface of a three-dimensional topological NCS in the presence of magnetic surface disorder with $\gamma = \Delta t$. In (a), (b), and (c) the impurity spins are polarized along the $x$, $y$, and $z$ axes, respectively. Here, we discretized the Hamiltonian on a cubic lattice of size $50 \times 20 \times 30$. (d)-(f) show the same as (a)-(c) but for the (01) edge of a two-dimensional topological NCS on a square lattice of size $80 \times 40$.

V. CONCLUSIONS AND OUTLOOK

In this paper we have used large-scale exact diagonalization and the recursive Green’s function technique to study the effects of strong surface disorder on the Majorana surface bands of two- and three-dimensional topological superconductors in symmetry class DIII. In order to determine the effects of strong disorder, we have computed the level spacing statistics and the local density of states of single particle wave functions. Weak disorder with strength $\gamma$ smaller than the bulk superconducting gap $\Delta$, does not perturb the surface Majorana cone, since there exists no relevant or marginal symmetry-allowed term that can couple to the surface Dirac Hamiltonian. Very strong disorder with $\gamma$ much larger than the bandwidth $4t$, however, partly localizes the states in the outermost layer, while in the second and third inward layers extended states reappear, which form linearly dispersing Majorana bands. Interestingly, we find that at the crossover from weak to strong disorder (i.e., for $\gamma \approx 5t$) the surface state wave functions exhibit signs of critical delocalization, particularly around zero energy. We find that for $\gamma \approx 5t$, the density of states of the two-dimensional topological superconductor diverges at zero energy, which is similar to the Dyson singularity of disordered (quasi)-one-dimensional superconductors. Our numerical data show that for all disorder strengths and configurations two extended zero-energy states exist. These findings suggest that no diffusive state can be realized at the edge or surface of a topological superconductor.

The (de)localization properties of the wave functions at the crossover from weak to strong disorder, i.e., e.g., the (multifractal) scaling properties, deserve further investigation. Moreover, it would be interesting to study the (de)localization properties of weak topological superconductors or of three-dimensional topological superconductors with more than one Majorana cone (i.e., winding number $\nu > 1$). Our findings are of relevance for fully gapped superconductors with time-reversal symmetry and (dominant) spin-triplet pairing. For example, $\text{Li}_2\text{Pt}_3\text{Bi}$, $\text{CePt}_3\text{Si}$, $\text{Cu}_x\text{Bi}_2\text{Se}_3$, $\text{Cu}_x\text{(PbSe)}_2\text{(Bi}_2\text{Se}_3)_6$, and $\text{(Ag}_x\text{Pb}_1-x\text{Se}_5\text{(Bi}_2\text{Se}_3)_y}$ have been proposed as possible realization of this unconventional superconducting phase. Tunneling experiments on disordered surfaces of these systems can be used to confirm our predictions.

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Note that Eqs. (6) and (7) are only valid in the limit of vanishing spin-orbit coupling, $\lambda = 0$, and zero spin-singlet pairing amplitude, $\Delta_s = 0$.

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