Topological quantum wires with balanced gain and loss

Henri Menke* and Moritz M. Hirschmann†
Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, D-70569 Stuttgart, Germany
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We study a one-dimensional topological superconductor, the Kitaev chain, under the influence of a non-Hermitian but $\mathcal{PT}$-symmetric potential. This potential introduces gain and loss in the system in equal parts. We show that the stability of the topological phase is influenced by the gain/loss strength and explicitly derive the bulk topological invariant in a bipartite lattice as well as compute the corresponding phase diagram using analytical and numerical methods. Furthermore, we find that the edge state is exponentially localized near the ends of the wire despite the presence of gain and loss of probability amplitude in that region.

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I. INTRODUCTION

Since the successful fabrication of topological insulators [1] and superconductors [2] in the last decade, enormous progress has been made in understanding and optimizing these nontrivial topological phases of matter. The first reported topologically nontrivial state, the integer quantum Hall effect [3], exhibits a fully gapped bulk with gapless chiral edge states. It is distinct from other states like the quantum spin Hall effect in the sense that it does not rely on any symmetries of the Hamiltonian. The quantum spin Hall state is only robust against perturbations which do not break time-reversal symmetry [4]. This symmetry protection can be generalized and has been summarized in periodic tables of topological insulators and superconductors [5–9]. Topological superconductors are particle-hole symmetric and exhibit gapless surface states. The particlelike and holelike excitations are an analogy to particle and antiparticle pairs which allows a description in terms of Majorana fermions [10].

Symmetries of the Hamiltonian operator are relevant in the field of non-Hermitian quantum mechanics [11,12]. The postulates of quantum mechanics demand that observables are represented by Hermitian operators which have real eigenvalues. It was shown by Bender and Boettcher [13] that the weaker constraint of parity-time ($\mathcal{PT}$) symmetry is sufficient for an operator to have a purely real eigenspectrum. Still, the eigenstates of an *a priori* $\mathcal{PT}$-symmetric Hamiltonian can spontaneously break the $\mathcal{PT}$ symmetry [14]. These non-Hermitian systems play an important role in physics and have been studied in the context of localization-delocalization transitions of flux lines in type-II superconductors [15], the disordered Anderson model [16], dissipative quantum systems [17,18], and most recently in topological insulators [19–23] and topological superconductors [24–27]. Experimental realizations have been achieved in photonic lattices and photonic crystals [28–31].

An open quantum system where the probability amplitude is not conserved and which is subject to in and out flux in the time evolution but still supports stationary solutions is called a system with balanced gain and loss. Gain and loss effects are usually studied with the non-Hamiltonian approach of a Lindblad master equation [32]. In a mean-field description this can be substituted by imaginary potentials fulfilling $\mathcal{PT}$ symmetry, as has been studied for Bose-Einstein condensates [33,34].

In this paper, we consider an extension of the well-known Kitaev chain [10] using $\mathcal{PT}$-symmetric potentials to introduce balanced gain and loss effects. This model has been investigated before in the context of the interplay between $\mathcal{PT}$-symmetry breaking and the topological phase [24–26]. We analytically derive the topological invariant given by the Pfaffian for a specific choice of the potential and compare it to numerical results. Furthermore, we study the localization properties of the edge state in the topological regime by the generating function approach [35]. Using this method, we analytically compute the decay constant of the edge state in the bulk and find a criterion for the topological phase transition.

II. KITAEV CHAIN WITH GAIN AND LOSS

The symmetries $\mathcal{P}$ and $\mathcal{T}$ are defined as the space-reflection (parity) and time-reversal operator with the actions $t \to t$, $x \to -x$, $i \to i$ and $t \to -t$, $x \to x$, $i \to -i$, respectively, with t denoting time and x denoting position. In the discrete lattice case, these actions can be described by $\mathcal{P} c_n \mathcal{P} = c_{N+1-n}$ and $\mathcal{T} i \mathcal{T} = -i$ with annihilation (creation) operators c_n ($c_n^\dagger$). A Hamiltonian operator is considered to be $\mathcal{PT}$ symmetric if it commutes with the union of the $\mathcal{P}$ and $\mathcal{T}$ operator $[\mathcal{PT}, H] = 0$. It is not necessary that H commutes with either of the operators alone.

Let us consider an in general non-Hermitian system which has $\mathcal{PT}$ symmetry. Furthermore, it is subject to particle-hole symmetry which means the Hamiltonian fulfills $H_{\mathrm{PHS}} = -\tau_1 H_{\mathrm{PHS}}^T \tau_1$ with τ_1 denoting the first Pauli matrix. $\mathcal{PT}$ symmetry of a Hamiltonian H implies $O^\dagger H^* O = H$ with a unitary matrix O.

The presence of particle-hole symmetry allows us to apply a basis transformation M to Majorana operators which relates the matrix H via $H = (i/4) M^\dagger X M$ to X which is skew symmetric. Under the change of basis the commuting $\mathcal{PT}$ symmetry $[\mathcal{PT}, H] = 0$ becomes an anticommuting one $\{U, X\} = 0$, where U is an antiunitary symmetry (see Appendix A). For the simplest case of an orthogonal matrix O

*h.menke@fkf.mpg.de
†m.hirschmann@fkf.mpg.de

and vanishing diagonal elements in X, we obtain

$$\mathrm{Pf}(X)^* = \mathrm{Pf}(OXO^T) = \mathrm{Pf}(X)\det(O) = \mathrm{Pf}(X), \quad (1)$$

i.e., a real Pfaffian. For a more detailed and general discussion we refer to the Appendixes. Therefore, we have shown that the sign of the Pfaffian is well defined in certain non-Hermitian systems with $\mathcal{PT}$ symmetry. The sign of the Pfaffian is known to be related to the $\mathbb{Z}_2$ topological invariant for the symmetry class D of Hermitian systems. Accordingly, we suggest that the same invariant may also be used to classify these $\mathcal{PT}$-symmetric non-Hermitian systems. We will elaborate this statement with an example where the continuity between a Hermitian and a non-Hermitian system is evident.

In the following, we consider a system described by a non-Hermitian Hamiltonian H with $\mathcal{PT}$ symmetry. It consists of a Hermitian part H_0 which is in our case given by the Kitaev chain Hamiltonian and a non-Hermitian U which commutes with the $\mathcal{PT}$ operator. In general, one has

$$H = H_0 + U, \quad U \neq U^\dagger. \quad (2)$$

We will refer to this full Hamiltonian as the extended Kitaev chain in this paper. The Kitaev chain Hamiltonian was introduced in Ref. [10] as a pedagogical model to describe topological superconductivity in a chain of spinless fermions. The Hamiltonian reads as

$$H_0 = \sum_n \left[t c_n^\dagger c_{n+1} + \Delta c_n c_{n+1} - \frac{\mu}{2} c_n^\dagger c_n + \mathrm{H.c.} \right] \quad (3)$$

with the hopping amplitude t, the p-wave pairing parameter $\Delta = |\Delta| e^{i\theta}$, and the chemical potential μ. The operators c_n ($c_n^\dagger$) are the fermionic annihilation (creation) operators of quasiparticles. In general, the Hamiltonian (3) is not $\mathcal{PT}$ symmetric, but for a choice of the superconducting phase $\theta = \pm\pi/2$ it is [24]. Therefore, we write (3) as

$$H_0 = \sum_n \left[t c_n^\dagger c_{n+1} + i\Delta c_n c_{n+1} - \frac{\mu}{2} c_n^\dagger c_n + \mathrm{H.c.} \right], \quad (4)$$

where the gap parameter Δ is real.

We investigate two choices for the potential U. One simple $\mathcal{PT}$-symmetric potential is given by alternating gain and loss at each site. This potential is chosen because the full Hamiltonian can then be diagonalized analytically by enlarging the unit cell. The expression reads as

$$U_1 = \sum_n (-1)^n i\gamma c_n^\dagger c_n, \quad (5)$$

where γ is a real number. The other choice breaks Hermiticity only in some regions of the chain. To consider a general way of in- and out-coupling fermions, we take the complex potential over a partitioning of $N/2 - f$ with $f \in \mathbb{N}_0$ starting from the edges

$$U_2 = i\gamma \left[-\sum_{n=1}^{N/2-f} c_n^\dagger c_n + \sum_{n=N/2+f}^{N} c_n^\dagger c_n \right]. \quad (6)$$

III. TOPOLOGICAL INVARIANT

In previous works [24,25], the influence of the $\mathcal{PT}$-symmetry-breaking transition on the topological phases of the Kitaev chain has been studied. However, the explicit computation of the topological invariant can be achieved for non-Hermitian systems as shown, for example, in Ref. [36]. Hu and Hughes [19] state a no-go theorem for topological insulator phases in $\mathcal{PT}$-symmetric systems showing that they cannot have a real eigenvalue spectrum but leave topological superconductors open for discussion. Purely real spectra of topological superconductors in the presence of a non-Hermitian potential have been discussed in Ref. [24].

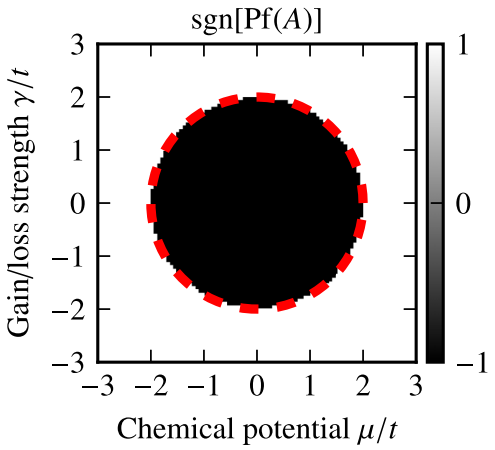

FIG. 1. Topological phase diagram for the Kitaev chain with $N = 100$ sites and the alternating potential (5) for $t = 1$ and $\Delta = 1$. The color map indicates the sign of the Pfaffian where -1 (black) means topological and $+1$ (white) means trivial. The dashed line corresponds to the analytically calculated phase boundary.

Depending on the gap parameter Δ, the Kitaev chain can belong to two different Altland-Zirnbauer symmetry classes [5–8]. For real $\Delta \in \mathbb{R}$ it belongs to class BDI whereas for complex $\Delta \in \mathbb{C}$ it is in class D. For class BDI the invariant is a winding number and has $\mathbb{Z}$ character. In class D the invariant is $\mathbb{Z}_2$ and is determined by the Pfaffian [10].

The Pfaffian is calculated by bringing the Hamiltonian itself into a skew-symmetric form and the topological invariant is determined by the sign of the Pfaffian. Now that the Hamiltonian contains non-Hermitian terms the Pfaffian is not necessarily real. It can be shown, however (see Appendix A), that in case of a non-Hermitian $\mathcal{PT}$-symmetric onsite potential the Pfaffian remains a real quantity which leaves the sign well defined and renders it eligible as a topological invariant for the model at hand.

For the potential in Eq. (5), the Pfaffian can be calculated analytically (see Appendix B). In this case, the Pfaffian is purely real and the sign of the Pfaffian is well defined. In addition, we find a circle criterion for the phase where the Pfaffian is negative

$$\mu^2 + \gamma^2 < 4t^2. \quad (7)$$

Due to the presence of edge states, we will refer to this as the topologically nontrivial phase. The sign of the Pfaffian can also be extracted from a real-space tight-binding calculation and it is found that the analytical and the numerical results coincide perfectly. The corresponding topological phase diagram is shown in Fig. 1.

For noninteracting Hermitian systems, the topological phase transition is accompanied by a gap closing. Therefore,

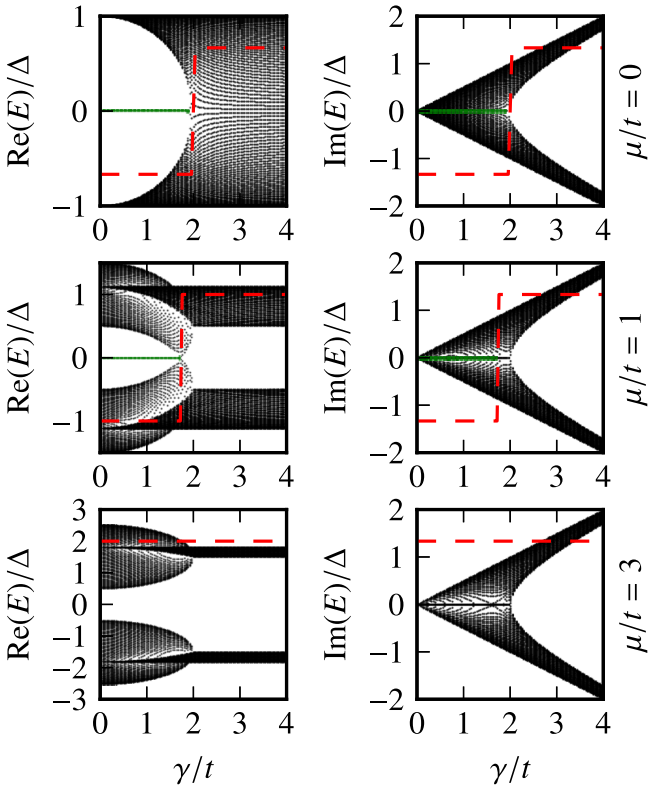

FIG. 2. We show spectra for a chain with $N = 100$ sites and the alternating potential (5) at different chemical potential over the gain/loss strength γ. The dashed line indicates the sign of the Pfaffian invariant. Zero modes [$\mathrm{Re}(E) = \mathrm{Im}(E) = 0$] are highlighted with green dots. Evidently, the potential can close the gap and lead to a topological phase transition. In the topological regime, we always have a state at zero energy.

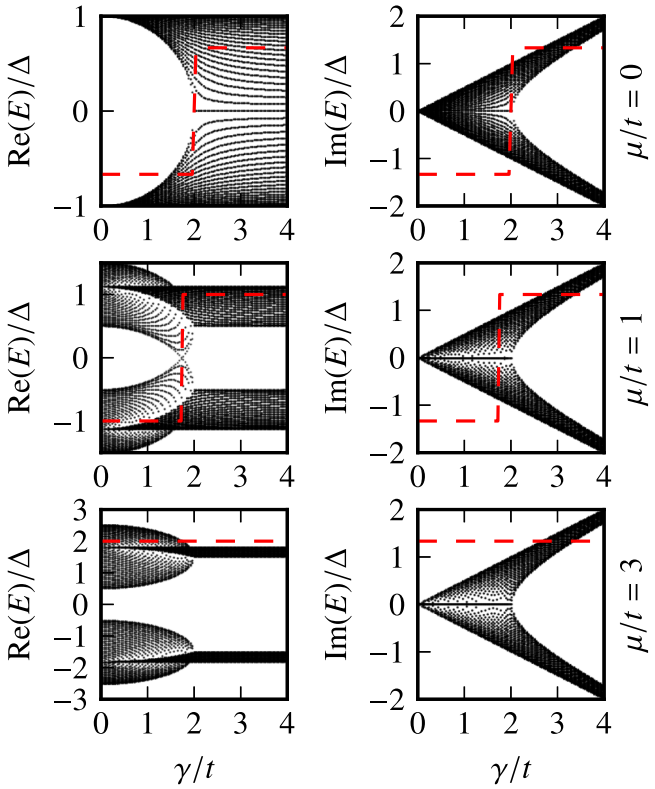

FIG. 3. We show bulk spectra for a chain with $N = 100$ sites and the alternating potential (5) at different chemical potential over the gain/loss strength γ. The dashed line indicates the sign of the Pfaffian invariant. For periodic boundary conditions, the spectra differ qualitatively from open boundary conditions.

we compute the spectrum of the extended Kitaev chain for various choices of the chemical potential and observe the real and imaginary parts of the eigenvalues as a function of the gain/loss strength γ. Relevant eigenvalue spectra are shown in Fig. 2. The $\mathcal{PT}$-unbroken states of the system are those with imaginary part $\mathrm{Im}(E) = 0$ which do not decay in the time evolution. The boundary states with zero energy are hence $\mathcal{PT}$ unbroken and robust against gain and loss even during time evolution. The bulk spectrum for this system, which we show in Fig. 3, differs qualitatively from the open chain, as has been observed before for a different system in Ref. [22]. Parameters $\mu/t = 0$ and 1 correspond to systems which can be topologically nontrivial according to Eq. (7) while $\mu/t = 3$ always corresponds to the trivial case. Figures 2 and 3 show that the gapless state of the open system is not present in the bulk system as it is expected for edge states. We find that at the topological phase transition, the real part undergoes a bulk gap closing whereas the imaginary part, which is zero in the topological regime, might open a gap, here for $\mu = 0$. The phase transition is characterized by a gap closing in the modulus of the energy eigenvalue.

IV. EDGE-STATE LOCALIZATION

Since a complex potential can be interpreted as particles added or removed from the system, it seems natural to expect a modified spatial dependence of the edge states. To verify this expectation we can apply the generating function method which relates the exponential decay of the edge states in the bulk to the poles of said function [35]. We will assume in the following calculation that the imaginary potential extends over a boundary region that is large compared to the extension of the edge state such that we can assume the potential as homogeneous, such as given for the partitioning potential in Eq. (6). Edge states of topological nature should reside at zero energy. Therefore, we start with the ground state of the system $|0\rangle$ which fulfills $H|0\rangle = E_g|0\rangle$ where we set the energy $E_g = 0$. On top of this, we then can start to look for edge states with an ansatz for the wave function $|\psi\rangle = \sum_{j=1}^{N}(c_j^\dagger \psi_j^A + c_j \psi_j^B)|0\rangle$ with $\psi_j^A, \psi_j^B \in \mathbb{C}$.

By applying the anticommutation relations for the fermion ladder operators as well as the previous relations, we can rewrite the eigenvalue equation $H\psi = E\psi$ into two coupled recursion relations for the coefficients ψ_j^A and ψ_j^B:

$$\Gamma_2 \psi_{j+1} + \Gamma_2^\dagger \psi_{j-1} - \Gamma_1 \psi_j = 0, \tag{8}$$

where $\psi_j = (\psi_j^A, \psi_j^B)^T$ and

$$\Gamma_1 = \begin{pmatrix} \mu + i\gamma + E & 0 \\ 0 & -\mu - i\gamma + E \end{pmatrix},$$
$$\Gamma_2 = \begin{pmatrix} t & -i\Delta \\ i\Delta & -t \end{pmatrix}. \tag{9}$$

Following the scheme laid out in the literature we multiply by z^j where $z \in \mathbb{C}$ and sum over j to rewrite the recursion relation as

$$g(z) = (\Gamma_2 - z\Gamma_1 + z^2\Gamma_2^\dagger)^{-1}\Gamma_2\psi_1, \tag{10}$$

where we defined the local generating function

$$g(z) = \sum_j z^{j-1}\psi_j. \tag{11}$$

Let us consider the edge of the system at $j = 1$. An edge state is expected to decay exponentially, i.e., $\psi_j \propto 1/z_1^j$ with increasing j. It can be proven [35] that poles of the generating function $g(z)$ are positioned at the decay constants z_1. The only poles our generating function may have arise in the determinant $\det(\Gamma_2 - z\Gamma_1 + z^2\Gamma_2^\dagger)$ which appears in the denominator during the calculation of the inverse matrix. The poles can be calculated analytically and for zero-energy edge states $E = 0$ they are given by

$$z_{a,b} = \frac{i\gamma + \mu + a\sqrt{4(-t^2 + \Delta^2) + (\mu + i\gamma)^2}}{2(t + b\Delta)} \tag{12}$$

with $a,b \in \{-1,1\}$.

There are four constants for each system parameter set, yet only those greater than 1 may contribute to a state localized at the edge $j = 1$. Those less than 1 correspond to the edge state that would appear at the opposite end of the chain. But, since the complex potential has a different sign at the other side, these solutions have to be discarded here. Obviously, similar results with a different sign of γ hold for the other edge. A comparison to numerical results validates the approach. The constants of exponential decay are given in Fig. 4(a). Clearly, a large complex potential, i.e., a large exchange of probability amplitude into or from the system, extends the edge states into the bulk which is as it is expected. Observe the divergence in Fig. 4(b) for $\mu = 0$ and $\gamma = 0$ which corresponds to perfectly localized Majorana edge states in the Hermitian system. At one value of γ at each μ the decay constants coalesce at magnitude 1. The notion of edge states is not valid anymore and the zero-energy state extends into the bulk at least as far as the approximation of constant complex potential holds true. Interestingly, the values of this intersection coincide with the sign change of the Pfaffian. For $t = \Delta$ the decay constants intersect at 1 for

$$\mu^2 + \gamma^2 = 4t^2, \tag{13}$$

which is the equation that gives the phase boundary as it appeared before in an analytical calculation of the Pfaffian invariant (see Appendix B for a comparison with numerical results).

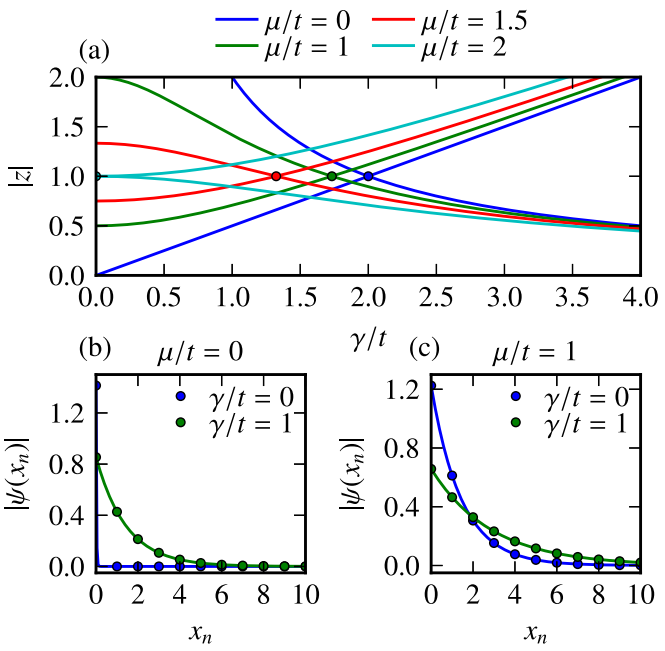

FIG. 4. (a) Modulus of the poles of the generating function for $t = \Delta$. The modulus of the pole gives the decay constant of the edge state. Their intersection at $|z| = 1$ corresponds to the topological phase transition which is also found in the numerical calculation of the Pfaffian (filled dots). In (b) and (c), the dots denote the unnormalized edge state from a numerical calculation with $N = 100$ sites overlayed with lines for the analytical solution.

V. CONCLUSION

We studied the Kitaev chain, a one-dimensional topological superconductor, hosting Majorana edge modes under the influence of balanced gain and loss from an imaginary $\mathcal{PT}$-symmetric potential. We explicitly showed that the Pfaffian invariant is well defined for a $\mathcal{PT}$-symmetric onsite potential and correctly reproduces the topological phase behavior. We computed the Pfaffian invariant analytically for an alternating non-Hermitian lattice and matched the results with numerical tight-binding calculations.

By the generating function approach we computed the decay constants of the edge state into the bulk. It is remarkable that despite the gain and loss effects at the boundaries of the system, the edge state is exponentially localized. The decay constants depend on the gain/loss strength γ and the intersection of the two solutions reproduces the phase boundary as found in numerical calculations.

The successful identification of a topological invariant in this non-Hermitian system is a step towards a symmetry-based classification of topological phases in non-Hermitian quantum systems. It is also conceivable that a similar system is realized experimentally with optical resonators [30,37].

ACKNOWLEDGMENT

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APPENDIX A: TOPOLOGICAL INVARIANT

For the Pfaffian invariant to be useful for the class of systems considered in this paper, it has to be well defined. In our case of non-Hermitian system the problem of a nonzero imaginary part could arise such that we cannot evaluate a sign of the Pfaffian.

The extended Kitaev chain is motivated by preserving $\mathcal{PT}$ symmetry of the non-Hermitian potential, which we will use in the following. A general particle-hole-symmetric matrix

$H_{\mathrm{PHS}} = -\tau_1 H_{\mathrm{PHS}}^T \tau_1$ can be written in Bogoliubov–de Gennes (BdG) form as

$$H = \psi^\dagger \begin{pmatrix} a & b \\ c & -a^T \end{pmatrix} \psi \quad \text{with} \quad b = -b^T, c = -c^T, \tag{A1}$$

where a, b, and c are matrices that fulfill the given relations and ψ refers to a Nambu spinor encompassing ladder operators for all sites. Introducing Majorana operators will lead to new spinors γ and a Hamiltonian in the form

$$H = \frac{i}{4} \gamma X \gamma. \tag{A2}$$

The matrix X is skew symmetric $X^T = -X$ and takes the form

$$X = \begin{pmatrix} -i(a - a^T + b + c) & -(a + a^T - b + c) \\ a + a^T + b - c & -i(a - a^T - b - c) \end{pmatrix}. \tag{A3}$$

If H is Hermitian, then $X^\dagger = -X$ and

$$\mathrm{Pf}(X)^* = \mathrm{Pf}(X^*) = \mathrm{Pf}(-X^T) = \mathrm{Pf}(X), \tag{A4}$$

such that the Pfaffian can only be a real number.

If the original Hamiltonian fulfills $\mathcal{PT}$ symmetry, each block will obey a similar relation

$$U^\dagger H^* U = H \Rightarrow u^\dagger d^* u = d, \quad d \in \{a, b, c\} \tag{A5}$$

where u is one diagonal block of the unitary matrix U

$$U = \begin{pmatrix} u & 0 \\ 0 & u \end{pmatrix}, \tag{A6}$$

which assumes that the time-reversal symmetry is chosen in such a way that it does not mix creation and annihilation operators:

$$X^* = U \begin{pmatrix} i(a - a^T + b + c) & -(a + a^T - b + c) \\ a + a^T + b - c & i(a - a^T - b - c) \end{pmatrix} U^\dagger. \tag{A7}$$

To see how the symmetry for H translates to a symmetry for X, we have to apply the unitary transformation M that relates the original basis to the Majorana basis

$$\mathcal{H} = \frac{i}{4} \psi^\dagger M^\dagger M(-4i) H M^\dagger M \psi =: \frac{i}{4} \gamma X \gamma, \tag{A8}$$

where $\psi = (\psi_I, \psi_I^\dagger)^T$ with ψ_I is the vector consisting of all annihilation operators in the system and $\gamma = M^\dagger \psi$ refers to the vector of Majorana operators which has $2n$ entries. With I we denote that the indices take values from 1 to the number of sites n. The matrix M can be written as

$$\psi = \begin{pmatrix} \psi_I \\ \psi_I^\dagger \end{pmatrix} = M^\dagger \gamma = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -i \\ 1 & i \end{pmatrix} \begin{pmatrix} \gamma_I \\ \gamma_{I+N} \end{pmatrix}. \tag{A9}$$

We can rewrite the definition of X into

$$H = \frac{i}{4} M^\dagger X M, \tag{A10}$$

and use it within the relation for $\mathcal{PT}$ symmetry to get

$$\begin{aligned} U^\dagger H^* U &= U^\dagger \frac{-i}{4} M^T X^* M^* U = \frac{i}{4} M^\dagger X M = H \\ &\Leftrightarrow U_M^\dagger X^* U_M = -X, \end{aligned} \tag{A11}$$

where we have used that

$$M^* U M^\dagger = \begin{pmatrix} u & 0 \\ 0 & -u \end{pmatrix} = U_M. \tag{A12}$$

Let us evaluate this expression for the components given in Eq. (A3) which yields

$$\begin{aligned} X^* &= \begin{pmatrix} -i(a - a^T + b + c) & -(a + a^T - b + c) \\ a + a^T + b - c & -i(a - a^T - b - c) \end{pmatrix}^* \\ &= U \begin{pmatrix} i(a - a^T + b + c) & -(a + a^T - b + c) \\ a + a^T + b - c & i(a - a^T - b - c) \end{pmatrix} U^\dagger. \end{aligned} \tag{A13}$$

1. Treat U and the signs separately

To see what we can expect of the unitary matrix U let us consider the general skew-symmetric matrix A:

$$\mathrm{Pf}(UAU^T) = \mathrm{Pf}(A) \det(U) = \det(u)^2 \mathrm{Pf}(A) = \mathrm{Pf}(A). \tag{A14}$$

If the matrix U is orthogonal instead and not only unitary, then we can remove it form the Pfaffian. Should this not be the case, we could also consider that u may commute with $a + a^T$ and $b - c$ and anticommute with $a - a^T$ and $b + c$. After summing or substracting these relations, the following is obtained:

$$bu + uc = 0, \quad cu + ub = 0, \tag{A15}$$

$$au + ua^T = 0, \quad \text{and} \quad a^T u + ua = 0. \tag{A16}$$

If U is treated by such means, then we can simply consider the matrix itself and we see that it will equal to X if the diagonals vanish. $a - a^T + b + c = 0$ and $a - a^T - b - c = 0$ leads to $a = a^T$, i.e., a is symmetric, and $b = -c$. If we connect this with the condition that u commutes with the blocks, then we see that u must commute with b and c and anticommute with a and a^T. If the diagonals have vanished and U is removed, we see from (A13) that $X^* = X$ and therefore $\mathrm{Pf}(X)^* = \mathrm{Pf}(X)$.

2. Treat U and the signs at the same time

Of course, there might be a way to treat U and the sign differences between X^* and X at the same time. If we state the necessary relations for each block and form differences and sums from them we end up with

$$bu + uc = 0, \quad cu + ub = 0, \tag{A17}$$

$$ua - a^T u = 0, \quad ua^T - au = 0, \tag{A18}$$

which will also give us a real Pfaffian. We see that $\mathcal{PT}$ symmetry alone is not enough.

Let us further consider the case where a non-Hermitian H_{nH} potential is added to a Hermitian operator H_H, which is the case we considered for the main part of this work. It is also the case that can be interpreted by particle exchange with the environment. Our PHS Hamiltonian is now written with a

non-Hermitian onsite potential $\tilde{a}$,

$$H_H + H_{nH} = \begin{pmatrix} a+\tilde{a} & b \\ -b^* & -a^T - \tilde{a}^T \end{pmatrix}, \tag{A19}$$

where b obeys the previously given relations. The skew-symmetric matrix X_{total} for the whole Hamiltonian is

$$\begin{aligned} X_{\text{total}} &= X_H + X_{nH} \\ &= \begin{pmatrix} -i(a-a^T+b-b^*) & -(a+a^T-b-b^*) \\ a+a^T+b+b^* & -i(a-a^T-b+b^*) \end{pmatrix} \\ &\quad + \begin{pmatrix} 0 & -2\tilde{a} \\ 2\tilde{a} & 0 \end{pmatrix}. \end{aligned} \tag{A20}$$

Now, we have to apply the complex conjugation

$$X^*_{\text{total}} = X_H + U \begin{pmatrix} 0 & -2\tilde{a} \\ 2\tilde{a} & 0 \end{pmatrix} U^\dagger = X_H + U X_{nH} U^\dagger, \tag{A21}$$

where the first term originates from the Hermitian part, which makes X a real quantity, and the second part is unmodified due to two sign changes but still subject to the matrix U. The unitary matrix U can be removed if it is orthogonal and commutes with X_H or if it commutes with X_{nH}. The property that U commutes with X_{nH} is equivalent to the commutativity of $\tilde{a}$ and u. But, if we recall the $\mathcal{PT}$-symmetry condition $u^\dagger \tilde{a}^* u = \tilde{a}$, we see that this would lead to a real $\tilde{a}$. The assumption reduces the generally non-Hermitian part to an additional Hermitian one. Therefore, we have to consider the first option, e.g., U is orthogonal such that it can be removed from the Pfaffian

$$\begin{aligned} \text{Pf}(X_{\text{total}})^* &= \text{Pf}(X_H + U X_{nH} U^T) \\ &= \text{Pf}(X_H U U^T + U X_{nH} U^T) \\ &= \text{Pf}(U(X'_H + X_{nH}) U^T) \\ &= \text{Pf}(X'_H + X_{nH}), \end{aligned} \tag{A22}$$

where $X'_H = X_H$ if $[X_H, U] = 0$ and for this case the Pfaffian is real. Let us go one step further in our considerations. For the extended Kitaev model we have a corresponding matrix U that just inverts the order of lattice sites. The Hermitian part of this model is isotropic in all terms except those related to pairing. We see that for any term of the form $c_n c_m$ an inversion of the sites leads to $c_m c_n = -c_n c_m$ which is true for two arbitrary indices $n \neq m$. This sign will appear at arbitrary pairing terms, therefore, we can remove it by a unitary transformation W on H' which shall have the additional minus signs compared to H:

$$W H' W^\dagger = H, \tag{A23}$$

$$W = \begin{pmatrix} i\mathbf{1} & 0 \\ 0 & -i\mathbf{1} \end{pmatrix}, \tag{A24}$$

$$W_M := M W M^\dagger = \begin{pmatrix} 0 & \mathbf{1} \\ -\mathbf{1} & 0 \end{pmatrix}, \tag{A25}$$

where we have introduced the orthogonal matrix W_M which is W expressed in the Majorana basis. If we collect the intermediate steps, we see that

$$\begin{aligned} \text{Pf}(X_{\text{total}})^* &= \text{Pf}(X_H + U X_{nH} U^T) \\ &= \text{Pf}(X_H U U^T + U X_{nH} U^T) \\ &= \text{Pf}[U(X'_H + X_{nH}) U^T] \\ &= \text{Pf}(X'_H + X_{nH}) \\ &= \text{Pf}\left[W_M^T (X'_H + X_{nH}) W_M\right] \\ &= \text{Pf}(X_H + X_{nH}) \\ &= \text{Pf}(X_{\text{total}}), \end{aligned} \tag{A26}$$

where we have used that W_M commutes with X_{nH} and that $\det(W_M) = 1$. With this it is proven that for a Hamiltonian, which obeys PHS and has terms that are either Hermitian or $\mathcal{PT}$-symmetric onsite potentials, the Pfaffian is real if the transformation for the $\mathcal{PT}$ symmetry acts only as inversion on the sites.

APPENDIX B: CALCULATION OF THE PFAFFIAN INVARIANT

The invariant of the Hermitian Kitaev chain [10] for complex order parameter $\Delta \in \mathbb{C}$ is given in terms of the Pfaffian. Here, we analytically calculate the Pfaffian invariant for an alternating potential consisting of two sublattices A and B experiencing gain and loss, respectively. The Hermitian part of the Hamiltonian is given in Eq. (4), similar to [10], by

$$H_0 = \sum_n \left[t c_n^\dagger c_{n+1} + i\Delta c_n c_{n+1} - \frac{\mu}{2} c_n^\dagger c_n + \text{H.c.} \right] \tag{B1}$$

with the non-Hermitian potential but $\mathcal{PT}$-symmetric potential

$$U = \sum_n (-1)^n i\gamma c_n^\dagger c_n. \tag{B2}$$

This potential is alternating between adjacent sites and is therefore not translationally invariant. By dividing the system into two sublattices A and B it can still be diagonalized:

$$\begin{aligned} H = &\sum_n \left[t(c_{A,n}^\dagger c_{B,n} + c_{B,n}^\dagger c_{A,n+1}) + i\Delta(c_{A,n} c_{B,n} + c_{B,n} c_{A,n+1}) - \frac{\mu}{2}(c_{A,n}^\dagger c_{A,n} + c_{B,n}^\dagger c_{B,n}) + \text{H.c.} \right] \\ &+ \sum_n [i\gamma c_{A,n}^\dagger c_{A,n} - i\gamma c_{B,n}^\dagger c_{B,n}]. \end{aligned} \tag{B3}$$

We now write the above Hamiltonian in the Majorana basis using the substitution rule

$$c_{\eta,n} = \tfrac{1}{2}(a_{\eta,2n-1} + i a_{\eta,2n}), \quad c_{\eta,n}^\dagger = \tfrac{1}{2}(a_{\eta,2n-1} - i a_{\eta,2n}) \tag{B4}$$

with $\eta = A, B$ and the Majorana operators a. In this basis, the Hamiltonian reads as

$$H = \sum_n \Big[\frac{it}{2}\big(a^A_{2n-1}a^B_{2n} - a^A_{2n}a^B_{2n-1} + a^B_{2n-1}a^A_{2n+2} - a^B_{2n}a^A_{2n+1}\big) + \frac{i\Delta}{2}\big(a^A_{2n-1}a^B_{2n-1} - a^A_{2n}a^B_{2n} + a^B_{2n-1}a^A_{2n+1} - a^B_{2n}a^A_{2n+2}\big) - \frac{i\mu}{2}\big(a^A_{2n-1}a^A_{2n} + a^B_{2n-1}a^B_{2n}\big) - \frac{i(i\gamma)}{2}a^A_{2n-1}a^A_{2n} + \frac{i(i\gamma)}{2}a^B_{2n-1}a^B_{2n}\Big]. \tag{B5}$$

Now, we Fourier transform this Hamiltonian according to the prescription

$$a^\eta_{2n-1} = \frac{1}{\sqrt{N}}\sum_q e^{-iqn}b^\eta_{q,1}, \quad a^\eta_{2n} = \frac{1}{\sqrt{N}}\sum_q e^{-iqn}b^\eta_{q,2}, \tag{B6}$$

where again $\eta = A, B$. Also note that $b^\dagger_q = b_{-q}$. In the new basis $b_q = (b^A_{q,1}, b^B_{q,1}, b^A_{q,2}, b^B_{q,2})^T$ we can write the Hamiltonian in the quadratic form

$$H = \frac{i}{4}\sum_q b^\dagger_q A(q) b_q \tag{B7}$$

with the skew-symmetric matrix $A(q)$. The nonzero entries of $A(q)$ are

$$A_{12} = \Delta(1 - e^{iq}), \tag{B8}$$

$$A_{13} = -(\mu + i\gamma), \tag{B9}$$

$$A_{14} = t(1 + e^{iq}), \tag{B10}$$

$$A_{23} = t(1 + e^{-iq}), \tag{B11}$$

$$A_{24} = -(\mu - i\gamma), \tag{B12}$$

$$A_{34} = -\Delta(1 - e^{iq}). \tag{B13}$$

The Pfaffian of this 4×4 matrix then is given by

$$\mathrm{Pf}[A(q)] = -\Delta^2(1 - e^{iq})^2 - (\mu^2 + \gamma^2) + 2t^2(1 + \cos q). \tag{B14}$$

The topological invariant from the Pfaffian is the Majorana number $\mathcal{M}$ which is defined in Ref. [10] as

$$\mathcal{M} = \mathrm{sgn}(\mathrm{Pf}[A(0)]\,\mathrm{Pf}[A(\pi)]), \tag{B15}$$

where $\mathcal{M} = -1$ indicates topologically nontrivial and $\mathcal{M} = 1$ topologically trivial behavior. Here, we obtain

$$\mathcal{M} = \mathrm{sgn}[(\mu^2 + \gamma^2 - 4t^2)(\mu^2 + \gamma^2 + 4\Delta^2)]. \tag{B16}$$

The second term consists of a sum of positive numbers which is itself always positive. Therefore, it does not contribute to the sign of the overall expression and the dependence on the gap parameter Δ drops out. From the final expression for the Majorana number

$$\mathcal{M} = \mathrm{sgn}(\mu^2 + \gamma^2 - 4t^2), \tag{B17}$$

we then derive the circle criterion $\mu^2 + \gamma^2 < 4t^2$ for the topological phase presented in the main text.

APPENDIX C: PARTITIONING POTENTIAL

In the main text we investigate a potential which breaks Hermiticity at both ends of the wire over the range f. The

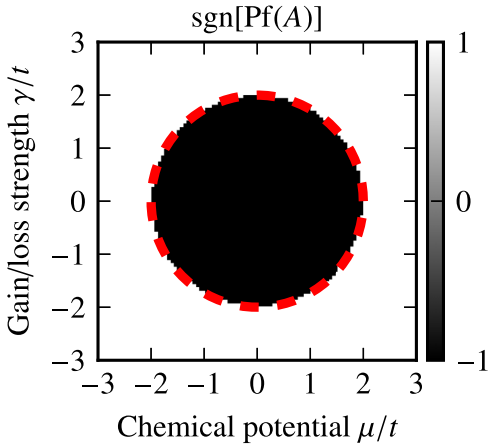

FIG. 5. Topological phase diagram for the partitioning potential (C1) in a chain with $N = 100$ sites and a partitioning fraction of $f = 0$. The color map indicates the sign of the Pfaffian, the dashed line corresponds to the analytical phase boundary as extracted from the generating function approach.

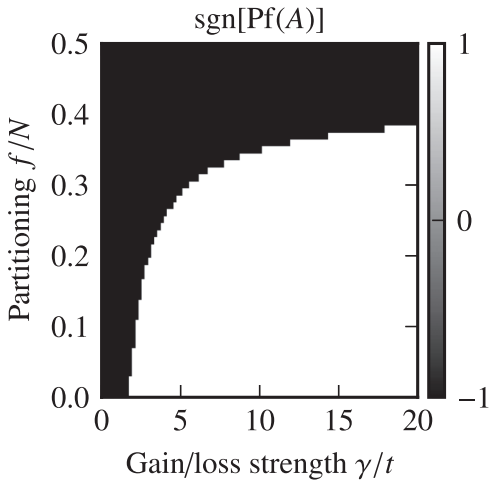

FIG. 6. Topological phase diagram for the partitioning potential (C1) in a chain with $N = 100$ sites. A partitioning fraction of $f/N = 0$ corresponds to half loss/half gain, whereas $f/N = 0.5$ corresponds to the Hermitian model without any potential. The color map indicates the sign of the Pfaffian. The left edge of the phase diagram corresponds to the Hermitian Kitaev chain. Clearly, the phase diagram changes with the partitioning.

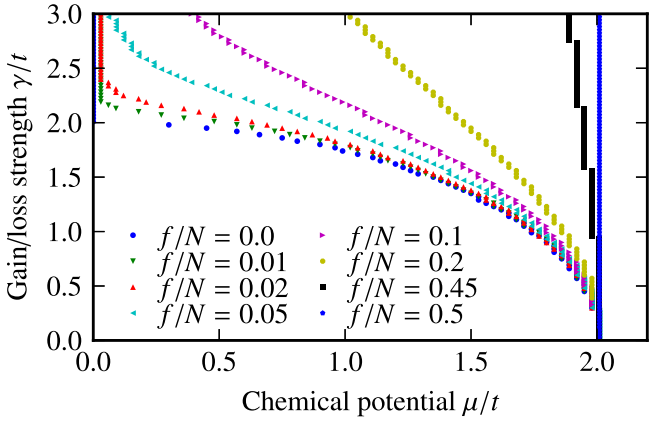

FIG. 7. Numerically determined phase boundary for the potential (C1) at different partitioning fractions f/N in a chain with $N = 100$ sites. With increasing partitioning fraction we approach the phase boundary of the Hermitian case ($f/N = 0.5$).

potential is given by

$$U_2 = i\gamma\left[-\sum_{n=1}^{N/2-f} c_n^\dagger c_n + \sum_{n=N/2+f}^{N} c_n^\dagger c_n\right]. \tag{C1}$$

For this potential we can numerically compute the phase diagram for a partitioning $f = 0$, i.e., half the wire experiences gain, the other half loss. This resembles the setup used for the analytical calculation with the generating function approach. Indeed, we recover the same criterion as derived from said method which we superimpose with our numerical findings in Fig. 5.

Because the phase diagram is again a circle one might get the impression that the phase diagram is a circle for all $\mathcal{PT}$-symmetric potentials. This would require that the topological phase is independent of the partitioning f. We investigate this in a numerical calculation of the Pfaffian and find that this is not the case (cf. Fig. 6).

It is interesting to study the behavior of the aforementioned partitioning potential under a change of the partitioning fraction f/N to see how it changes as we approach the Hermitian limit ($f/N = 0.5$). This can be seen in Fig. 7.

APPENDIX D: NON-$\mathcal{PT}$-SYMMETRIC POTENTIALS

We would like to add some comments regarding potentials which do not fulfill $\mathcal{PT}$ symmetry based on the observations in numerical simulations. We assume the potential

$$U = \sum_n -i\gamma c_n^\dagger c_n. \tag{D1}$$

This is obviously not $\mathcal{PT}$ symmetric. However, in numerical calculations we nevertheless find edge modes and were able to extract a rule of thumb for the topological invariant. As

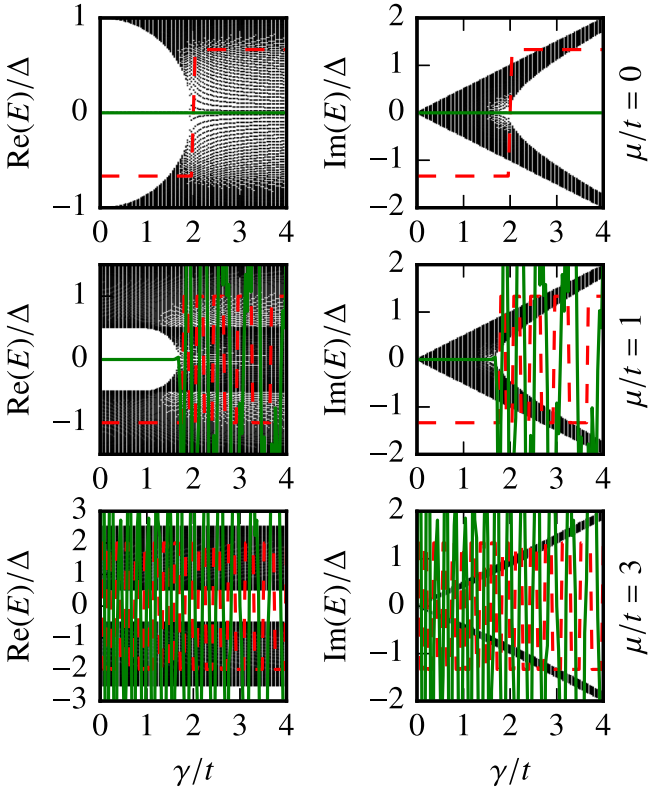

FIG. 8. We show spectra for the non-$\mathcal{PT}$-symmetric potential in Eq. (D1) in a chain with $N = 100$ sites at different chemical potential over the gain/loss strength γ. The dashed line corresponds to the sign of the real part of the Pfaffian, the solid line to the value of the imaginary part.

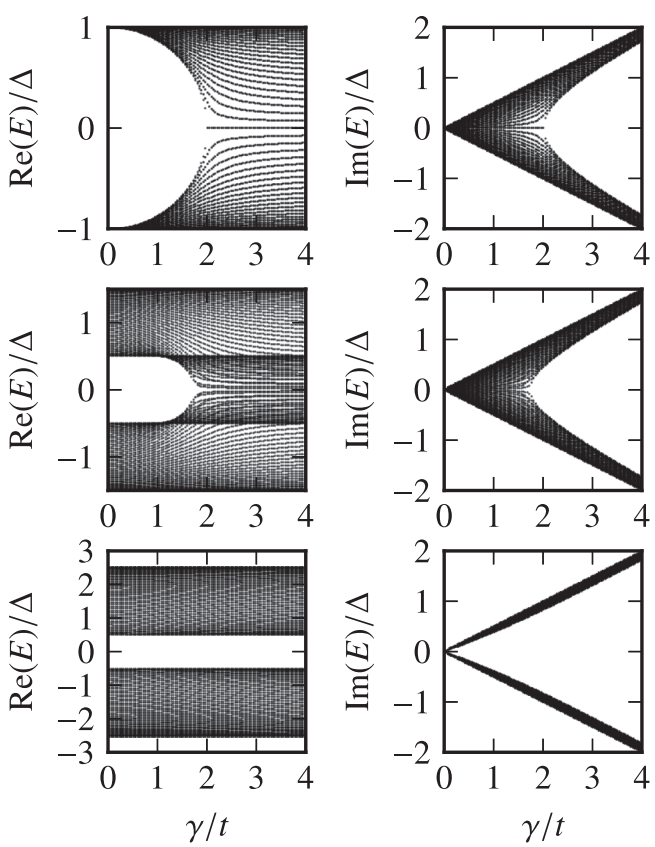

FIG. 9. We show bulk spectra for the non-$\mathcal{PT}$-symmetric potential in Eq. (D1) in a chain with $N = 100$ sites at different chemical potential over the gain/loss strength γ.

in the $\mathcal{PT}$-symmetric case, the edge modes are characterized by a vanishing real and imaginary part of the eigenvalues. In the topological regime, the Pfaffian is real and has a sign of -1, correctly indicating topological behavior. In the trivial regime, however, the Pfaffian becomes imaginary and the sign of the real part is no longer strictly positive, making the sign of the real part alternate. Therefore in this case we extended the condition for a topological phase to the following statement. For a topological phase to exist, the Pfaffian must be real and its sign must be negative. Imaginary Pfaffian or a positive sign of the Pfaffian corresponds to the trivial phase.

For the potential in Eq. (D1), we show the eigenvalue spectra overlayed with the sign of the real part and the bare value of the imaginary part of the Pfaffian in Fig. 8.

As described in the main text for the potential U_1, the bulk spectrum for this system differs qualitatively from its open counterpart (see Fig. 9). In the case $\mu/t = 0$ the real part of the spectrum becomes gapless in the topologically trivial phase.

This does also not conform with analytical predictions. If we calculate the Pfaffian of the present model we find

$$\mathrm{Pf}[A(q)] = 2t\cos q - (\mu + i\gamma) + 2i\Delta\sin q. \tag{D2}$$

Simply evaluating the condition for the Majorana number would in this case yield

$$\begin{aligned}\mathcal{M} &= \mathrm{sgn}(\mathrm{Pf}[A(0)]\,\mathrm{Pf}[A(\pi)]) \\ &= \mathrm{sgn}(\mu^2 - 4t^2 - \gamma^2 + 2i\gamma\mu).\end{aligned} \tag{D3}$$

The argument of the sign function is complex and the result is thus undefined. Even if we apply the same demands as for the real-space tight-binding results, namely that the imaginary part of the Pfaffian vanishes, this would lead to a contradiction with the numerical results. Here, this would mean that $\gamma\mu = 0$ which implies that either $\gamma = 0$ or $\mu = 0$. In Fig. 8, however, we find that for $\mu/t = 1$ the topological phase transition does not take place at $\gamma = 0$ as would be required by the ill-defined argument. We hence conclude that the Pfaffian is not a good topological invariant for non-$\mathcal{PT}$-symmetric systems.

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