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Driving topological phases by spatially inhomogeneous pairing centers

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We investigate the effect of periodic and disordered distributions of pairing centers in a one-dimensional itinerant system to obtain the microscopic conditions required to achieve an end Majorana mode and the topological phase diagram. Remarkably, the topological invariant can be generally expressed in terms of the physical parameters for any pairing center configuration. Such a fundamental relation allows us to unveil hidden local symmetries and to identify trajectories in the parameter space that preserve the nontrivial topological character of the ground state. We identify the phase diagram with topologically nontrivial domains where Majorana modes are completely unaffected by the spatial distribution of the pairing centers. These results are general and apply to several systems where inhomogeneous perturbations generate stable Majorana modes.

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Introduction. A topological phase is generally marked by quantized macroscopic observables which are insensitive to perturbations of the local environment [1–3], as for the well-known example of the quantum Hall effect [4,5]. In many cases, however, there is a limitation on the allowed perturbations, leading to so-called symmetry protected topological phases [6–8]. Strong topological phases are due to global symmetries, such as time-reversal, particle-hole, or chirality, while translation or point group symmetries of the lattice lead commonly to weak and crystalline topological states [9–13]. Weak or strong character refers to what extent the protecting symmetry can be guaranteed in a realistic configuration. Indeed, while time-reversal symmetry can be controlled by avoiding magnetic impurities, for weak topological phases the translation symmetry can be broken by impurities in a crystal. However, even when disorder breaks the lattice symmetry, a weak topological phase can still be robust if the system remains symmetric on average [14–22].

Though harmful for some types of topological protections, inhomogeneous perturbations have recently provided new perspectives as a rich intrinsic source of topological phases or topological transitions. Some relevant examples of this type are topological Anderson insulators [23,24] and disorder-driven topological superconductivity [25,26]. Impurities with a periodic pattern placed on superconductors or insulators can generally lead to a robust zero energy crossing for increasing impurity strength [27], enabling, among others, topological phases with very large Chern numbers [28]. Thus the use of magnetic impurities represents a consolidated route to manipulate or induce topological phases. For instance, magnetically active dopants on the top of a topological insulator [29–32] are employed to break time-reversal symmetry and give rise to a topological magnetoelectric effect [33]. Even more striking is the example of a one-dimensional (1D) topological superconductor (TSC) obtained through the deposition of a chain of magnetic adatoms on the surface of a superconductor when they order magnetically, even if the superconductor is topologically trivial [34–47].

Remarkably, every TSC can be linked to a p-wave superconductor (PWS) in a suitable limit [6,48–50], as for the paradigmatic case of electrons forming Cooper pairs in the symmetric spin-triplet and orbitally antisymmetric configuration. Such a connection motivated the proposal of artificial TSCs [51–55] and the subsequent observation of Majorana modes in hybrid superconducting (SC) devices [47,56–63]. In this context, the issue of disorder in the employed effectively spinless PWSs is of great relevance, especially in view of any realistic implementation in devices for topological quantum computing. After the pioneering work of Ref. [64], this problem has been largely explored in the literature, mainly focusing on spatially varying the charge potential for periodic [65–68], quasiperiodic [68–70], or disordered [71–74] patterns, indicating that a sufficient strength of SC correlations is basically required to drive the system into a topological phase.

Apart from local charge density disorder, there is another fundamental route to explore the intricate relation between inhomogeneous perturbations and topological behavior in such a class of systems where Majorana modes may occur at the edge. Indeed, impurities can be introduced into a system of itinerant electrons as effective pairing centers (PCs), both by artificial or intrinsic means, thus focusing attention on the role of the profile of the pairing amplitude rather than of the charge density. Such a problem has a broader physical context if one considers the formation in a metallic host of local electronic states that prefers to be either empty or with two paired electrons. Indeed, due to a phononic [75,76] or excitonic [77] origin, PCs can lead to both pairing mechanisms and superconductivity [77–80] in various materials as well as drive superfluid-to-insulator transitions [81]. Furthermore, impurities on the surface of topological insulators or Dirac materials [75,76] have also been suggested as generators of local PCs. Finally, the same physics may arise in spin-orbital coupled quantum systems with a spatially inhomogeneous anisotropic exchange in the presence of impurities with different valence [82,83].

In this Rapid Communication, we investigate the effect of periodic and disordered (within a large unit cell) distributions of effective p-wave PCs in a 1D electron system to obtain the microscopic conditions required for the existence of an end

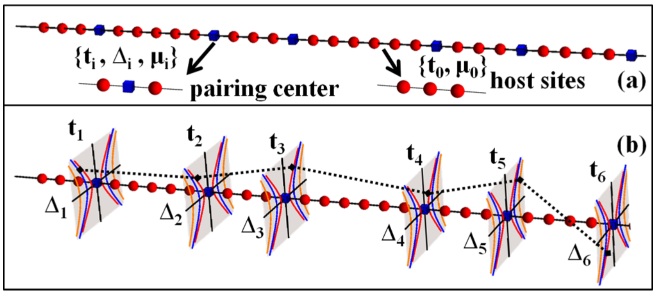

FIG. 1. (a) Schematic representation of a large unit cell of length $L = 30$ sites with $N = 6$ impurities within the 1D chain with spatially inhomogeneous distributed PCs (blue squares) which separate host sites (red circles) and reduce the translational invariance. (b) A representative trajectory (dashed line) in the parameter space connecting different impurities in (a). Local variation along the hyperbolic contours in the shadow plane at the impurity site can lead to topologically equivalent nontrivial trajectories.

Majorana mode. Remarkably, the topological invariant can be generally expressed in terms of the physical parameters for any distribution of the PCs. A striking consequence of the emerging symmetries in the parameter space is the finding of a physical regime where Majorana modes can be completely unaffected by the overall spatial distribution of the PCs.

The model. We investigate a ring described by a 1D tight-binding model of spinless electrons with an inhomogeneous distribution of PCs. The Hamiltonian is a modification of the one originally introduced by Kitaev [84], and includes inhomogeneities generated by diluted PCs distributed in the unit cell of length L. Using system periodicity which introduces momentum k, we get

$$\mathcal{H} = \sum_{\substack{p=1\\k}}^{L} \{t_p c^\dagger_{k,p} c_{k,p+1} + \Delta_p c^\dagger_{k,p} c^\dagger_{-k,p+1} + \text{H.c.} + \mu_p c^\dagger_{k,p} c_{k,p}\}, \tag{1}$$

with boundary conditions $c_{L+1,k} \equiv e^{ik} c_{1,k}$ and $\{t_p, \Delta_p\}$ being the nearest-neighbor (NN) hopping and on-bond pairing amplitudes, respectively. We assume that there are N impurities in the unit cell labeled by i at generic (but non-neighboring) positions $\{p_i\}$ along the chain such that $\Delta_p \neq 0$ only at the bonds around them, i.e., $\Delta_{p_i - 1} = \Delta_{p_i} \equiv \Delta_i$. The hopping and chemical potential for the host subsystem take uniform values, $t_p \equiv t_0$ and $\mu_p \equiv \mu_0$ (which can be transformed to an alternating $\mu_p = (-1)^p \mu_0$; see the Supplemental Material [85]), while at the host-impurity bonds these parameters are given by arbitrary amplitudes, $t_{p_i - 1} = t_{p_i} \equiv t_i$ and $\mu_{p_i} = \mu_i$ (see Fig. 1). The Hamiltonian belongs to the BDI class of the Altland-Zirnbauer classification [48] and it can have a nontrivial topological phase characterized by a $\mathbb{Z}$ winding number—finite $\mathbb{Z}$ implies end Majorana modes in an open chain, as explicitly demonstrated in the Supplemental Material [85] for a representative case.

For real values of the parameters, due to the chiral symmetry, $\mathcal{H}$ Eq. (1) can be cast into a purely block-off diagonal form with antidiagonal blocks given by matrices $\mathbf{u}_k$ and $\mathbf{u}_k^\dagger$. Hence, as long as the eigenvalues of $\mathbf{u}_k$ are gapped, its determinant $\det \mathbf{u}_k$ can be used to get the winding number $\mathbb{Z}$ by evaluating its trajectory in the complex plane. We observe that the phase of the determinant is a topological invariant because it is not related to any symmetry breaking and it can only change when it goes through zero. In general, by a Laplace transformation we have that $\det \mathbf{u}_k = \alpha(\mathcal{A} + \mathcal{B} \cos k + i\,\mathcal{C} \sin k)$, with α, $\mathcal{A}$, $\mathcal{B}$, and $\mathcal{C}$ being real coefficients that are independent of k. Then, a general condition for a nontrivial $\mathbb{Z}$ is provided by having both (i) $|\mathcal{A}| < |\mathcal{B}|$ and (ii) $\mathcal{C} \neq 0$, giving $\mathbb{Z} = \pm 1$ for positive/negative $\mathcal{C}$.

Symmetry features of the topological invariant. The central result obtained in this Rapid Communication is the general analytical expression for the topological invariant of an inhomogeneous quantum system. This outcome allows us to unveil the emergent symmetries in the parameter space and to predict the key physical regimes for the occurrence of Majorana end modes. By means of an inductive construction and a recursive relation in terms of the number of impurities within the unit cell, the coefficient $\mathcal{A}$ is

$$\begin{aligned}\mathcal{A} = {} & \cos(L\eta_0) + \sum_{i=1}^{N} y_i \sin(L\eta_0) \\ & + 2^1 \sum_{i<j} y_i y_j \sin(d_{ij}\eta_0) \sin(d_{ji}\eta_0) \\ & + 2^2 \sum_{i<j<k} y_i y_j y_k \sin(d_{ij}\eta_0) \sin(d_{jk}\eta_0) \sin(d_{ki}\eta_0) + \cdots \\ & + 2^{N-1} y_1 y_2 \cdots y_N \sin(d_{12}\eta_0) \sin(d_{23}\eta_0) \cdots \sin(d_{N1}\eta_0),\end{aligned} \tag{2}$$

where d_{ij} are the *ordered* distances between impurities which cover the unit cell for each term of this expansion, i.e., $d_{ij} \equiv p_j - p_i$ for $j > i$ and $d_{ji} \equiv L - p_j + p_i$ for the second line, etc. (see the Supplemental Material [85]). The above equation can be written in a compact form, $\mathcal{A} = \cos(L\eta_0) + \mathrm{Tr}\{(\mathbf{1} - 2\mathbf{M}_1\mathbf{Y})^{-1}\mathbf{M}_2^T\mathbf{Y}\}$, in terms of two triangular matrices of the impurities' distances $\mathbf{M}_1$ and $\mathbf{M}_2$, and a diagonal matrix $\mathbf{Y}$. These matrices have the following nonvanishing entries: $(\mathbf{M}_1)_{ij} = \sin(\eta_0 d_{ij})$, $(\mathbf{M}_2)_{ij} = \sin[\eta_0(L - d_{ij})]$ for $j \geqslant i$ and $\mathbf{Y}_{ii} = y_i$. Here, $\eta_0 = \arccos[\mu_0/(2t_0)]$ is the effective inverse Fermi length of the host, and y_i are dimensionless variables related to the parameters at the impurity and in the host via

$$y_i = \frac{t_0\left(J_i^{-1} - J_0^{-1}\right)}{\sqrt{4 - \mu_0^2/t_0^2}}, \tag{3}$$

with $J_i = (t_i^2 - \Delta_i^2)/\mu_i$ being a renormalized energy scale that includes effectively the particlelike and holelike transfer processes between the impurities and the host. Similarly, for the host, one has $J_0 = t_0^2/\mu_0$. Concerning $\mathcal{B}$ and $\mathcal{C}$, it is convenient to parametrize the set $\{t_i, \Delta_i, \mu_i\}$ at each host-impurity bond using hyperbolic coordinates as $t_i = r_i \cosh \phi_i$, $\Delta_i = r_i \sinh \phi_i$, and $\mu_i = r_i^2 J_i^{-1}$, because they explicitly manifest their unique dependence on the hyperbolic angles as

$$\mathcal{B} = \cosh\left(2\sum_{i=1}^{N} \phi_i\right), \quad \mathcal{C} = \sinh\left(2\sum_{i=1}^{N} \phi_i\right). \tag{4}$$

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Hence, the topological invariant has a highly symmetric structure in the parameter space. The coefficient $\mathcal{A}$ depends both on impurity-host and host bonds whereas the coefficients $\mathcal{B}$ and $\mathcal{C}$ contain only information about the impurity-host bonds through the sum of all hyperbolic angles. Note that the same properties hold in a general case of $\{t_p,\Delta_p,\mu_p\}$ taking an arbitrary value on every bond/site (see the Supplemental Material [85]). Benefiting from the analytical expression of the winding number, we can easily unveil hidden symmetries for the trajectories in the parameter space.

First, a variation in the local angles $\{\phi_i\}$, akin to a relativistic Lorentz rotation, will not affect the amplitude of $\mathcal{B}$ as far as the sum of all angles stays unchanged. In this respect a given value of $\mathcal{B}$ corresponds to many equivalent trajectories in the $\{t_i,\Delta_i,\mu_i\}$ multidimensional space [see Fig. 1(b)]. In general, it is always possible to turn the system topological by changing one hyperbolic angle to satisfy the condition $|\mathcal{A}| < |\mathcal{B}|$. This uncovers a nonlocal way to employ inhomogeneous perturbations for either driving a topological transition or for keeping unchanged the topological character of the ground state. The second symmetry aspect is related to the amplitude scaling of the impurity parameters. Indeed, a local scaling of μ_i and r_i^2 by the same factor will leave unchanged the amplitudes $\{y_i\}$. Moreover, either a cyclic translation of all the impurities in the unit cell or having a multiplied unit cell will not affect the coefficient $\mathcal{A}$.

Finally, from the inspection of Eq. (2), we observe that there exists a special point in the parameter space where all $\{y_i\}$ vanish, i.e., at $J_i \equiv J_0$, which is a resonance condition between the host and impurities. Then, a special critical point emerges in the phase diagram where the interference between the impurities and the host makes $\mathcal{A}$ insensitive to the actual spatial distribution of impurities.

Periodic and disordered impurity pattern. A topological domain can be obtained by imposing the condition $|\mathcal{A}| < 1$. By construction, $|\mathcal{B}| \geqslant 1$, so for any choice of hyperbolic angles $\{\phi_i\}$ such a region in the parameter space will be topologically nontrivial. For values $|\mathcal{A}| > 1$ there can be regions with an end Majorana mode, nevertheless their boundaries would be exponentially unstable to small changes in the parameters. In Figs. 2(a)–2(d) we report the evolution of the topological domains for a single impurity unit cell in terms of the key physical parameters related to the impurity-host competition, i.e., $y_i \equiv y_{\rm imp}$ and μ_0/t_0. The domains always extend around the line of the impurity-host resonance at $y_{\rm imp} = 0$ for which $|\mathcal{A}| \leqslant 1$. We observe that the topological domains evolve around the nodal lines of $\mathcal{A}$, and their number is $\lceil L/2 \rceil$. Finally, for all the cases the topological regions never extend beyond $|\mu_0| = |2t_0|$, where the trigonometric functions in $\mathcal{A}$ become hyperbolic—this corresponds to the topological boundary of the pure Kitaev model [84].

The question of having slightly different y_i's at the two PCs is addressed in Fig. 2(e) when we double the unit cell of length $L = 4$ [compare with Fig. 2(c)] and set $y_1 = y_{\rm imp}$, $y_2 = 0.9 y_{\rm imp}$. We see that the topological domains split into halves with narrow inclusions of the trivial phase and the number of nodal lines of $\mathcal{A}$ doubles. More splitting appears when we impose a small perturbation of the impurity positions [see Fig. 2(f)] by taking a tenfold unit cell of $L = 5$ [compare with Fig. 2(d)] and by moving one impurity (out of $N = 10$) by one site.

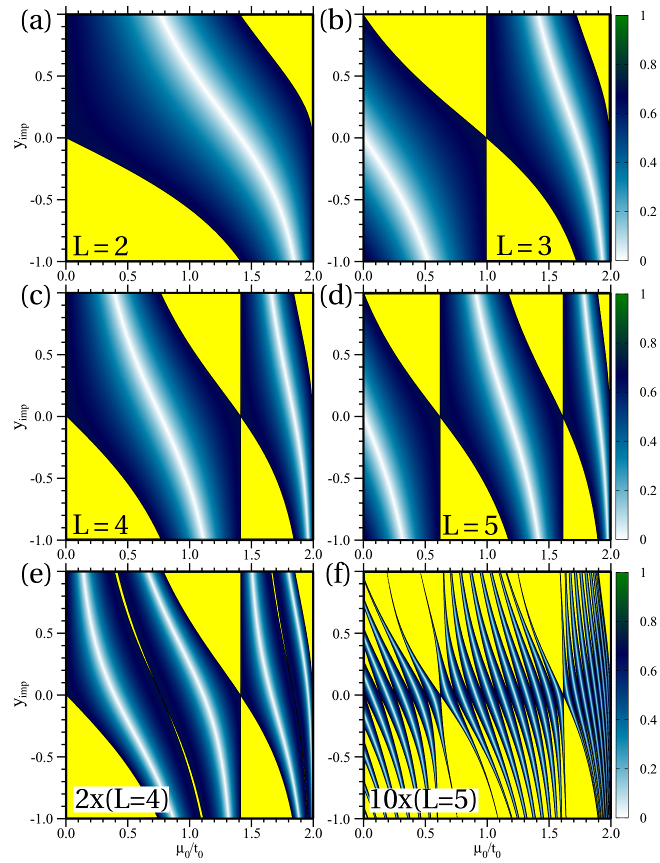

FIG. 2. Topological domains (blue regions) with (a)–(d) small unit cells of the lengths $L = 2, \ldots, 5$ with a single impurity and $y_i \equiv y_{\rm imp}$, (e) doubled unit cell of $L = 4$ and perturbed y_i, i.e., $y_1 = y_{\rm imp}$ and $y_2 = 0.9\, y_{\rm imp}$ with impurities at regular position $p_i = 4i$, and (f) tenfold unit cell of $L = 5$ and perturbed position of the last impurity by one bond, i.e., $p_i = 5i$ for $i = 1, \ldots, 9$ and $p_{10} = 51$ with $y_i \equiv y_{\rm imp}$. The color map indicates values of $|\mathcal{A}|$ in the topological domains. Yellow regions are for topologically trivial configurations.

Topological domains persist for dilute impurities in large unit cells ($N \ll L$), as seen for a dimerized system with two distances between NN PCs, $d_{12} = 40$ and $d_{21} = 60$ ($L = 100$) and $y_i \equiv y_{\rm imp}$ [see Fig. 3(a)]. Next, we randomize the NN distances so that for every bond $d_{i,i+1} = \{40,60\}$ with the same probability and implement the constraint that the total number of short/long bonds is the same. After averaging over 1000 random configurations of unit cells with $L = 1000$ and $N = 20$, we obtain a complex interference pattern of many harmonics of η_0, which destroys some of the vertical legs of the initial topological region of Fig. 3(a) and adds a subtle parabolic modulation on top of it [see Fig. 3(b)]. Introducing complete randomness of the positions of PCs modifies the domains further [see Fig. 3(c)]. The long vertical legs are gone and the entire topological region does not extend beyond $|y_{\rm imp}| < 0.25$. Interestingly, the subtle parabolic features remain with some characteristic points on the horizontal axis (such as $\mu_0/t_0 = 0.6, 1.5, 1.9$) around which the tips of many vertically shifted parabolas seems to accumulate. We note that adding even a significant random modulation of y_i around $y_{\rm imp}$

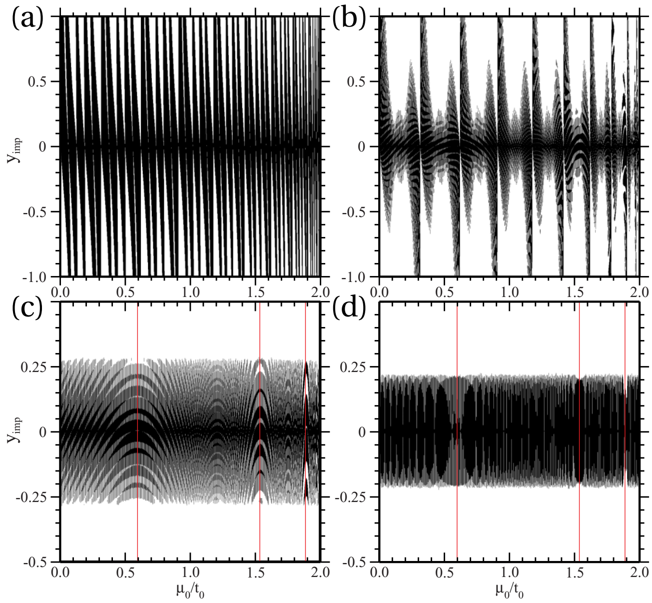

FIG. 3. Topological domains (black) for equivalent PCs, $y_i \equiv y_{\rm imp}$, in (a) a dimerized system with alternating distance between NN impurities $d_{1,2} = 40$, $d_{2,1} = 60$, and $L = 100$, (b) a system with the unit cell of $L = 1000$ and $N = 20$ impurities with NN distances taking random and equiprobable values of 40 or 60, and (c) the same system with random distribution of impurities and $d_{ij} > 1$. The random signs of y_i, i.e., $y_i \equiv \pm y_{\rm imp}$, are added to the case (c) in plot (d). Red lines indicate $\mu_0/t_0 \simeq 0.6, 1.54, 1.9$, for which a zoomed view of the interference fringes is reported in the Supplemental Material [85].

does not change this result much as long as the signs of y_i are fixed.

The parabolic features are suppressed and the domains gain a mirror symmetry around $y_{\rm imp} = 0$ when the signs of $\{y_i\}$ are random [see Fig. 3(d)]. Quite surprisingly, the characteristic μ_0/t_0 points still host some distinct interference features. The overall width of the topological window is further reduced, but only slightly. Note that lowering the concentration of PCs does not change much the subtle features of topological regions of Figs. 3(c) and 3(d)—only the width of the topological window is increased as the number of terms in $\mathcal{A}$ drops with N.

Conclusions. We provide a different perspective on the way to get Majorana end modes in 1D itinerant systems by means of an inhomogeneous distribution of PCs. The structure of the topological invariant uncovers the reasons why domains in the parameter space can be so robust to the local variations of impurity PCs. Such a response to inhomogeneous perturbations is a generalization of the Kitaev model within the Altland-Zirnbauer classification and goes beyond the expectation from density disorder.

An interesting aspect of our analysis points to the possibility of having zero energy modes in the interior of the 1D diluted Kitaev chain. Such an occurrence can be captured by searching for a parameter configuration satisfying $\mathcal{C} = 0$ and $|\mathcal{A}| < |\mathcal{B}|$. This condition implies that the determinant $\det[\mathbf{u}_k]$ vanishes at a given k. Hence, if the obtained zero energy states are not accidentally occurring at the boundary, they must be in the interior of the system. Therefore, the combination of $\mathcal{C} = 0$ and the topological regions for which $|\mathcal{A}| < |\mathcal{B}|$ makes a guide for the search for nontrivial states in the interior of the 1D diluted Kitaev chain. Another path to engineer inhomogeneous topological phases can be achieved by designing the system as a series of topologically inequivalent domains. For instance, by selecting the microscopic parameters for the impurity and the host such that the neighboring domains have different winding numbers (e.g., they are topologically inequivalent), Majorana modes would occur at the domain boundary in the interior of a quantum system.

Furthermore, for completeness, we observe that the modification of the kinetic term with the inclusion of long-range hopping is expected to lead to multiple Majorana end modes both in spinless [86] and spinful p-wave SC chains [87]. We also point out that for the case of intrinsic diluted pairing centers, the model Hamiltonian in Eq. (1) would strictly apply only in the weak-coupling regime. Therefore, it is challenging to investigate to what extent the overall scenario will be modified by including finite NN interactions without any decoupling [88].

Various realizations of the presented topological states may be possible. One way is to design a mesoscopic array of SC dots coupled to a metallic host in such a way that close to the dot an effective spin-triplet pairing is induced, e.g., by employing a spin orbit and external magnetic field. Here, a local tuning of the superconducting amplitude can be achieved by external perturbations, while the hopping connectivity among the pairing centers might be tailored by the distance between the dots, or by suitably varying the conducting channels linking the dots. Another possible realization is in doped 1D spin-orbital quantum systems where the coupling between the host and dopants could be converted into effective pairing terms for the spin or the orbital channel. One could then atomically design doped quantum chains that map onto the Kitaev model [84] with diluted PCs. Then, the present study may stimulate different directions of research on the generation and manipulation of Majorana states and their design for topological quantum computing [89,90].

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