Relation between $\mathcal{PT}$-symmetry breaking and topologically nontrivial phases in the Su-Schrieffer-Heeger and Kitaev models

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Non-Hermitian systems with $\mathcal{PT}$ symmetry can possess purely real eigenvalue spectra. In this work two one-dimensional systems with two different topological phases, the topological nontrivial phase (TNP) and the topological trivial phase (TTP), combined with $\mathcal{PT}$-symmetric non-Hermitian potentials are investigated. The models of choice are the Su-Schrieffer-Heeger (SSH) model and the Kitaev chain. The interplay of a spontaneous $\mathcal{PT}$-symmetry breaking due to gain and loss with the topological phase is different for the two models. The SSH model undergoes a $\mathcal{PT}$-symmetry breaking transition in the TNP immediately with the presence of a nonvanishing gain and loss strength γ, whereas the TTP exhibits a parameter regime in which a purely real eigenvalue spectrum exists. For the Kitaev chain the $\mathcal{PT}$-symmetry breaking is independent of the topological phase. We show that the topologically interesting states—the edge states—are the reason for the different behaviors of the two models and that the intrinsic particle-hole symmetry of the edge states in the Kitaev chain is responsible for a conservation of $\mathcal{PT}$ symmetry in the TNP.

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I. INTRODUCTION

One of the best known relations of topology in solid-state systems is the explanation of the quantized Hall effect, which was discovered by von Klitzing *et al.* [1,2], in terms of a topological invariant [3]. Today topological many-body systems are a strongly investigated and well understood subject [4], and in recent works a topological periodic table has been proposed [5,6] to relate topological systems depending on their symmetries, e.g., electron-particle hole symmetry or time-reversal symmetry, to different classes.

Two simple and one-dimensional topological systems are the Su-Schrieffer-Heeger (SSH) model [7], initially introduced to investigate the one-dimensional polyacetylene, and the Kitaev [8] chain, a model for the description of a one-dimensional spinless superconductor. They possess an energy spectrum exhibiting a band gap. In dependence of a certain parameter two different topological phases can arise, which can be distinguished by energies lying within the band gap. The corresponding eigenstates of the gap-connecting energies are called edge states. These edge states show a strong localization at the edge of the system and can only exist in the topologically nontrivial phase (TNP). Besides the TNP the two one-dimensional systems feature a topologically trivial phase (TTP), which is characterized by a fully gapped energy spectrum, in which consequently no edge states appear.

In reality any topological system will always interact with its nearby environment, which leads to dissipative effects. A common way to handle such environmental effects in many-body systems is the solution of the dynamics via Lindblad master equations [9]. However, this can become numerically very expensive, and in many cases an effective description in terms of the stationary Schrödinger equation is sufficient. An often used and elegant way of describing interactions with an environment on the stationary level is given by the application of non-Hermitian potentials [10]. Examples range from electromagnetic waves [11–15], dissipative electric circuits [16], and optomechanics [17] to quantum mechanics, where it is applied in atomic [18–21] or molecular [22] physics, the scattering of particles [23–25], the explanation of fundamental relations [26,27], and in many-body systems [28,29].

A special class of non-Hermitian operators, viz. those possessing a parity-time symmetry, has been introduced by Bender and Boettcher in 1998 [30] because these operators feature the interesting property that they can posses purely real eigenvalues despite their non-Hermiticity. However, in general the eigenvalues of the non-Hermitian $\mathcal{PT}$-symmetric operators can be complex. A Hamiltonian is considered to be $\mathcal{PT}$ symmetric if it commutes with the combined action of the parity operator $\mathcal{P}$ and the time-reversal operator $\mathcal{T}$, i.e., $[\mathcal{PT},H]=0$. The $\mathcal{PT}$ symmetry of the system can become spontaneously broken, and this symmetry breaking is related to the realness of the eigenvalues [31]. It can be shown that $\mathcal{PT}$-symmetric eigenstates of a $\mathcal{PT}$-symmetric Hamiltonian always possess purely real eigenvalues, while eigenstates that are not $\mathcal{PT}$ symmetric appear in pairs with complex and complex conjugate eigenvalues. It turned out that $\mathcal{PT}$ symmetry is a powerful concept to effectively describe systems interacting with an environment in such a way that they experience balanced gain and loss. In particular, it was shown in optical experiments that $\mathcal{PT}$ symmetry and $\mathcal{PT}$-symmetry breaking can be realized in the laboratory [32–34]. Proposals for the realization in quantum mechanics exist for Bose-Einstein condensates [35,36].

Recently some models of topological insulators have been investigated under gain and loss effects in terms of non-Hermitian operators. This leads to interesting questions. In particular, it has to be understood whether topologically protected states can be found in the presence of the gain and loss [37–44]. In an optical experiment of a modified SSH model topological interface states were observed [45]. Even though the SSH and Kitaev models are equivalent in some special cases [46] they behave completely differently when complex on-site potentials are applied. Zhu *et al.* [47] and

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Wang *et al.* [48] have studied the connection between the TNP and spontaneous $\mathcal{PT}$-symmetry breaking due to external gain and loss in the SSH and Kitaev models, respectively. Comparing the results of the two investigations leads to a discrepancy in the interplay between topological phases and spontaneous $\mathcal{PT}$-symmetry breaking. In the Kitaev chain the $\mathcal{PT}$ symmetry is protected within the TNP when a non-Hermitian potential is applied. On the other hand the SSH model shows an instantaneous $\mathcal{PT}$-symmetry breaking within the TNP for every arbitrarily small gain and loss effect. Also in further models it was sometimes found that completely real eigenspectra do not appear in the TNP, whereas this was possible in other models.

It is the purpose of this paper to give an unambiguous answer to the question of how the relation between topologically nontrivial edge states and the effects of $\mathcal{PT}$-symmetry breaking can be established. To do so, we investigate the SSH and Kitaev models in the presence of two different non-Hermitian potentials generating $\mathcal{PT}$-symmetric gain-loss effects. In particular we study the eigenstates of the system and the symmetries of the edge states. It will turn out that there is no general relation between the $\mathcal{PT}$ symmetry of the system and the topological phase as assumed previously [48]. The symmetry of the specific edge states in the systems decides whether or not these states spontaneously break the $\mathcal{PT}$ symmetry. The symmetry the states exhibit in the Hermitian case survives in the presence of the gain-loss effect. However, in dependence of the imaginary potential applied to the system also the bulk states may lead to a spontaneous $\mathcal{PT}$-symmetry breaking in both the TNP and the TTP.

The paper is organized as follows. In Sec. II the two different Hamiltonians are introduced. In Sec. III energy spectra of the two models are shown without and with the application of external gain and loss potentials. This is used to analyze the cause of $\mathcal{PT}$-symmetry breaking in the TTP and the TNP. In particular, the different symmetry behaviors of the topologically interesting edge states are presented. For the Kitaev chain the number of edge states is counted for certain parameter values to investigate their dependence on the imaginary potentials. The last section, Sec. IV, provides conclusions.

II. MODELS

In this paper we consider two different one-dimensional models with a lattice distance $a = 1$ and N lattice sites. The Su-Schrieffer-Heeger model [7] is given by

$$H_{\mathrm{SSH}} = \sum_n (t_- c_{2n-1}^\dagger c_{2n} + t_+ c_{2n}^\dagger c_{2n+1} + \mathrm{H.c.}), \tag{1}$$

where the alternating hopping strengths $t_\pm = t(1 \pm \Delta \cos\Theta)$ contain the hopping amplitude t and the dimerization strength $\Delta\cos\Theta$, which can vary from $-\Delta$ to Δ. The second system is the one-dimensional Kitaev chain [8], which is a toy model for a topological p-wave superconductor,

$$H_{\mathrm{Ki}} = \mu \sum_n c_n^\dagger c_n + \sum_n (t c_n^\dagger c_{n+1} - i\delta c_n c_{n+1} + \mathrm{H.c.}), \tag{2}$$

where the chemical potential is given by μ, t is again the nearest-neighbor hopping, and δ is the p-wave pairing amplitude. In both models the operator $c_n^\dagger$ (c_n) is the creation (annihilation) operator for electrons at lattice site n. In the following all energies are measured in units of t, i.e., $t = 1$ is always set, which defines the dimensionless units used in this work.

In our study the two systems are described by the total Hamiltonians

$$H = H_0 + U, \tag{3}$$

where H_0 is either the Hamiltonian of the Kitaev model H_{Ki} or the SSH model H_{SSH}. The term U represents the gain and loss effects via an additional $\mathcal{PT}$-symmetric part. In this work we distinguish between two potentials,

$$U_1 = i\gamma c_1^\dagger c_1 - i\gamma c_N^\dagger c_N, \tag{4}$$

in which electrons gain in probability amplitude at the first site and lose at the last site. The second $\mathcal{PT}$-symmetric potential,

$$U_2 = i\gamma \sum_n (-1)^n c_n^\dagger c_n, \tag{5}$$

corresponds to an alternating gain and loss effect of the whole chain.

Due to the superconducting term in the Kitaev Hamiltonian (2) a coupling between electrons and holes arises. The basis of the Kitaev chain has to be expanded to respect the particle-hole coupling. The particle number operator of an electron at site i is given by the relation $n_{\mathrm{e},i} = c_i^\dagger c_i$, whereas the number operator for holes reads $n_{\mathrm{h},i} = c_i c_i^\dagger$. A matrix representation of the Hamiltonian (2) can be achieved by choosing vectors in the form of

$$|\psi\rangle = (\boldsymbol{c}, \boldsymbol{c}^\dagger)^T \tag{6}$$

with $\boldsymbol{c} = (c_1, c_2, \ldots c_n)$ and $\boldsymbol{c}^\dagger = (c_1^\dagger, c_2^\dagger, \ldots c_n^\dagger)$. The projection $\langle\psi|\psi\rangle$ corresponds to all number operators of electrons and holes.

III. ENERGY SPECTRA AND PHASE DIAGRAMS

In this section the numerical solutions of the single-particle eigenvalue equation

$$H\,|\psi\rangle = E\,|\psi\rangle$$

are calculated under open boundary conditions (OBCs). The Hamiltonian is given by $H = H_0 + U$, where H_0 is the Hamiltonian of the considered model and U is one of the two $\mathcal{PT}$-symmetric potentials U_1 or U_2. Due to the $\mathcal{PT}$ symmetry of the Hamiltonian solving the eigenvalue equation for an applied gain and loss effect can lead to purely real eigenvalues, however, in general the eigenvalues are complex numbers $E = \mathcal{E} + i\Gamma$ with the real energy part $\mathcal{E}$ and the decay or growth rate Γ.

A. Hermitian system

For the reader's convenience we briefly recapitulate the essential properties of both models. In the case of the isolated models, i.e., $H = H_0$, both energy spectra show domains, in which a vanishing energy emerges. The presence of a zero energy is connected to edge states. The parameter regime

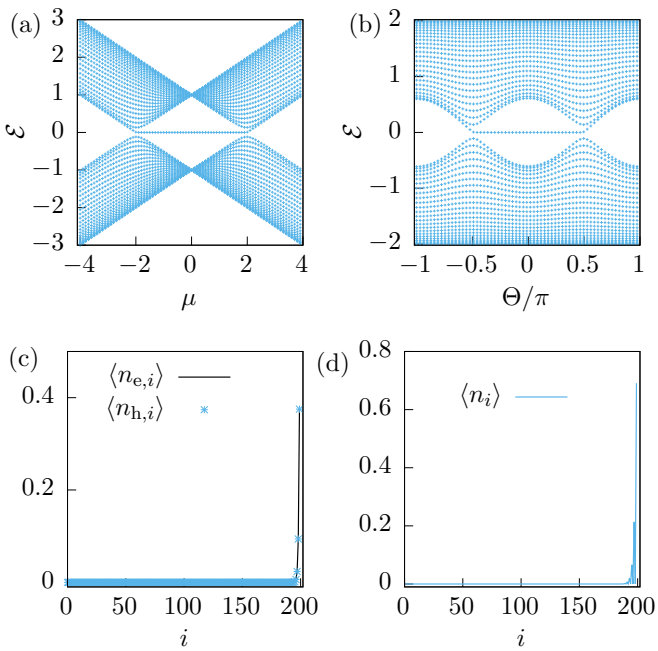

FIG. 1. First row: isolated ($\gamma = 0$) energy spectrum for (a) the Kitaev chain with the parameters $t = 1.0$, $\delta = 1.0$ and (b) the SSH chain with $t = 1.0$, $\Delta = 0.3$. In both cases the spectrum is computed for a chain with $N = 200$ sites. Second row: One of the two edge states for (c) the Kitaev model with the parameters $\mu = 1.0$, $t = 1.0$, and $\delta = 1.0$ and (d) for the SSH model with $\Theta = 0.1\pi$, $t = 1.0$, and $\Delta = 0.3$. The edge states shown feature a vanishing energy eigenvalue.

hosting edge states belongs to the topological nontrivial phase (TNP). This phase is called topologically nontrivial since a topological invariant can be found. The edge states differ in this invariant from the bulk states [8,49–52]. In the Kitaev chain the topologically nontrivial phase ranges from $\mu = -2 \ldots 2$, whereas the TNP reaches from $\Theta = -\pi/2 \ldots \pi/2$ in the SSH model; see Fig. 1 for $N \to \infty$ lattice sites. The calculation of the expectation value of each particle number operator at every lattice site can be used to illustrate the localization of the electrons in a certain eigenstate along the chain. The states of interest are the edge states. For the SSH model the required expectation value of the occupation of lattice site i is calculated via

$$\langle n_i\rangle = \langle\psi_{\rm ed}|c_i^\dagger c_i|\psi_{\rm ed}\rangle, \tag{7}$$

where $|\psi_{\rm ed}\rangle$ is one of the two edge states with zero energy. For the Kitaev chain one has to distinguish between the expectation values of particles and holes,

$$\langle n_{{\rm e},i}\rangle = \langle\psi_{\rm ed}|c_i^\dagger c_i|\psi_{\rm ed}\rangle, \quad \langle n_{{\rm h},i}\rangle = \langle\psi_{\rm ed}|c_i c_i^\dagger|\psi_{\rm ed}\rangle. \tag{8}$$

In Fig. 1 one edge state for each model is shown. As one can see the edge state of the Kitaev model fulfills particle-hole symmetry, i.e., $\langle n_{{\rm e},i}\rangle = \langle n_{{\rm h},i}\rangle$. Even though no potential is applied the $\mathcal{PT}$ symmetry of the edge states shown can be explored. In the SSH model the $\mathcal{PT}$ symmetry is broken by the edge states, whereas the edge states of the Kitaev model conserve the $\mathcal{PT}$ symmetry. Though every single expectation value $\langle n_{\rm e}\rangle$, respectively $\langle n_{\rm h}\rangle$, of the Kitaev edge state is not $\mathcal{PT}$ symmetric, it is the particle-hole symmetry which ensures the $\mathcal{PT}$ symmetry of the edge state. Due to the anticommutation relation of fermions $\{c_i, c_j^\dagger\} = \delta_{i,j}$ a gain γ of an electron at site i corresponds to the equal loss of a hole at the same lattice site. Applying a $\mathcal{PT}$-symmetric potential generates gain and loss effects to specific lattice sites in the Kitaev chain depending on the potential U_1, respectively U_2. For one lattice site the net gain-loss effect is zero if a particle-hole symmetry in the occupation probabilities is present. If an eigenstate preserves particle-hole symmetry throughout the whole system, the net gain is zero and therefore the corresponding eigenstate accomplishes $\mathcal{PT}$ symmetry. The crucial question now is whether this symmetry survives in the case that imaginary potentials are indeed applied.

B. Small gain and loss effects

For small gain and loss strengths γ the spectra of the energy real parts do not change much under variation of the imaginary potential as compared to the isolated cases. Moreover the parameter regimes of the TNP stay the same in the Kitaev model as well as in the SSH model, and therefore also edge states are available in the case of small imaginary potential strengths. The calculation of the edge state expectation values generates the same localization as in the isolated case. Thus the total situation does not change and the edge states remain $\mathcal{PT}$ symmetric in the Kitaev chain, whereas both edge states of the SSH model are $\mathcal{PT}$-broken eigenstates.

A purely real energy spectrum can only occur if every eigenstate of the system obeys $\mathcal{PT}$ symmetry. Due to the fact that even for any arbitrarily small gain and loss effect at least the two edge states of the SSH model break $\mathcal{PT}$ symmetry the energy spectrum has to show complex energies in the TNP. This is indeed the case which is illustrated in the first row of Fig. 2. For both potentials two complex energies emerge in the case of the SSH model. The spectrum performs a $\mathcal{PT}$ phase transition at the same parameter, at which a topological phase transition occurs in the isolated case, i.e., at $\Theta = \pm\pi/2$.

In the second row of Fig. 2 the imaginary parts of the energy spectrum for the Kitaev chain with applied potentials U_1 and U_2 are shown. In contrast to the SSH model the potential U_1 preserves a purely real spectrum. Both topological phases show the same behavior related to the $\mathcal{PT}$ symmetry, and therefore the imaginary parts of the eigenvalues cannot be used to distinguish between the TNP and TTP. For the Kitaev model with applied potential U_2 the imaginary part of the energy shows a nonvanishing value for disappearing chemical potential $\mu = 0$. Still the energy spectrum of the imaginary part cannot be used to provide any information about the topological phases. Taking a closer look at the eigenstates corresponding to the violation of the $\mathcal{PT}$ symmetry for $\mu = 0$ reveals the fact that all states with complex energies are bulk states.

The important finding is that the properties of the edge states in both models are not altered immediately by the presence of the gain-loss effect. In particular, the symmetries of the edge states survive, which leads to an immediate $\mathcal{PT}$-symmetry breaking in the SSH model by the edge states and a preserved $\mathcal{PT}$ symmetry in the Kitaev chain. This explains that it is the symmetry of the actual edge states that is connected to

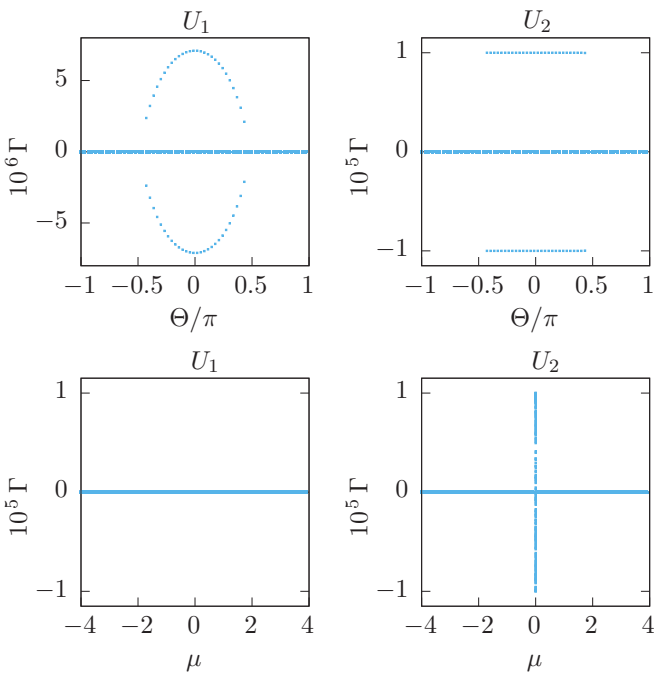

FIG. 2. First row: Imaginary parts of all energies of the SSH model with potentials U_1 (left) and U_2 (right). In both calculations the parameters $t = 1.0$, $\Delta = 0.3$, $N = 200$, and $\gamma = 10^{-5}$ were used. Second row: Imaginary parts of all energies of the Kitaev chain with the parameters $t = 1.0$, $\delta = 1.0$, $N = 200$, and $\gamma = 10^{-5}$.

the $\mathcal{PT}$ symmetry of the whole system not the existence of a topologically nontrivial phase alone.

C. $\mathcal{PT}$-symmetry breaking in dependence of γ

Leaving the field of a low gain and loss effect a $\mathcal{PT}$ phase diagram can be realized by plotting the imaginary parts of the energies over the potential strength γ. In the case of the SSH model the phase diagrams for both the potentials U_1 and U_2 are shown in Fig. 3. For the dimerization strength $\Theta = 0.1\pi$, i.e., in the TNP, the potential U_1 only shows one pair of complex conjugate eigenvalues, which vanish for $\Theta = 0.9\pi$ in the TTP. The same pair also appears if the potential U_2 is applied. The corresponding eigenstates for the two complex eigenvalues appearing in both potentials are the two existing edge states. In contrast to the potential U_1 both of the dimerization strengths shown for U_2 possess a critical value, at which the system gets completely $\mathcal{PT}$ broken and therefore not a single energy eigenvalue remains purely real.

For the Kitaev chain with applied potentials U_1 and U_2 the imaginary parts of the eigenvalues are shown in Fig. 4 for two different chemical potentials, where each value represents one of the topological phases in the isolated case, i.e., $\mu = 0.5$ for the TNP and $\mu = 2.5$ for the TTP. For both potentials there is no obvious difference in the imaginary part of the energies for the different values of μ. As in the scenario of the SSH model the potential U_2 also exhibits a critical parameter value γ at which no purely real energy eigenvalue exists. Due to the fact that the chemical potential has no appreciable influence on the behavior of the imaginary parts of the eigenvalues the bulk states are responsible for breaking the $\mathcal{PT}$ symmetry. The edge states in the Kitaev model are particle-hole symmetric and therefore always conserve the $\mathcal{PT}$ symmetry as long as they exist. Due to a complete $\mathcal{PT}$-symmetry breaking in the case of the potential U_2 the chemical potential capable of hosting edge states is dependent on the potential strength.

D. Phase diagram for the Kitaev model

Since the potential U_2 shows a completely $\mathcal{PT}$-broken regime when the gain and loss strength is increased, the chemical potential at which topological edge states can be present has to be a function of the potential strength, i.e.,

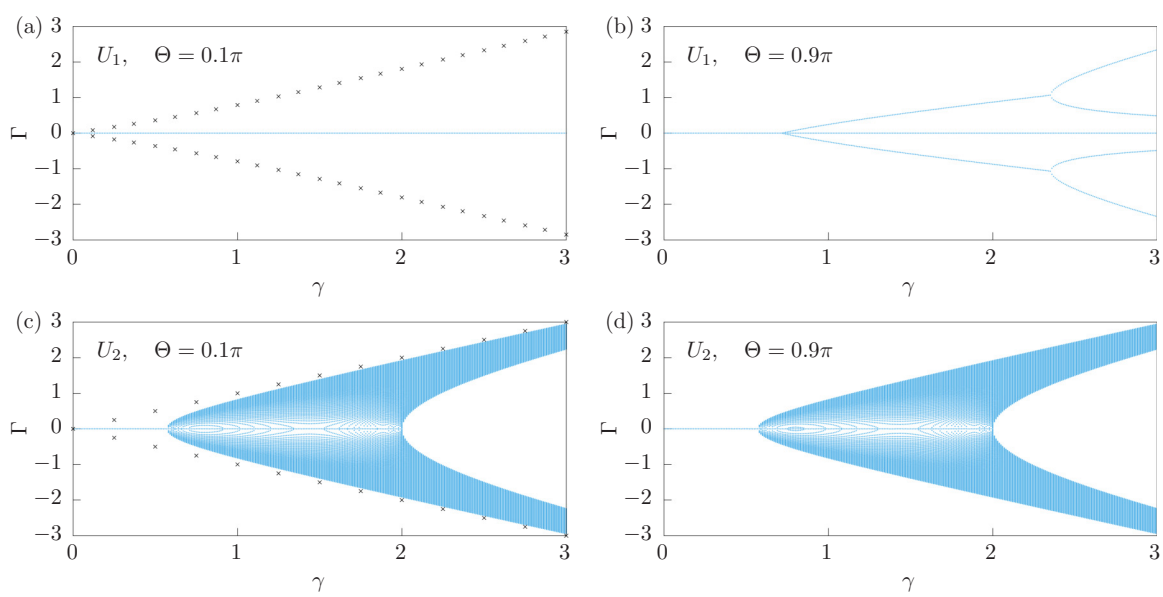

FIG. 3. Imaginary parts of all energies in dependence on the gain and loss strength of all eigenstates of the SSH model. For each plot the parameters $t = 1.0$, $\Delta = 0.3$, and $N = 200$ are used. For (a) and (b) the potential U_1 is used, whereas for (c) and (d) the potential U_2 is applied. The black crosses in (a) and (c) represent the purely imaginary energies of the two edge states appearing in the TNP.

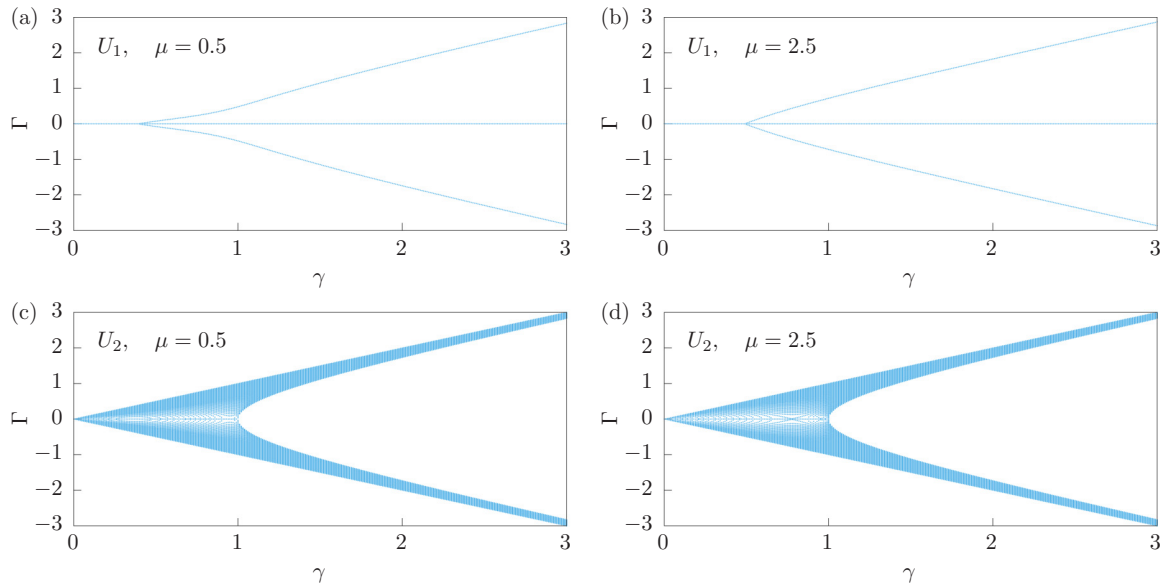

FIG. 4. Imaginary parts of all energy eigenvalues for the Kitaev chain with length $N = 200$ and the parameters $t = 1.0$ and $\delta = t$. The data in (a) and (b) are calculated with the potential U_1. In (c) and (d) U_2 is applied.

$\mu(\gamma)$. For each μ a critical parameter value γ_c can be found at which the topological edge states disappear. The definition of topological edge states in the sense of the Kitaev chain is the fact that the energy has to fulfill the property

$$E = \mathcal{E} = \Gamma = 0, \tag{9}$$

i.e., it has a vanishing real and imaginary part. To obtain a phase diagram a constant gain and loss effect γ is assumed and for a chemical potential representing the TTP in the isolated model, e.g., $\mu = 4.0$, the energy is calculated. Then the chemical potential is decreased in steps of equal size and for each step the number of eigenvalues fulfilling Eq. (9) is counted. This is repeated for further values of γ. In general, numerical calculations do not supply accurate zero values, and therefore in this work we measure a numerical zero if the modulus is smaller than 10^{-8}. The value selected for zero is in this way not a critical choice because the energy spectra show a pronounced jump to small numbers if any topological edge state is present. In Fig. 5 the number of states, which are in agreement with Eq. (9) are counted for the ranges $\mu = 0 \ldots 4$ and $\gamma = 0 \ldots 2$. By applying the potential U_2 one can find values of γ for which no chemical potential supports the existence of edge states. This is in contrast to the Kitaev chain in the case that electrons gain in probability at the first site and lose at the last site as described with the potential U_1. In fact the number of edge states does in the latter case not depend on the value of γ and is only limited by the chemical potential as in the isolated problem. The TNP can host two edge states for $\mu \lessapprox 2.0$. In total, the Kitaev chain is an example, in which gain and loss effects can have an influence on the parameter regime with edge states. However, the two model potentials U_1 and U_2 show that this behavior of the TNP depends on the shape of the gain and loss effects, and therefore there is no general statement on the existence of edge states in the presence of non-Hermitian potentials in the Kitaev chain.

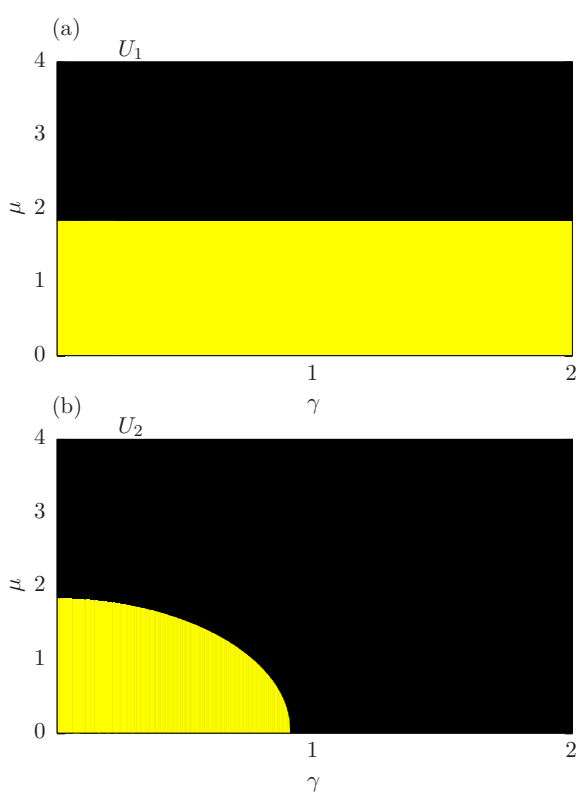

FIG. 5. The number of states fulfilling the property of Eq. (9) for the Kitaev chain with $N = 200$ lattice sites and the parameters $t = 1.0$ and $\delta = t$ in combination with the potential U_1 in (a) and U_2 in (b). The color represents the number of states, where yellow (bright) stands for the value 2 and black (dark) for the value 0.

IV. SUMMARY

In conclusion we studied both the Kitaev and the SSH model with two different $\mathcal{PT}$-symmetric non-Hermitian potentials.

Our investigation of the topological interesting edge states explains why the topological nontrivial phase in the SSH model shows an instantaneously $\mathcal{PT}$-broken spectrum for an arbitrary small potential strength γ, and that the edge states in the case of the Kitaev chain are protected from violating $\mathcal{PT}$ symmetry due to an intrinsic particle-hole symmetry. The important fact is that this symmetry survives in presence of the gain-loss effect. For the Kitaev chain the number of existing edge states at a certain value pair (μ,γ) depends on the applied gain and loss effect, and therefore the range of the topological nontrivial phase can be a function of the potential strength γ.

Both results clearly demonstrate that the previously assumed connection between a spontaneously broken $\mathcal{PT}$ symmetry and the topological phase [47,48] does not exist in general. Only the symmetry of the individual edge states decides whether their presence has an influence on the $\mathcal{PT}$ symmetry of the whole system. Their existence alone does not give a useful answer. It is necessary to always determine the states and to investigate their probability distribution.

Even though this work can explain the role of the edge states in non-Hermitian $\mathcal{PT}$-symmetric systems there remain a few open questions. The imaginary potentials are an effective description of the in- and outfluxes of the probability amplitude and thus for the interaction with an environment. Much more realistic is the addition or removal of electrons, which can be simulated very well in the context of master equations [9,53,54]. It will be interesting to see whether signatures of the results of this work can be found in the dynamics of the master equation, and investigations in this direction are under way. Furthermore, for non-Hermitian operators the often used Berry phase [55] or its formulation in the Brillouin zone, i.e., the Zak phase [56], needs extensions to understand the influence of imaginary potential contributions. Some extensions exist [57,58], however, they are restricted to special cases. A more general way of identifying topologically different states would be valuable. Since similar Bosonic systems with topologically nontrivial states are known [59] and in the case of cold atoms much better controllable in an experiment it seems also worthwhile to extend these studies to Bosons. This might be in particular interesting since Bosonic many-body systems already with very simple interactions feature an unusual dynamics such as purity oscillations in the presence of balanced gain and loss [60,61].

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