Spectrum of localized states in fermionic chains with defect and adiabatic charge pumping.

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In this paper, we study the localized states of a generic quadratic fermionic chain with finite-range couplings and an inhomogeneity in the hopping (defect) that breaks translational invariance. When the hopping of the defect vanishes, which represents an open chain, we obtain a simple bulk-edge correspondence: the zero-energy modes localized at the ends of the chain are related to the roots of a polynomial determined by the couplings of the Hamiltonian of the bulk. From this result, we define an index that characterizes the different topological phases of the system and can be easily computed by counting the roots of the polynomial. As the defect is turned on and varied adiabatically, the zero-energy modes may cross the energy gap and connect the valence and conduction bands. We analyze the robustness of the connection between bands against perturbations of the Hamiltonian. The pumping of states from one band to the other allows the creation of particle-hole pairs in the bulk. An important ingredient for our analysis is the transformation of the Hamiltonian under the standard discrete symmetries, $C$, $P$, $T$, as well as a fourth one, peculiar to our system, that is related to the existence of a gap and localized states.
I. INTRODUCTION

Topology has played an outstanding role in condensed matter physics since the discovery of quantum Hall effect and topological phase transitions [1]. Among the systems whose topological properties have been widely studied, we find topological insulators [2–4]. These are systems of non-interacting fermions that possess gapped phases with zero-energy edge states. These modes are spatially localized at the boundaries of the system and they are topologically protected in the sense that they are robust against deformations of the Hamiltonian, as long as the gap of the bulk does not close and certain symmetries are preserved. A prominent example is the open Kitaev chain, which hosts Majorana modes at its end-points [5] that according to some studies may be detected experimentally, see e.g. [6–10]. The robustness of the edge modes under small perturbations or disorder has turned topological insulators into essential ingredients of quantum devices [11–13].

Topological insulators can be classified in terms of the behaviour of its Hamiltonian under charge conjugation (C), parity (P) and time reversal (T) symmetries. According to the ten-fold classification [14–16], these discrete symmetries allow to arrange them in a “periodic table” of ten generic classes, provided the Hamiltonian is Hermitian, each one related to one of the ten Cartan symmetric spaces. A consequence of this classification is that topologically inequivalent systems can not be adiabatically connected without breaking some of the classifying symmetries. The different phases within a topological insulator can be characterized by a topological invariant. The topological invariant typically establishes a relation between a property of the bulk and another one of the edge—the so-called bulk-edge correspondence [17].

In this paper, we present a comprehensive and systematic analysis of the edge states in one-dimensional chains of spinless fermions described by a generic homogeneous quadratic Hamiltonian with finite-range couplings. The end-points of the chain are connected by a hopping term parametrized by $q$, which will be referred as the contact. We may see this special bond as a defect in the chain which breaks the translational invariance [18–20]. Its existence will be very important for us, as it produces, under certain circumstances, localized states in the vicinity of the defect.

In particular, we will analyze the zero modes of the open chain, $q = 0$, through the discrete symmetries $P$, $C$, and $T$. The dimension of the space of zero-energy modes char-
acterizes the universality class of the corresponding Hamiltonian. We will see that these modes are associated to the roots of a polynomial defined on the analytical continuation of the momentum space to the Riemann sphere and with coefficients given by the bulk Hamiltonian. This result leads to a simple bulk-edge correspondence for these systems and, as we will show, the determination of the topological phase reduces to a counting of the roots of the aforementioned polynomial.

We will also study the spectrum of localized states when the defect is turned on, \( q \neq 0 \). We obtain that, when \( P \) and \( C \) are symmetries of the chain, there are localized states that traverse the bulk gap as the contact \( q \) varies, allowing the pumping of states between the valence and conduction bands. In other systems, this mechanism may induce a quantized transport of charge across the bulk without applying any bias voltage—a genuine topological phenomenon known as adiabatic charge pumping [27–33]—or may switch the fermionic parity of the edge states—a fermion parity pump [34, 35]. In our case, the pumping of a localized state to the conduction band allows to create a free particle-hole pair delocalized in the bulk. An important difference is that, while in the usual topological pumping the parameter that is changed refers to a feature of the bulk, e.g. modulating their hopping amplitudes, here we vary adiabatically the value of the contact that characterizes the defect.

The rest of the paper is organized as follows. In Sec. II, we introduce the family of quadratic fermionic systems under study, as well as a formalization of the well-known diagonalization procedure for this kind of systems in terms of Bogoliubov modes. In Sec. III, we discuss the discrete symmetries \( C, P \) and \( T \), as they are crucial in the analysis of the edge modes. In fact, they will be used in Sec. IV to determine the number of zero-energy modes present in the open chain. In Sec. V, we describe how to construct the edge states; providing a rigorous definition for them in the thermodynamic limit, and we analyze their basic properties. Using this framework, in Sec. VI, we rederive in an analytic way the algebraic results of Sec. IV and, moreover, we formulate a bulk-edge correspondence and introduce a topological index, which identifies the different phases of this class of systems. Sec. VII is devoted to the analysis of the spectrum of localized states in terms of the contact \( q \) and to the charge pumping phenomenon for different topological phases. Finally, in Sec. VIII we end with the conclusions and future prospects.
II. LONG RANGE FERMIONIC CHAIN. SPACE OF BOGOLIUBOV MODES.

We consider a fermionic chain of length $N$. Its Hilbert space $\mathcal{H} = (\mathbb{C}^2)^{\otimes N}$ is endowed with the standard scalar product. In this space, the creation and annihilation operators, $a_n^\dagger$ and $a_n$, act with anticommutation relations

$$\{a_n, a_m\} = \{a_n^\dagger, a_m^\dagger\} = 0, \quad \{a_n, a_m^\dagger\} = \delta_{nm} \text{id},$$

and id is the identity operator in $\mathcal{H}$.

Our system is a homogeneous chain with range $L$ couplings and quadratic Hamiltonian. The two ends of the chain are connected with a tight binding type of interaction with real hopping parameter $q$, we will call it contact. This is our main tunable parameter and, in particular, we recover the open chain by taking $q = 0$.

According to the previous description, the most general form of the Hamiltonian is

$$H = \frac{1}{2} \sum_{n=1}^{N} \sum_{l=-L}^{L} \left( 2A_l a_n^\dagger a_{n+l} + B_l a_n a_{n+l}^\dagger - B_l' a_n a_{n+l} ight) + q (a_1^\dagger a_N + a_N^\dagger a_1),$$

where $\sum'$ stands for the sum restricted to terms such that $1 \leq n + l \leq N$ and, without loss of generality, we may take $B_{-l} = -B_l$, $B'_{-l} = -B'_l$. We will always assume that $N > 2L$.

Of course, in general $H$ is not self-adjoint. In due time, for actual computations, we will restrict to the self-adjoint case that requires

$$A_{-l} = \overline{A}_l, \quad B'_l = \overline{B}_l.$$  

However, and in order to study the symmetries of the system, we prefer for the moment to keep the most general form for $H$.

The usual strategy in order to find the spectrum of this kind of quadratic systems is to write the Hamiltonian in terms of the Bogoliubov modes which render it diagonal \[36\]. A convenient way to formalize this procedure is by the introduction of another Hilbert space, different from $\mathcal{H}$, that for the lack of a better name we will call space of Bogoliubov modes and will be denoted by $\mathcal{B}$. It is simply the space generated by the linear span of the creation and annihilation operators, that is

$$\mathcal{B} = \text{span}\{a_1^\dagger, \ldots, a_N^\dagger, a_1, \ldots, a_N\}.$$
Note that $\mathcal{B}$ is a subspace of $\mathcal{L}(\mathcal{H})$, the linear operators in $\mathcal{H}$.

Using the anticommutation of operators we may introduce a scalar product in $\mathcal{B}$, namely
\[
\langle \xi | \xi' \rangle \text{id} = \{\xi, \xi'\}, \quad \xi, \xi' \in \mathcal{B}.
\] (1)

One immediately sees that the standard basis $\{a_1^\dagger, \ldots, a_N^\dagger, a_1, \ldots, a_N\}$ is orthonormal with respect to $\langle \cdot | \cdot \rangle$.

Now, the Hamiltonian acts naturally in $\mathcal{B}$ by the adjoint. We denote by $H_\mathcal{B}$ the corresponding operator, so that
\[
H_\mathcal{B}\xi = [H, \xi].
\]
Here the right hand side should be understood as the commutator of operators in $\mathcal{L}(\mathcal{H})$ that, for $\xi \in \mathcal{B}$ and due to the quadratic nature of $H$, also belongs to $\mathcal{B}$.

The matrix for $H_\mathcal{B}$ in the standard basis can be written as
\[
(H_\mathcal{B}) = \begin{pmatrix} A & B \\ -B' & -A^\dagger \end{pmatrix},
\]
where $^\dagger$ stands for transposition and $A, B$ are Toeplitz matrices given by
\[
A = \begin{pmatrix}
A_0 & A_1 & \cdots & A_L & 0 & \cdots & 0 & q \\
A_{-1} & A_0 & \cdots & \cdots & \cdots & \cdots & \cdots & \vdots \\
\vdots & \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\
0 & \cdots & \cdots & \cdots & A_L & \cdots & \cdots & 0 \\
q & 0 & \cdots & 0 & A_{-L} & \cdots & A_{-1} & A_0
\end{pmatrix},
\]
\[
B = \begin{pmatrix}
0 & B_1 & \cdots & B_L & 0 & \cdots & 0 & 0 \\
B_{-1} & 0 & \cdots & \cdots & \cdots & \cdots & \cdots & \vdots \\
\vdots & \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\
0 & \cdots & \cdots & \cdots & B_L & \cdots & \cdots & 0 \\
0 & 0 & \cdots & 0 & B_{-L} & \cdots & B_{-1} & 0
\end{pmatrix},
\]
and $B'$ is like $B$ with $B_l'$ replacing $B_l$.

We will use the symbol $^\dagger$ for the adjoint in the Hilbert space $\mathcal{B}$ and keep the more standard $^\dagger$ for the adjoint in $\mathcal{H}$. Then notice that
\[
(H_\mathcal{B})^\dagger = \begin{pmatrix} A^+ & -\overline{B'} \\ -\overline{B} & -(A^+)^\dagger \end{pmatrix},
\]
where we have used the antisymmetry of $B$ and $B'$. Therefore, $H_\mathcal{B}$ is Hermitian if and only if $A^+ = A$ and $\overline{B'} = B$ or, in other words, if and only if $A_{-l} = \overline{A}_l$ and $B'_l = \overline{B}_l$, which are
precisely the conditions for the Hermiticity of $H$. This can also be proven using the definition of the scalar product in terms of the anticommutator,

$$\langle \xi | H_B \xi' \rangle = \{\xi^\dagger, [H, \xi']\} = \{[\xi^\dagger, H], \xi'\} = \{[H^\dagger, \xi], \xi'\}.$$ 

This implies that

$$H_B \xi = [H^\dagger, \xi]$$

and we recover the previous result: the Hermiticity of $H$ in $\mathcal{H}$ is equivalent to that of $H_B$ in $B$.

Now the Bogoliubov modes are the eigenvectors of $H_B$

$$H_B \xi_n = -E_n \xi_n$$

and provided $H$ is Hermitian they form an orthogonal basis.

In this case (Hermitian Hamiltonian) there is also the (anti)symmetry under the adjoint operation that inverts the sign of the energy for a Bogoliubov mode

$$H_B \xi_n^\dagger = [H, \xi_n^\dagger] = -[H, \xi_n]^\dagger = E_n \xi_n^\dagger.$$ 

From all the previous considerations we may divide the Bogoliubov modes into those with negative energy $\xi_n$ and their adjoint $\xi_n^\dagger$ with positive energy (for the present consideration we can forget about the possible states with zero energy, although they will be studied at length later on). As stated before, they are orthonormal, which, given the definition of the scalar product in (1), implies that they satisfy canonical anticommutation rules,

$$\{\xi_n^\dagger, \xi_m\} = \delta_{nm} \text{id},$$

while

$$\{\xi_n, \xi_m\} = 0 \quad \text{and} \quad \{\xi_n^\dagger, \xi_m^\dagger\} = 0.$$ 

Of course, the importance of the Bogoliubov modes is that they diagonalize the Hamiltonian in the sense that the latter can be written in the form

$$H = \sum_n E_n \xi_n^\dagger \xi_n,$$

and from this expression one easily finds the energy of the multiparticle states in the associated Fock space.
III. DISCRETE SYMMETRIES

After this brief formalization of the Bogoliubov procedure for solving quadratic Hamiltonians, we want to study the discrete symmetries of the system. Later we will see that they play an important role in the discussion of the localized states.

**Parity**

The first discrete symmetry that we consider is parity or space reflection. We represent it with a unitary operator $P \in \mathcal{L}(B)$ and, if it satisfies $P^2 = I$, then it must be also Hermitian. It implements a spatial reflection with respect to the defect and therefore it should have the general form

$$P : a_n \mapsto \eta a_{N+1-n}, \quad P : a_n^\dagger \mapsto \rho a_{N+1-n}^\dagger,$$

where in order to satisfy the requirements of unitarity and Hermiticity $\rho$ and $\eta$ should be $1$ or $-1$. A global factor of $-1$ is irrelevant, therefore we can always take $\rho = 1$. The matrix for $P$ in the standard basis is

$$(P) = \begin{pmatrix} J & 0 \\ 0 & \eta J \end{pmatrix}, \quad \text{with} \quad J = \begin{pmatrix} 0 & \cdots & 0 & 1 \\ \vdots & \ddots & \ddots & \vdots \\ 0 & \ddots & \ddots & 0 \\ 1 & 0 & \cdots & 0 \end{pmatrix},$$

the antidiagonal $N \times N$ matrix. It is immediate to check that $J A J = A^\dagger$, $J B J = -B$ and $J B^\dagger J = -B^\dagger$. Therefore, we have

$$(PH_B P) = \begin{pmatrix} A^\dagger & -\eta B \\ -\eta B^\dagger & -A \end{pmatrix},$$

and, if we fix the value of $\eta$ to $-1$, then parity is a symmetry of the Hamiltonian, $PH = HP$, if and only if $A^\dagger = A$ or $A_l = A_{-l}$. Notice that, if we restrict to Hermitian Hamiltonians (that is the case of interest), this is equivalent to having $A_l \in \mathbb{R}$.

**Time reversal**

As it is well known time reversal, denoted by $T$, is represented by an antiunitary operator and it should be also involutive: $T^2 = I$. Under these conditions, as proved already by Wigner [37], there is always a basis on which $T$ acts as the identity. Therefore, the only effect of the antilinear operator in a general vector is to take the complex conjugation of its components in that basis.
We shall assume that the standard basis is left unchanged by $T$. Hence $T$ is simply the complex conjugation of the coefficients which may be expressed as $(T) = \overline{\cdot}$, where we use the overline for complex conjugation. Therefore, $T$ is a symmetry of the Hamiltonian in the sense that $TH = HT$ if and only if the couplings are real, $A_l, B_l, B'_l \in \mathbb{R}$.

Notice also that, due to the fact that the matrix of $P$ in the standard basis has real entries, it commutes with time reversal, $TP = PT$.

**Charge conjugation**

The last of the three discrete transformations exchanges creation and annihilation operators. It will be implemented by a unitary, involutive linear map that we denote by $C$.

If we call by $b_k$ and $b_k^\dagger$ respectively the annihilation and creation operators of a particle with momentum $k$,

$$b_k = \sum_{n=1}^{N} e^{-ikn} a_n, \quad b_k^\dagger = \sum_{n=1}^{N} e^{ikn} a_n^\dagger,$$

we require that the charge conjugation operator transforms one into the other (up to a phase)

$$C : b_k \mapsto \varphi b_k^\dagger.$$

It is clear that in order to achieve this goal we must combine the transformation of creation and annihilation operators in the space representation with a reflection, namely

$$C : a_n \mapsto \eta a_{N-n+1}^\dagger, \quad C : a_n^\dagger \mapsto \rho a_{N-n+1},$$

with phases $\eta$ and $\rho$. This transformation implies that $b_k$ is mapped into $e^{-ik(N+1)} \eta b_k^\dagger$ as required.

Now we want $C^+ = C^{-1} = C$, therefore the most general form for $C$ in the standard basis is

$$(C) = \begin{pmatrix} 0 & \eta J \\ \eta J & 0 \end{pmatrix}.$$ 

The transformed Hamiltonian is given by

$$(CH_B C) = - \begin{pmatrix} A & -\eta^2 B' \\ \eta^2 B & -A' \end{pmatrix},$$

and therefore $C$ reverses the sign of the energy,

$$CH_B = -H_B C, \quad \text{if and only if} \quad \eta^2 B' = -B.

(2)$$

So far the value of $\eta$ is undetermined. It is related to the relative phase between creation and annihilation operators and can be modified by redefining them. The only effect of the latter
redefinition in the Hamiltonian is to multiply the coefficients $B_l$ and $B'_l$ by the corresponding phase. However, and in view of the condition in (2), it is very natural to fix $\eta = i$ and then we have that $C$ anticommutes with $H_B$ if $B = B'$.

If we include the condition for Hermiticity of the Hamiltonian, $\mathcal{H} = \mathcal{H}'$, the result is that an Hermitian Hamiltonian anticommutes with $C$ if $B_l \in \mathbb{R}$.

To summarize, in this section we have introduced the $P$, $T$ and $C$ transformations. Their commutation relations are

$$PT = TP, \quad CP = -CP, \quad TC = -CT.$$ 

We have also found the following relations

$$PH_B = H_B P \quad \text{if} \quad A_l = A_{-l},$$

$$TH_B = H_B T \quad \text{if} \quad A_l, B_l, B'_l \in \mathbb{R},$$

$$CH_B = -H_B C \quad \text{if} \quad B_l = B'_l,$$

which, if we restrict to the case of Hermitian Hamiltonian, take the more symmetric form

$$PH_B = H_B P \quad \text{if} \quad A_l \in \mathbb{R},$$

$$TH_B = H_B T \quad \text{if} \quad A_l, B_l \in \mathbb{R},$$

$$CH_B = -H_B C \quad \text{if} \quad B_l \in \mathbb{R}.$$

Finally, it is interesting to consider the combination of the three transformations, that we will denote by $\Theta$ for short, that is $\Theta \equiv CPT$. Its matrix in the standard basis is

$$\begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix}$$

which is a self-adjoint, antiunitary operator. Notice that except for a factor $i$ it acts on $\mathcal{B}$ like the adjoint, i.e. $\Theta \xi = i \xi^\dagger$. If we compute the transformation of $H_B$ under $CPT$ we find

$$\begin{pmatrix} A^+ & \mathcal{B} \\ -\mathcal{B} & -(A^+)^\dagger \end{pmatrix} = -(H_B)^\dagger,$$

and, therefore, if $H$ is Hermitian we always have

$$\Theta H_B = -H_B \Theta$$

even if $H$ has none of the three discrete symmetries. This is our form of the $CPT$ theorem [38].
IV. ZERO MODES

In this section, we will show how the symmetries that we introduced above determine the states of zero energy. We will see that the dimension of the space of zero modes characterizes the universality class of the corresponding Hamiltonian in a sense that will be made precise below.

We recall that the general Hermitian Hamiltonian that we will consider in the sequel is

\[ H = \frac{1}{2} \sum_{n=1}^{N} \sum_{l=-L}^{L} \left( 2A_l a_n^\dagger a_{n+l} + B_l a_n^\dagger a_{n+l} - B_l^* a_n a_{n+l} \right) + q (a_1^\dagger a_N + a_N^\dagger a_1), \]

with \( A_{-l} = \overline{A}_l \) and \( B_{-l} = -B_l \) and acts by the adjoint in the space of Bogoliubov modes.

We decompose the Hamiltonian as the sum of the unperturbed part (the Hamiltonian for \( q = 0 \)) and the rest

\[ H_B = H_0 + qV. \]

Besides, in order to achieve the thermodynamic limit, it will be convenient to divide \( H_0 \) into the piece in the bulk and that in the edge. By that we mean the following: first decompose the Hilbert space into the subspace in the bulk, corresponding to those sites that for range \( L \) couplings do not interact with the defect, and the rest, i.e. \( \mathcal{B} = \mathcal{B}_b \oplus \mathcal{B}_e \) with

\[ \mathcal{B}_b = \text{span}\{a_{L+1}^\dagger, \ldots, a_{N-L}^\dagger, a_{L+1}, \ldots, a_{N-L}\} \]

and

\[ \mathcal{B}_e = \text{span}\{a_1^\dagger, \ldots, a_L^\dagger, a_{N-L+1}^\dagger, \ldots, a_N^\dagger, a_1, \ldots, a_L, a_{N-L+1}, \ldots, a_N\}. \]

Now consider the orthogonal projectors associated to this decomposition \( \Pi_b \) and \( \Pi_e \) and define

\[ H_b = \Pi_b H_0 \quad \text{and} \quad H_e = \Pi_e H_0. \]

In this section, we are interested in the states of zero energy for \( q = 0 \). That is, we must compute the kernel of \( H_0 \). It is clear that \( \text{Ker} \, H_0 = \text{Ker} \, H_b \cap \text{Ker} \, H_e \). We proceed to characterize \( \mathcal{K} = \text{Ker} \, H_b \).

In the standard basis for \( \mathcal{B} \) and \( \mathcal{B}_b \), the matrix of \( H_b \) can be written as

\[ (H_b) = \begin{pmatrix} A_b & B_b \\ -B_b^* & -A_b^* \end{pmatrix}. \]
where $A_b$, $B_b$ are $(N - 2L) \times N$ dimensional matrices given by

$$A_b = \begin{pmatrix}
A_{-L} & \cdots & A_0 & \cdots & A_L & 0 & \cdots & 0 \\
0 & A_{-L} & \cdots & A_0 & \cdots & A_L & 0 & \cdots & 0 \\
\vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \cdots & \vdots \\
0 & \cdots & 0 & A_{-L} & \cdots & A_0 & \cdots & A_L & 0 \\
0 & \cdots & 0 & A_{-L} & \cdots & A_0 & \cdots & A_L & 0
\end{pmatrix},$$

and

$$B_b = \begin{pmatrix}
B_{-L} & \cdots & 0 & \cdots & B_L & 0 & \cdots & 0 \\
0 & B_{-L} & \cdots & 0 & \cdots & B_L & 0 & \cdots & 0 \\
\vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \cdots & \vdots \\
0 & \cdots & 0 & B_{-L} & \cdots & 0 & \cdots & B_L & 0 \\
0 & \cdots & 0 & B_{-L} & \cdots & 0 & \cdots & B_L & 0
\end{pmatrix}.$$

Given the form of $(H_b)$, one easily sees that, if the non degeneracy condition $|A_L|^2 \neq |B_L|^2$ is met, the rank of $(H_b)$ is maximal, which implies dim$\mathcal{K} = 4L$. This is the first piece of information we need.

Now, let us consider the simplest case in which the chain enjoys $P$, $T$ and $C$ symmetries. This means that $H_B$ commutes with $P$ and $T$ and anticommutes with $C$. It is equivalent to assuming that all the couplings are real.

We must introduce one more transformation that we denote $\Gamma$ and acts on the standard basis in the following way

$$\Gamma a_n^\dagger = \begin{cases} a_n^\dagger & \text{for } n \leq N/2 \\ -a_n^\dagger & \text{for } n > N/2 \end{cases}, \quad \Gamma a_n = \begin{cases} a_n & \text{for } n \leq N/2 \\ -a_n & \text{for } n > N/2 \end{cases}.$$

That is, $\Gamma$ leaves invariant the first half of the chain and reverts the sign of the second half.

It is clear that $\Gamma$ commutes with $H_e$ and anticommutes with $V$. Besides, if the system has a gap between the valence and conduction bands or, in other words, if the zero energy states of $H_b$ are localized at the edges with exponential decay, then, in the thermodynamic limit, $\Gamma$ preserves $\mathcal{K}$. In the following section, when we define properly the thermodynamic limit, we will make these statements more precise. For the moment, it is enough to assume that

$$\Gamma \mathcal{K} \subset \mathcal{K}.$$
From its definition, one has $\Gamma = \Gamma^\dagger = \Gamma^{-1}$ and satisfies the following commutation relations

$$\Gamma P = -P\Gamma, \quad \Gamma T = T\Gamma, \quad \Gamma C = -C\Gamma.$$  

Due to the symmetries of the system, $K$ is left invariant by $P$, $C$ and $T$ transformations. From the commutation relations above, one may check that $\Gamma$ and $iCP$ commute, hence we can classify the vector in the kernel of $H_b$ according to the respective charges $+1$ or $-1$ with respect to each of both symmetries. Then, if we write the $\Gamma$ charge upstairs and that of $iCP$ downstairs, we have

$$K = K_+^+ \oplus K_+^- \oplus K_-^+ \oplus K_-^-,$$

and we denote by $n_+^+$, $n_+^-$, $n_-^+$ and $n_-^-$ the respective dimensions.

Note that $P$ or $C$ act inside $K$ and reverse both $\Gamma$ and the $iCP$ charges. This implies that $n_+^+ = n_-^-$ and $n_-^+ = n_+^-$ and hence $n_+^+ + n_-^+ = n_+^- + n_-^- = 2L$.

Now, in order to determine the zero modes of $H_0$, we must consider the restriction to $K$ of the Hamiltonian at the edge

$$H_e : K \to \mathcal{B}_e$$

and compute its kernel.

First, notice that $\mathcal{B}_e$ is preserved by $P$, $C$, $T$ and $\Gamma$ and therefore it can be decomposed into invariant subspaces under the simultaneous action of the two commuting operators $\Gamma$ and $iCP$. Using the same notation as before, we have

$$\mathcal{B}_e = \mathcal{B}_+^+ \oplus \mathcal{B}_+^- \oplus \mathcal{B}_-^+ \oplus \mathcal{B}_-^-$$

and, given the definitions of the different operators, we find

$$\dim \mathcal{B}_+^+ = \dim \mathcal{B}_+^- = \dim \mathcal{B}_-^+ = \dim \mathcal{B}_-^- = L.$$  

Second, we may use that $\Gamma$ commutes with $H_e$ while $iCP$ anticommutes, then we have

$$H_e : K_+^+ \to \mathcal{B}_-^+, \quad H_e : K_+^- \to \mathcal{B}_+^+, \quad H_e : K_-^+ \to \mathcal{B}_-^+, \quad H_e : K_-^- \to \mathcal{B}_+^-.$$  

Therefore if, for instance, $n_+^+ > L$ then the restriction of $H_e$ to $K_+^+$ has a kernel of dimension at least $n_+^+ - L$ and the same is true when considering $K_-^-$ and $n_-^-$ that, as shown before, is equal to $n_-^-$. Given that $L = (n_+^+ + n_-^-)/2$ and taking into account the two subspaces, we finally get

$$\dim \text{Ker} H_0 \geq |n_+^+ - n_-^-|,$$
where the absolute value has been introduced to cover the case \( n^+ > L \). Our result here is a lower bound for the number of independent zero modes, but using a genericity argument one sees that for typical Hamiltonians the lower bound is saturated. In the next section, we will explicitly show that this is indeed the case for our family of Hamiltonians.

It is interesting to observe that the zero modes for a given Hamiltonian (at \( q = 0 \)) have all the same \( iCPT \) charge: +1 if \( n^+ > n^+ \) or -1 in the opposite case.

In the next sections, we will compute explicitly the indices introduced above, that determine the number of zero modes, we will also show that it is possible to derive them as a topological charge and establish the bulk-edge correspondence.

V. BOGOLIUBOV STATES

This section is devoted to the construction of the Bogoliubov modes of the fermionic chain, i.e. the solutions of the eigenvalue equations

\[
H_B \xi = -E \xi, \quad H_B \xi^\dagger = E \xi^\dagger.
\]

So that in the particular case of \( E = 0 \) we must recover the results of the previous section.

We first consider the part of the Hamiltonian in the bulk, and study the equation

\[
H_b \xi = -E \Pi_b \xi.
\]

It is immediate to see that we can solve it with the ansatz

\[
\xi_z = \sum_n (\alpha z^{n-1} a_n^\dagger + \beta z^{n-1} a_n),
\]

where

\[
\begin{pmatrix}
E + \Phi(z) & \Xi(z) \\
-\Xi(z) & E - \overline{\Phi}(z)
\end{pmatrix}
\begin{pmatrix}
\alpha \\
\beta
\end{pmatrix} = 0.
\]

We have introduced the Laurent polynomials of degree \((-L, L)\) \[41, 42\]

\[
\Phi(z) = \sum_{l=-L}^L A_l z^l, \quad \Xi(z) = \sum_{l=-L}^L B_l z^l,
\]

and \(\overline{\Phi}(z)\) in \[4\] stands for the Laurent polynomial in \( z \) with complex conjugate coefficients. That is

\[
\overline{\Phi}(z) = \overline{\Phi(\overline{z})}.
\]
and analogously for $\Xi(z)$.

Using the properties of their coefficients (for Hermitian Hamiltonians), we can establish reflection relations when we replace the arguments $z$ by $z^{-1}$. Indeed, one has

$$\Phi(z^{-1}) = \overline{\Phi}(z), \quad \Xi(z^{-1}) = -\Xi(z),$$

which will be useful in the future.

In order to have non-trivial solutions for (4), the determinant of the matrix has to vanish,

$$(E + \Phi(z))(E - \overline{\Phi}(z)) + \Xi(z)\overline{\Xi}(z) = 0,$$

and if we take $z = e^{i\theta}$ the expression above is, of course, the dispersion relation in implicit form.

The latter can be easily solved for $E$ to get

$$E_{\theta} = \pm \sqrt{\Phi_+^2(e^{i\theta}) + |\Xi(e^{i\theta})|^2 - \Phi_-(e^{i\theta})},$$

where

$$\Phi_{\pm}(z) = \frac{\Phi(z) \pm \overline{\Phi}(z)}{2}$$

are the even and odd part of $\Phi$ under inversion of its argument and both are real for $z = e^{i\theta}$. It is then clear that $E$ is always real for $z = e^{i\theta}$.

The possible values of $E_{\theta}$ determine the bands of positive and negative energy and, therefore, the gap between them is given by

$$\Delta = 2 \min_{\theta} |E_{\theta}|.$$

The bands can be identified respectively with the conduction and valence band, hence if $\Delta = 0$ our system is a model for a conductor and if $\Delta > 0$ it corresponds to an insulator.

The latter is the situation we are interested in: when the gap opens there may appear Bogoliubov modes localized in the vicinity of the defect whose energy lays between the bands. As the value of the contact, $q$, changes, the energy of the localized modes may vary from the valence band to the conduction one, allowing for the adiabatic pumping phenomenon. This is also analogous to what happens for topological insulators in higher dimensions, where states localized at the boundary interpolate between the bands rendering the material a conductor [28].

States with energy between the bands correspond to solutions of (5) with $|z| \neq 1$. Notice that, if the non-degenerate condition $|A_L|^2 - |B_L|^2 \neq 0$ is met, the Laurent polynomial in equation (5)
has degree \((-2L, 2L)\) and hence it is equivalent to a polynomial equation of degree \(4L\), therefore it has exactly \(4L\) complex solutions including multiplicities. Although there is no difficulty in dealing with the general case, with the aim of making the exposition simpler, we will assume that all the roots are simple so we have \(4L\) different solutions for (5).

It will be useful to distinguish the roots with modulus greater than one, that we will denoted by \(z^r\); from those which have modulus smaller than one, to be denoted by \(z^r\). Due to the properties of the Laurent polynomials \(\Phi\) and \(\Xi\), it is clear that if \(z\) is a solution of (5) then \(\bar{z}^{-1}\) is also a solution. This implies that we have the same number of roots of every type, exactly \(2L\).

The distinction of the two types of solutions is important because, for \(z^r\) and due to its exponential decay, \(\xi^r\) is supported, in the thermodynamic limit, in the first half of the chain, from 1 to \(N/2\), while for the other roots we have \(\xi^r\) supported in the second half. This fact can be expressed through the action of the operator \(\Gamma\), so that we have

\[
\Gamma \xi^< = \xi^>, \quad \Gamma \xi^> = -\xi^<.
\]

The general solution for the bulk equations is a linear combination of those for the different roots, hence the Bogoliubov mode has the form

\[
\xi = \sum_{r=1}^{2L} (\lambda^< r \xi^+ r + \lambda^> r \xi^- r),
\]

where

\[
\xi^< r = \sum_{n=1}^{N} (z^< r)^{n-1} (\alpha^< r a_n^\dagger + \beta^< r a_n), \quad \xi^> r = \sum_{n=1}^{N} (z^> r)^{N-n} (\alpha^> r a_n^\dagger + \beta^> r a_n).
\]

Now we have to consider the piece of the Hamiltonian near the defect

\[
(H_e + qV)\xi = -E \Pi_0 \xi.
\]

We can remove the dependence on \(E\) by applying to \(\xi\) the relations in the bulk and using again the non degeneracy condition we obtain, in the thermodynamic limit, the equivalent equations
for \( \lambda_\xi \) and \( \lambda_\zeta 
\)
\[
\sum_{r=1}^{2L} \lambda_\xi^z \alpha_\xi^z (z_\xi^r)^{-L} = q \sum_{r=1}^{2L} \lambda_\xi^z A L \alpha_\xi^z + B L \beta_\xi^z, \\
\sum_{r=1}^{2L} \lambda_\xi^z \beta_\xi^z (z_\xi^r)^{-L} = q \sum_{r=1}^{2L} \lambda_\xi^z A L \beta_\xi^z + B L \alpha_\xi^z,
\]
\[
\sum_{r=1}^{2L} \lambda_\zeta^z \alpha_\zeta^z (z_\zeta^r)^{-l} = 0, \\
\sum_{r=1}^{2L} \lambda_\zeta^z \beta_\zeta^z (z_\zeta^r)^{-l} = 0, \quad l = 1, \ldots, L - 1,
\]
\[
\sum_{r=1}^{2L} \lambda_\zeta^z \alpha_\zeta^z (z_\zeta^r)^l = 0, \\
\sum_{r=1}^{2L} \lambda_\zeta^z \beta_\zeta^z (z_\zeta^r)^l = 0, \quad l = 1, \ldots, L - 1,
\]
\[
\sum_{r=1}^{2L} \lambda_\zeta^z \alpha_\zeta^z (z_\zeta^r)^L = q \sum_{r=1}^{2L} \lambda_\zeta^z A L \alpha_\zeta^z - B L \beta_\zeta^z, \\
\sum_{r=1}^{2L} \lambda_\zeta^z \beta_\zeta^z (z_\zeta^r)^L = q \sum_{r=1}^{2L} \lambda_\zeta^z A L \beta_\zeta^z - B L \alpha_\zeta^z.
\]

The previous, together with the equations in the bulk in [41] for \( z_\xi^r, \alpha_\xi^r \) and \( \beta_\xi^r \), can be considered as the rigorous definition of the spectrum of the localized modes in the thermodynamic limit (notice that all the equations mentioned here are independent of \( N \)).

It is interesting to observe how \( P, T \) and \( C \) transformations act in the space of localized states:

\[
P : z_\xi^r \mapsto (z_\xi^r)^{-1} \quad T : z_\xi^r \mapsto z_\zeta^r \quad C : z_\zeta^r \mapsto (z_\zeta^r)^{-1}
\]

\[
\alpha_\zeta^r \mapsto \alpha_\xi^r \quad \beta_\zeta^r \mapsto -\beta_\xi^r
\]

And analogously with the exchange of \( \gg \) and \( \ll \). One easily checks that these transformations are symmetries of the equations in [0] for \( A_1 \in \mathbb{R} \) (\( P \)), for \( A_1, B_l \in \mathbb{R} \) (\( T \)), and for \( B_l \in \mathbb{R} \) (\( C \)).

Finally, we have the action of the operator \( \Gamma \),

\[
\Gamma : \lambda_\xi^z \mapsto -\lambda_\xi^z \\
\lambda_\zeta^r \mapsto \lambda_\zeta^r \\
q \mapsto -q,
\]

which always leaves the equations invariant.

Naturally the unknowns \( \lambda_\xi^z \) and \( \lambda_\zeta^r \) are uncoupled when \( q = 0 \). In this case, the equations read simply

\[
\sum_{r=1}^{2L} \lambda_\xi^z \alpha_\xi^z (z_\xi^r)^{-l} = 0, \\
\sum_{r=1}^{2L} \lambda_\xi^z \beta_\xi^z (z_\xi^r)^{-l} = 0, \quad l = 1, \ldots, L,
\]
\[
\sum_{r=1}^{2L} \lambda_\zeta^z \alpha_\zeta^z (z_\zeta^r)^l = 0, \\
\sum_{r=1}^{2L} \lambda_\zeta^z \beta_\zeta^z (z_\zeta^r)^l = 0, \quad l = 1, \ldots, L.
\]
Their solutions will be discussed in the next sections.

Now we are interested in the opposite situation $q \to \pm\infty$. One can show that the energy of the localized states in these limits coincide with those for $q = 0$. To do that one must consider the following ansatz

$$\xi' = \sum_{r=1}^{2L} (\lambda'_{r}^\leq \xi_{r}^\leq + \lambda'_{r}^\geq \xi_{r}^\geq),$$

where

$$\xi_{r}^\leq = \sum_{n=2}^{N} (z_{r}^\leq)^{n-2} (\alpha_{r}^\leq a_{n}^\dagger + \beta_{r}^\leq a_{n}), \quad \xi_{r}^\geq = \sum_{n=1}^{N-1} (z_{r}^\geq)^{n-N+1} (\alpha_{r}^\geq a_{n}^\dagger + \beta_{r}^\geq a_{n}).$$

The important point here is that the term for $n = 1$ is missing in $\xi_{r}^\leq$ and that for $n = N$ is absent in $\xi_{r}^\geq$.

If we introduce this ansatz into the equation for the defect and use $|A_{L}|^2 - |B_{L}|^2 \neq 0$, we arrive when $q \to \pm\infty$ at a set of equations identical to that for $q = 0$, namely

$$\begin{align*}
2L \sum_{r=1}^{2L} \lambda'_{r}^\leq \alpha_{r}^\leq (z_{r}^\leq)^{-l} &= 0, \\
2L \sum_{r=1}^{2L} \lambda'_{r}^\leq \beta_{r}^\leq (z_{r}^\leq)^{-l} &= 0, \quad l = 1, \ldots, L, \\
2L \sum_{r=1}^{2L} \lambda'_{r}^\leq \alpha_{r}^\geq (z_{r}^\geq)^{l} &= 0, \\
2L \sum_{r=1}^{2L} \lambda'_{r}^\geq \beta_{r}^\geq (z_{r}^\geq)^{l} &= 0, \quad l = 1, \ldots, L.
\end{align*}$$

Therefore, the solutions are the same and the spectrum of localized states at $q = 0$ and $q = \pm\infty$ coincide. This fact is apparent when one examines the numerical resolution of the system.

VI. BULK-EDGE CORRESPONDENCE

In this section, we shall apply the machinery presented above to rederive in an analytic way the algebraic results obtained in Sec. [IV]. With the new analytic tools we will be able to characterize the universality classes of the system which depend on the symmetries preserved by the deformations.

First of all we will consider the zero modes of the $C, P$ and $T$ symmetric chain at $q = 0$, as we did in Sec. [IV]. In this case, the Laurent polynomials have real coefficients and the solutions are of the form

$$\xi_{z} = \sum_{n} (\alpha \ z^{n-1} a_{n}^\dagger + \beta \ z^{n-1} a_{n})$$

for the bulk Hamiltonian should satisfy

$$\begin{pmatrix}
\Phi(z) & \Xi(z) \\
-\Xi(z) & -\Phi(z)
\end{pmatrix}
\begin{pmatrix}
\alpha \\
\beta
\end{pmatrix} = 0,$$

(9)
FIG. 1: In these plates we show the roots of (10) inside the unit circle. The different plates correspond to Hamiltonians with different values of the topological index $\nu$. Their non vanishing couplings are respectively: (a) $A_0 = 0.9, A_1 = 1.0, A_3 = -1.0, B_1 = 1.0, B_2 = 0.5, B_3 = 0.5$; (b) $A_1 = 0.5, B_1 = 0.5, B_3 = -0.1$; (c) $A_2 = 0.5, A_3 = 0.1, B_2 = 0.5, B_3 = -0.05$ and (d) $A_3 = 0.5, B_3 = 0.4$.

while $z$ is a solution of

$$(\Phi(z) + \Xi(z))(\Phi(z) - \Xi(z)) = 0.$$  \hspace{1cm} (10)

Now we may distinguish two kinds of roots depending on whether it is a solution of the first factor, in which case it will be denoted by $z_+$, or of the second one denoted by $z_-$. It is immediate to see that the solution for (9) in the first case satisfies $\alpha_+ = \beta_+$ and the Bogoliubov mode is even under the combined action of charge conjugation and parity i.e. $iCP\xi_{z_+} = \xi_{z_+}$, while for the second case we have $\alpha_- = -\beta_-$ and $iCP\xi_{z_-} = -\xi_{z_-}$. On the other hand, recall from the previous section that $\Gamma_{\xi_{z^\flat}} = \xi_{z^\flat}$ for $|z^\flat| < 1$ and $\Gamma_{\xi_{z^\dagger}} = -\xi_{z^\dagger}$ if $|z^\dagger| > 1$.

Therefore, in order to determine the number of zero modes for the open chain, it is enough to focus on the roots of (10) inside the unit circle and classify them into those that make zero its first factor, $z_+$, and those that annihilate the second one, $z_-$. Their respective numbers are $n_+$ and $n_-$ using the notation of Sec. IV.

Now, according to the results in that section, the number of zero modes is simply $|n_+ - n_-|$. It is not difficult to rederive this result by plugging into Eq. (7) our solutions and examining the resulting system of equations. One immediately sees that the subsystem for $\lambda^\flat_z$ has a kernel of dimension $\max(n_+, n_-) - (n_+ + n_-)/2$, and the same for those for $\lambda^\dagger_z$. From this the result follows. In passing we have shown that the bound for the limit on the dimension of $\text{Ker} H_0$ is saturated, as announced in Sec. IV. In Fig. 1 we represent the roots of (10) inside the unit circle for different values of the coupling constants and the index $\nu$. $\oplus$ stands for a root of the
first factor of 10 and \( \ominus \) for one of the second.

The number of zero modes as well as the index \( \nu = (n_+ - n_-)/2 \) are topologically protected. The latter takes integer values from \(-L\) to \(L\), and it can be written as a complex integral (or a difference of the complex phase when traversing the Brillouin zone). In concrete terms, consider the rational function

\[
R(z) = \frac{\Phi(z) + \Xi(z)}{\Phi(z) - \Xi(z)}
\]

then one has

\[
\nu = \frac{1}{4\pi i} \oint_{|z|=1} \frac{R'(z)}{R(z)} \, dz
\]

where the contour is travelled anticlockwise.

Now it is clear that, as long as the gap exists and the \( C, P \) and \( T \) symmetries are preserved, this number is topologically protected. In fact, if we deform the Hamiltonian while keeping the symmetries, the roots \( z_+^\pm \) and \( z_-^\pm \) may move but they can not change suddenly their character associated to the \( \Gamma \) and \( iCP \) charges. The only way of varying the amount of solutions of each type inside the disc is by letting the roots cross the unit circle, but in that moment the gap closes (there are zero modes in the continuum spectrum) and the topological protection associated to the existence of a gap disappears.

Notice that our proof of the topological protection and the universality classes requires that \( P \) and \( C \) are preserved so we have real couplings. One may wonder what happens if these symmetries are absent.

In general, if the symmetries are lost, there are no zero modes at \( q = 0 \) except for some exceptions which are still protected and will be discussed later on. But we may ask what is the fate of the universality classes. The concrete question is the following: can we interpolate between two \( C, P \) and \( T \) invariant theories with different topological indices without closing the gap? The answer is affirmative provided the two indices have the same parity, i.e. \( \nu - \nu' = 2k \).

It is also true that in order to do so the interpolating Hamiltonians must lose the \( C \) symmetry. The previous implies the existence of a \( \mathbb{Z}_2 \) charge that is robust under any perturbation that maintains the existence of a gap.

We first show that if we preserve the \( C \) symmetry in the intermediate theories, then the topological index does not change. To see it, we first notice that if \( C \) is preserved, then the
pairings $B_l$ are real and the dispersion relation can be written as

$$(E + \Phi_-(z))^2 = \Phi_+^2(z) - \Xi^2(z).$$

Now if for some of the interpolating Hamiltonians $\Phi_+^2(e^{i\theta}) - \Xi^2(e^{i\theta}) = 0$ for some $\theta$, then it is also so for $-\theta$ and, due to the properties of $\Phi_-$ under inversion, $E_\theta = -E_{-\theta}$. This means that going around the unit circle the sign of the energy changes, which implies that it vanishes at some $\theta_0$ and the gap closes. If $\theta = -\theta$, i.e. if it is 0 or $\pi$, one has that always $\Phi_\pm(\pm 1) = 0$ and $E_0 = 0$ or $E_\pi = 0$ and the gap also closes.

Then the roots of $(\Phi_+(z) + \Xi(z))(\Phi_+(z) - \Xi(z)) = 0$ can not approach the boundary of the unit disc without closing the gap. It implies that

$$R(z) = \frac{\Phi_+(z) + \Xi(z)}{\Phi_+(z) - \Xi(z)}$$

is analytic around the unit circle for every intermediate Hamiltonian and therefore the index defined from $R$ can not change at any step.

The second question is the invariance of the $\mathbb{Z}_2$ topological charge under any perturbation. In order to show that, we abandon for the moment the complex plane and move to the Bogoliubov modes space. In this context, we will prove that starting from a $P$, $C$, and $T$ invariant Hamiltonian with odd $\nu$, then we necessarily have a pair of zero-energy states that does not disappear under any perturbation of the couplings.

The reason is the following. As we saw in Sec. IV, in every $P$, $C$, $T$ invariant theory with gap we can decompose the space of zero modes at $q = 0$ into eigenspaces of $\Gamma$,

$$\text{Ker } H_0 = \mathcal{V}_0^+ \oplus \mathcal{V}_0^-$$

and dim $\mathcal{V}_0^\pm = |\nu|$.

Then the theory is deformed, call $H_t$ the deformed Hamiltonian, in such a way that the gap does not disappear, i.e. we still have states that are localized at the edge and its energy is preserved under the transformation $\Gamma$. The subspace $\text{Ker } H_0$ is deformed into a new $H_t$ invariant subspace $\mathcal{V}_t$ that can be decomposed, as before, according to the eigenvalues of $\Gamma$, which still is a symmetry of the theory,

$$\mathcal{V}_t = \mathcal{V}_t^+ \oplus \mathcal{V}_t^-,$$

and both $\mathcal{V}_t^+$ and $\mathcal{V}_t^-$ are $H_t$ invariant. Let us focus on $\mathcal{V}_t^+$. Under a continuous deformation, its dimension must be independent of $t$, therefore it is $|\nu|$. Now let us consider a basis of $\mathcal{V}_t^+$.
formed by eigenstates of $H_t$ and denote them by $\xi_E$. As $\Theta$ anticommutates with any Hermitian $H_t$, therefore

$$\Theta \xi_E = \xi_{-E}$$

and, if all the states have $E \neq 0$, then we must have an even number of them, which implies that $|\nu| = \dim V^+_t$ is even. Or, reciprocally, if $\nu$ is odd then there must be a state of zero energy invariant under $CPT$. This shows the topological protection of the zero modes. Of course, it ceases to be true when the gap closes and we lose the symmetry under $\Gamma$.

It may be interesting to see this from a more constructive or geometrical point of view that, besides, will give us an argument to prove that all $P$, $C$ and $T$ symmetric theories with odd (even) $\nu$ are accessible by the continuous deformation of any of them, maintaining the gap $\Delta > 0$ in all the process.

Consider a Hamiltonian with real couplings of range $L$. The theory is fully determined by the $(-L, L)$ degree, Laurent polynomial

$$Q(z) = \Phi(z) + \Xi(z).$$

Actually we can single out $\Phi$ as the even part of $Q$ under inversion of $z$ and $\Xi$ as the odd part and from them we can recover the hopping and pairing constants $A_l$ and $B_l$ respectively.

$Q(z)$ is, in turn, determined up to a trivial scaling by its roots $z_r$. These, in order to have a gapped theory, should have modulus different from one. By changing the $P$, $C$, $T$ invariant Hamiltonian and as long as they do not cross the unit circle (in which moment the theory would be gapless), we can move the roots freely with the only restriction of being real numbers or forming complex conjugate pairs. Then the only difficulty is how to interpolate continuously between two theories whose polynomials $Q(z)$ have a different number of roots inside the unit disc. The latter is given by $L + \nu$, hence the task is to interpolate between two Hamiltonians with different index $\nu$ or, in more physical terms, different number of zero modes.

Explicitly, consider the following $t$ dependent family of Laurent polynomials

$$Q_t(z) = \frac{1}{2}(e^{-t}z + e^{t}z^{-1})P(z), \quad t \in [-1, 1]$$

where $P(z)$ has degree $(-L + 1, L - 1)$ and real coefficients. Assume that $P(z)$ is associated to a $L - 1$ range Hamiltonian with a gap between the valence and conduction bands, and denote its corresponding index by $\nu_0$ (that is, we assume that $P(z)$ has $L + \nu_0 - 1$ roots inside the unit
disc and $L - \nu_0 - 1$ outside). Notice that if $z_1, \ldots, z_{2L-2}$ are the roots of $P$, then those of $Q_t$ are $z_1, \ldots, z_{2L-2}, ie^t, -ie^t$. Therefore, the family of polynomials interpolates between a theory with index $\nu - 1 = \nu_0 + 1$ (or equivalently $L + \nu_0 + 1$ roots inside the unit disc for $t = -1$) and another one with $\nu_1 = \nu_0 - 1$ (or $L + \nu_0 - 1$ roots).

The problem with this interpolation is that the gap closes at $t = 0$. In fact, we have

$$\Delta_t^2 = 4 \min_\theta |Q_t(e^{i\theta})|^2,$$

but for $t = 0$ one has $Q_0(e^{i\pi/2}) = 0$, hence $\Delta_0 = 0$, which is not allowed.

This inconvenience can be overcome if we consider a modification of the interpolating Hamiltonians. If $Q_t$ is associated to the couplings $A_l(t)$ and $B_l(t)$ we replace the pairing between nearest neighbours $B_1(t)$ by

$$B'_1(t) = B_1(t) + ib\sqrt{1 - t^2},$$

where $b$ is a constant to be appropriately fixed. Notice that this new family of Hamiltonians also interpolate between $Q_{-1}$ and $Q_1$, $B'(\pm 1) = B(\pm 1)$. Next we will show that $H_t$ has a non zero gap for every $t \in [-1, 1]$.

In fact, using the dispersion relation one can compute the new gap

$$\Delta'_t^2 = 4 \min_\theta \left( (\cosh^2 t \cos^2 \theta + \sinh^2 t \sin^2 \theta) |P(e^{i\theta})|^2 + 4b^2 (1 - t^2) \sin^2 \theta \right).$$

We have assumed that $P(e^{i\theta}) \neq 0$ for any $\theta$, then there is a positive constant $a$ such that

$$|P(e^{i\theta})|^2 > a^2 > 0, \text{ for any } \theta \in [-\pi, \pi],$$

and if we choose $b = a/2$ we have

$$\Delta'_t^2 \geq 4a^2 \min_\theta (\cosh^2 t \cos^2 \theta + \sinh^2 t \sin^2 \theta + (1 - t^2) \sin^2 \theta)$$

$$\geq 4a^2 \min_\theta (1 + \sinh^2 t - t^2 + t^2 \cos^2 \theta)$$

$$\geq 4a^2(1 + \sinh^2 t - t^2) \geq 4a^2. \quad (11)$$

Therefore, throughout the whole process the gap is bounded below by a positive constant which means that we have constructed a legitimate, topological protective, interpolation.

It is interesting to pause a little and discuss why, while this procedure can be used to connect a Hamiltonian with index $\nu_0 + 1$ with another one with $\nu_0 - 1$, we never could end up with a system of index $\nu_0$.

To understand why it is so, notice that if we move a single root (instead of a pair of complex conjugate) from inside the unit disc to its exterior it should be real and cross the unit circle...
at $z = 1$ or $z = -1$. Now, due to its antisymmetric properties, $\Xi(\pm 1) = 0$, which implies that we can not open the gap at $z = \pm 1$ with a modification of the couplings $B_l$, as we did before (the same applies to $\Phi_-$, the antisymmetric part of $\Phi$), and necessarily the interpolating Hamiltonians have, at some point, zero gap. This is an alternative explanation to the strong topological protection of the $\mathbb{Z}_2$ charge determined by the parity of the index $\nu$.

VII. CHARGE PUMPING

In this section, we will study how the spectrum of the localized states changes when we modify the value of the contact. We will see that for certain Hamiltonians there are states that travel from the valence band to the conduction one, providing a mechanism for the so called adiabatic charge pumping.

Let us illustrate this with an example. Consider the chain with topological index $\nu = 0$ corresponding to plate a. in Fig. 2. Assume that initially $q = -3$ and the system is at its minimum energy state, i.e. we have all negative energy modes filled (alternatively we can interpret this state as the vacuum of the Fock space $|\Omega\rangle$ given by $\xi_n |\Omega\rangle = 0$, $n = 1, \ldots, N$). Now we proceed by slowly increasing the value of $q$. At some point, approximately for $q = -2.053$, one of the modes with negative energy crosses the $E = 0$ level and produces a hole in the Fermi sea. This represents the creation of a particle-hole pair, but they are still localized at the defect. If we keep adiabatically increasing $q$ there is a moment (near $q = 1.256$ in our case) in which the mode of positive energy enters into the conduction band giving rise to a free (unlocalized) particle-hole pair. This is what we mean by the charge pumping phenomenon.

We will see that all $P, C, T$ invariant theories enjoy the charge pumping property, but their behaviour under perturbations that break the symmetries differs from one universality class to another.

For definiteness, we will consider the family of Hamiltonians with range $L = 3$, so that we have seven universality classes (if we restrict to the $P, C, T$ invariant Hamiltonians), which correspond to $\nu = 0, \pm 1, \pm 2, \pm 3$. Now, the theories with $\nu$ of opposite sign and their perturbations are related by the change of $B_l$ to $-B_l$ that preserves the full spectrum. So in order to explore the whole zoo of theories we may restrict to four classes with $\nu = 0, 1, 2, 3$.

The spectrum of localized states, as a function of the contact $q$, for a representative of any of
FIG. 2: In these plates we show part of the one particle spectrum that includes the gap, as a function of the contact. The different plates correspond to Hamiltonians with different values of the topological index $\nu$. Their non vanishing couplings are respectively: (a) $A_0 = 0.9, A_1 = 1.0, A_3 = -1.0, B_1 = 1.0, B_2 = 0.5, B_3 = 0.5$; (b) $A_1 = 0.5, B_1 = 0.5, B_3 = -0.1$; (c) $A_2 = 0.5, A_3 = 0.1, B_2 = 0.5, B_3 = -0.05$ and (d) $A_3 = 0.5, B_3 = 0.4$. The two figures in the lower row look similar, but they have the important difference that the horizontal line at $E = 0$ represents a doubly degenerate state in the plate (c) and a four times degenerate one in (d).

At first sight, the plots corresponding to $\nu = 2$ and $\nu = 3$ look quite similar. This is only apparent because, while in the case of $\nu = 2$ the states at zero energy that are present for any value of the contact are doubly degenerate, those of $\nu = 3$ are four times degenerate. This will be manifest when we break the degeneracy by perturbing the respective Hamiltonians with non symmetric terms.

**Trivial case $\nu = 0$.**

In the first place, we shall consider the so called trivial phase in which we have no edge states at zero energy in the open chain, $q = 0$. As it was discussed in the previous sections, this occurs
FIG. 3: In the figure we show the spectrum around the gap for two Hamiltonians in the trivial phase. Plate (a) is the same than the one in Fig. and corresponds to a $C$ and $P$ symmetric Hamiltonian with couplings listed there. Plate (b) represents the spectrum for a deformation of the previous theory obtained by changing only $A_1 = 1.0 + 0.3i$ and $B_1 = 1.0 + 0.8i$. The addition of an imaginary part to the couplings breaks $C$ and $P$ symmetries.

in $P$, $C$ and $T$ symmetric theories with an index $\nu = 0$.

The energy spectrum as a function of $q$ is plotted in Fig. There we see that, while there are no zero modes at $q = 0$, we have them at some definite value of the contact.

We will show that this is a general property in the sense that for our family of Hamiltonians there is always a zero energy state at some value of $q$. In other words, we claim that there is always some value of $q$ such that

$$(H_0 + qV)\xi = 0$$

has a solution with $\xi \neq 0$.

To prove it, let us consider the subspace of $\mathcal{B}$ containing the sites contiguous to the defect and denote it by $\mathcal{B}_{\text{def}}$. Explicitly

$$\mathcal{B}_{\text{def}} = \text{span}\{a_1^+, a_N^+, a_1, a_N\}$$

and call $\Pi_{\text{def}}$ the orthogonal projector onto that space.

Of course, the relevant role played by $\mathcal{B}_{\text{def}}$ is due to the properties of the operator $V$, namely we immediately see

$$\Pi_{\text{def}}V = V\Pi_{\text{def}} = V.$$
Note also that $B_{\text{def}}$ is left invariant by the operators $\Gamma$ and $\Theta$, that act on the standard basis respectively as

$$
\Gamma a_1^\dagger = a_1^\dagger, \quad \Gamma a_1 = a_1, \quad \Gamma a_N^\dagger = -a_N^\dagger, \quad \Gamma a_N = -a_N,
$$

$$
\Theta a_1^\dagger = ia_1^\dagger, \quad \Theta a_1 = ia_1, \quad \Theta a_N^\dagger = ia_N, \quad \Theta a_N = ia_N^\dagger.
$$

Now we have two possibilities: either $H_0$ has a non trivial kernel (as it happens, for instance, with Hamiltonians in the universality class of odd $\nu$), in which case

$$
(H_0 + qV)\xi = 0
$$

has a non trivial solution for $q = 0$ or, if the previous does not hold, $H_0$ is invertible.

In this second case, we will consider the equation

$$
(VH_0^{-1} + q^{-1}I)\xi' = 0
$$

that is equivalent to (12) if $q \neq 0$ and we take $\xi' = H_0\xi$.

Of course, due to the properties of $V$, any solution of (13) should belong to $B_{\text{def}}$ and its equation can be equivalently written as

$$
(V\Pi_{\text{def}}H_0^{-1}|_{B_{\text{def}}} + q^{-1}I)\xi' = 0.
$$

Our next task is to determine the most general form of the map

$$
\Pi_{\text{def}}H_0^{-1}|_{B_{\text{def}}} : B_{\text{def}} \rightarrow B_{\text{def}}.
$$

In order to do that, we use the relations

$$
H_0\Gamma = \Gamma H_0, \quad H_0\Theta = -\Theta H_0
$$

where, as argued earlier, the first one is true for localized states and the second one holds for any Hermitian Hamiltonian. These relations are also valid for its projected inverse. Therefore, we can deduce the following properties for the matrix elements of $\Pi_{\text{def}}H_0^{-1}|_{B_{\text{def}}}$

$$
\langle a_1^\dagger | H_0^{-1} a_1^\dagger \rangle = -\langle a_1 | H_0^{-1} a_1 \rangle = \gamma_1 \in \mathbb{R},
$$

$$
\langle a_N^\dagger | H_0^{-1} a_N^\dagger \rangle = -\langle a_N | H_0^{-1} a_N \rangle = \gamma_N \in \mathbb{R},
$$

and all the others vanish.
From which we get the following expression for $VH_0^{-1}|_{\mathcal{B}_{\mathrm{def}}}$ in the standard basis of $\mathcal{B}_{\mathrm{def}}$

$$(VH_0^{-1}|_{\mathcal{B}_{\mathrm{def}}}) = \left( \begin{array}{cccc} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 \end{array} \right) \left( \begin{array}{cccc} \gamma_1 & 0 & 0 & 0 \\ 0 & \gamma_N & 0 & 0 \\ 0 & 0 & -\gamma_1 & 0 \\ 0 & 0 & 0 & -\gamma_N \end{array} \right) = \left( \begin{array}{cccc} 0 & \gamma_N & 0 & 0 \\ \gamma_1 & 0 & 0 & 0 \\ 0 & 0 & 0 & \gamma_N \\ 0 & 0 & \gamma_1 & 0 \end{array} \right).$$

Thus the eigenvalue equation (13) has non trivial solutions if and only if

$$\det(VH_0^{-1}|_{\mathcal{B}_{\mathrm{def}}} + q^{-1}I) = (q^{-2} - \gamma_1\gamma_N)^2 = 0.$$ 

We will show below that for our cases of interest (invertible $H_0$ continuously connected with a $P$ invariant Hamiltonian without zero modes at $q = 0$) $\gamma_1\gamma_N > 0$ and hence there are two opposite real values of $q = \pm(\gamma_1\gamma_N)^{-1/2}$ for which (13) has non trivial solutions or equivalently $H_0 + qV$ has eigenstates localized at the defect with zero energy.

First we will prove that $\gamma_1$ and $\gamma_N$ must be different from zero. Let us assume the contrary and take for instance $\gamma_1 = 0$. If we denote by $\Pi_{\mathrm{def}}^1$ the orthogonal projector onto

$$\mathcal{B}_{\mathrm{def}}^1 = \text{span}\{a_1^+, a_1\}$$

and take $\xi_0 = H_0^{-1}a_1^+$, then when $\gamma_1 = 0$ we have $\xi_0 \in (\mathcal{B}_{\mathrm{def}}^1)^\perp$ and also

$$(I - \Pi_{\mathrm{def}}^1)H_0\xi_0 = (I - \Pi_{\mathrm{def}}^1)a_1^+ = 0.$$ 

This means that the operator in $(\mathcal{B}_{\mathrm{def}}^1)^\perp$ defined by $H_0' = (I - \Pi_{\mathrm{def}}^1)H_0(\mathcal{B}_{\mathrm{def}}^1)^\perp$ has a zero energy eigenstate given by $\xi_0$. But the operator $H_0'$ is exactly like $H_0$ only in a chain in which the site 1 has been removed. In the thermodynamic limit and for localized states, this suppression does not make any difference, therefore it is contradictory that $H_0'$ has a localized state of zero energy and $H_0$ has not. The consequence of this is that $\gamma_1, \gamma_N$ can not vanish.

To argue that $\gamma_1\gamma_N > 0$ we use an argument of continuity. In fact, for a $P$ invariant Hamiltonian $\gamma_1 = \gamma_N$ and the positivity of the product is guaranteed. As we just showed, it can not vanish and therefore any deformation of this system has also $\gamma_1\gamma_N > 0$ and necessarily a state of zero energy at some value of the contact $q$, as we stated before.

We discussed and explained the similarities between the two plates in Fig. 3, namely the existence of zero modes of the Hamitonian for some value of $q$. As it is apparent, the main difference between them is the existence of degenerate, localized states at $q = 0$ in the plate on
the left, while the degeneracy is broken in the plate on the right. Of course, the difference is related to the breaking of \( C \) and \( P \) symmetries as we will explain now.

Consider first a \( P \) symmetric Hamiltonian \( H_B \), then we have in particular \( PH_0 = H_0P \) and for localized states also \( \Gamma H_0 = H_0 \Gamma \). Then every \( H_0 \)-eigenspace \( S_E \) of localized states is left invariant by \( P \) and can be obtained from eigenvectors of \( \Gamma \). But, as \( \Gamma \) and \( P \) anticommute, we have that if we take \( \xi \in S_E \) with \( \Gamma \xi = \xi \), then \( P\xi \in S_E \) and \( \Gamma P\xi = -P\xi \). Therefore, \( \xi \) and \( P\xi \) are independent and \( S_E \) has dimension at least two, which explains the degeneracy of the energy level.

In the case that \( C \) is not broken, we can repeat the previous argument but replacing \( P \) by \( PT \) which, due to the \( CPT \) theorem, commute in this situation with \( H_B \) and anticommutes with \( \Gamma \).

Finally, if both \( C \) and \( P \) are broken there is no reason for the existence of degenerate states at \( q = 0 \) and, as it is shown in the plate on the right, the two curves split.

Note in passing, that in this last case the charge pumping phenomenon is not possible, as the adiabatic evolution fails to transfer states from the valence band to the conduction one.

We finally would like to remark the coincidence of the spectrum of localized states for \( q = 0 \) and \( q = \infty \). This was explained in Sec. V and is clearly illustrated in the two plates of Fig. 3.

**Nontrivial phase \( \nu = 1 \).**

We move now to the case in which we have localized states of zero energy for the open chain \((q = 0)\). Two examples of this situation that correspond to the topological index \( \nu = 1 \) are plotted in Fig. 4.

As we already discussed, and due to the fact that \( \nu \) is odd, we can not remove the zero modes at \( q = 0 \) by any continuous perturbation of the system that maintains a gap between the bands along the whole process. This is illustrated in Fig. 4 in the left plate we depict the spectrum of a \( C, P, T \) symmetric chain while that of the right has \( P \) and \( T \) symmetries broken. We observe that in both cases there are two states of zero energy for the open chain.

The main difference between the two plots is that in the left one we have the possibility of pumping charge adiabatically from the valence to the conduction band, while in the right one this is not possible. In fact in the \( C, P, T \) symmetric case, as we change \( q \), a state moves continuously from one band to the other while in the non symmetric one there is a gap and there are not states that connect both bands.
FIG. 4: In the figure we show the spectrum around the gap for a Hamiltonian with topological index \( \nu = 1 \) and its deformation. Plate (a) is identical to that in Fig. 2 and corresponds to a \( C \) and \( P \) symmetric Hamiltonian with the coupling constants specified there. Plate (b) represents the spectrum for a deformation of the previous, obtained by changing the nearest neighbours hopping into \( A_1 = 0.5 + 0.1i \), which breaks \( P \) invariance.

The two different regimes are determined by the properties of the system under parity. One can show that if the chain is parity invariant (\( PH_B = H_B P \)), then there is necessarily a pair of states interpolating between the two bands. To see this, let us denote by \( \xi_q \) a localized eigenstate for \( H_B = H_0 + qV \) with energy \( E_q \) between the bands and assume that it is even under parity, i.e. \( P\xi_q = \xi_q \). Now due to the Hellmann-Feynman theorem we have

\[
\frac{d}{dq} E_q = \langle \xi_q | V \xi_q \rangle.
\]

Then if we denote

\[
\xi_q = \sum_{n=1}^{N} (\alpha_n a_n^\dagger + \beta_n a_n)
\]

and take into account the form of \( V \) we have

\[
\langle \xi_q | V \xi_q \rangle = \overline{\alpha}_1 \alpha_N + \alpha_1 \overline{\alpha}_N - \overline{\beta}_1 \beta_N - \beta_1 \overline{\beta}_N.
\]

But \( P\xi_q = \xi_q \) implies that \( \alpha_1 = \alpha_N \) and \( \beta_1 = -\beta_N \). Therefore,

\[
\langle \xi_q | V \xi_q \rangle = 2|\alpha_1|^2 + 2|\beta_1|^2.
\]

Now if \( \alpha_1 \neq 0 \) or \( \beta_1 \neq 0 \) for any \( q \), then the energy as a function of \( q \) has a positive slope and it interpolates between the lower and the upper band.
Before proceeding, let us pause a little to discuss the possibility $\alpha_1 = \beta_1 = 0$. In that case, we have $V\xi_q = 0$ and then $E_q = E_0$ and $\xi_q = \xi_0$, i.e. both the energy and the state are independent of $q$. This would be represented in our plots by a horizontal line at the given constant value of the energy $E_0$. It is also interesting to notice that in the thermodynamic limit we can obtain two eigenstates $\xi'_0$ and $\Gamma\xi'_0$ with the same energy $E_0$ for $H_0$ by the transformation

$$
\alpha'_1 = \alpha_2, \quad \alpha'_2 = \alpha_3, \ldots, \quad \alpha'_{N-1} = \pm \alpha_{N-2}, \quad \alpha'_N = \pm \alpha_{N-1},
$$

where the $+$ and $-$ sign corresponds, respectively, to $\xi'_0$ and $\Gamma\xi'_0$. To be more precise, and using the notation of Sec. V where we give a rigorous definition of the thermodynamic limit,

$$
\lambda_r^+ = z_r^+ \lambda_r^-, \quad \text{and} \quad \lambda_r^-' = \pm (z_r^-)^{-1} \lambda_r^-.
$$

This is precisely the situation that we have for $E = 0$ and $q = 0$ in the third and fourth plates of Fig. 2 where, together with the horizontal line at $E = 0$, we have two oblique curves with parity $+$ and $-$ respectively, which correspond to the states $\xi'_0$ and $\Gamma\xi'_0$, forming altogether a $\nabla$ shape. So far, this multiply degenerate situation for stationary states at $q = 0$ has been observed uniquely in these particular cases ($P$, $C$ and $T$ symmetric theories with $\nu \geq 2$ and $E = 0$). We do not know if they may appear elsewhere.

After this little digression, we proceed to conclude the analysis of the differences between the two plates of Fig. 4. We already showed that for a $P$ invariant theory there are always lines with a slope of constant sign in the plot of $E$ against $q$. This is not necessarily so if parity is broken, as it is illustrated in the plate on the right where the different curves in the region between the bands reach a maximum or minimum and change the sign of their slope. A consequence of this is that the connection between the bands is interrupted and the phenomenon of charge pumping is not possible any more. This is similar to what we observed in the trivial ($\nu = 0$) case with the difference that there we had to break both $C$ and $P$ symmetries to destroy the connection between the bands.

**Nontrivial phases $\nu = 2$ and $\nu = 3$.**

We finally discuss the cases of higher topological index $\nu$ where the complexity of the $E - q$ diagrams is shown in full lore. Most of the features of the different plots and its relation with the breaking of symmetries have been discussed already. Here we will review how they actually manifest in these cases.
FIG. 5: In these four plates we represent the spectrum around the gap for different deformations of the $C, P, T$ symmetric Hamiltonian corresponding to the third plot in Fig. 2 with topological index $\nu = 2$. As listed there, the non-vanishing couplings are $A_2 = 0.5, A_3 = 0.1, B_2 = 0.5, B_3 = -0.05$ for the plate (a); we add to the previous Hamiltonian an imaginary nearest neighbour pairing $B_1 = 0.3i$, breaking $C$, in plate (b); a hopping $A_1 = 0.15i$, that breaks $P$ in plate (c) and, finally, we add both perturbations $A_1$ and $B_1$ together in plate (d).

If we start with the four plates of Fig. 5 corresponding to $\nu = 2$, we have in the upper-left the fully symmetric theory. As we already mentioned, the horizontal line represents a doubly degenerate level.

The upper-right plot depicts the spectrum of a $P$ and non-$C$ symmetric theory. We observe that the four degenerate states that we had at $q = 0$ and $E = 0$ split into two pairs, as expected. On the other hand, the adiabatic charge pumping is still possible if we consider the compactification of the $q$-axis to form a circle.

In the lower-left plate, we show the spectrum for a $C$ and non-$P$ symmetric theory. Here the splitting of the four states in the middle still occurs into pairs, but the connection between the
FIG. 6: In these four plates we represent the spectrum around the gap for different deformations of the $C, P, T$ symmetric Hamiltonian corresponding to the fourth plot in Fig. 2 with topological index $\nu = 3$. The spectrum of the undeformed Hamiltonian with the only non vanishing couplings given by $A_3 = 0.5, B_3 = 0.4$ is represented in plate (a); the previous, perturbed with an imaginary nearest neighbour pairing $B_1 = 0.3i$ breaking $C$ is plotted in plate (b); the original Hamiltonian supplemented with a hopping $A_1 = 0.17i$ that breaks $P$ in plate (c) and, finally, the result of adding both perturbations $A_1$ and $B_1$ together is shown in plate (d).

bands and the charge pumping phenomenon is destroyed due to the breaking of parity.

Finally, in the lower-right plate, all the symmetries are broken and consequently there are not any degeneration, except for the doubly degenerate states of zero energy at opposite values of $q$, whose necessary existence can be proven as we did in the $\nu = 0$ case. Notice also the coincidence of the spectrum at $q = 0$ and at $q = \pm \infty$ in all four plates.

To conclude, let us briefly discuss the four plates of Fig. 6. They represent the spectrum of localized states for different perturbations of a Hamiltonian with topological index $\nu = 3$. As it is indicated in the plates, they differ by its behaviour under $C$ and $P$ symmetries. Here
we see a situation very similar to the case $\nu = 2$ (see Fig. 5), but a little more intricate. The main difference with the previous case is the persistence of a pair of zero modes at $q = 0$ as it is expected according to the arguments given in Sec. VI. Again, when the Hamiltonian is $P$ symmetric, we have the possibility of adiabatic charge pumping from the valence band to the conduction one and this disappears when the $P$ symmetry is broken.

VIII. CONCLUSIONS

In this paper, we have studied the localized modes in a general free-fermionic chain with possible finite-range couplings and a single defect which breaks the translational invariance. The defect consists in a tunable hopping coupling $q$ that connects the end points of the chain. We have obtained a set of equations that allow to construct the edge modes for any values of the couplings and $q$ and can be directly extended to the thermodynamic limit.

For generic open chains ($q = 0$) with $P$, $C$ and $T$ symmetries, we have determined the number of independent zero-energy modes, which characterizes the topological phase of the system. This analysis has been performed both algebraic and analytically. Through the latter approach, we have derived a bulk-edge correspondence. The zero-modes can be associated with the roots of a polynomial. This polynomial is defined on the analytical continuation of the momentum space, their coefficients are determined by the couplings of the Hamiltonian in the bulk and its degree by the the range $L$ of the couplings. Using this fact, we have introduced a topological index which can be calculated by counting the roots of the polynomial and identifies the topological phases in agreement with the ten-fold classification [16]. We have found that the number of different topological phases depends on the range $L$, there are $2L + 1$ phases for $C$, $P$ and $T$ symmetric theories. It is interesting to point out that the analytical approach considered here is reminiscent of the geometric framework developed in Refs. [39,42] to analyze the entanglement entropies in this kind of systems. This may have some connection with previous results that relate entropic and topological properties of this kind of systems [43, 44].

When we turn on the contact $q$, we have found that the zero-energy modes may acquire energy, and they can cross the gap of the bulk as $q$ varies, connecting the valence and conduction bands. By pumping a localized state from one band to the other, one can create a free and delocalized particle-hole pair. We have shown that this phenomenon occurs in any topological phase as
long as the chain enjoys $P$ symmetry. In fact, the states that interpolate between bands have a defined parity. In general, when we introduce perturbations in the couplings that break $P$ and $C$ symmetries, the connection between bands is lost. As we already mentioned in the introduction, an interesting aspect is that in our case we pump states by modifying adiabatically a parameter of the edge instead of one related to the bulk, as usually happens in the topological pumping.

Here we have only considered chains with finite long-range couplings, i.e. the range $L$ of the couplings does not diverge when we take the thermodynamic limit. But it would be interesting to extend the machinery and results presented in this paper to chains in which the couplings extend through the whole chain, and the range $L$ diverges in the thermodynamic limit, such as the long-range Kitaev [45]. The presence of infinite-range couplings may give rise to unconventional features, see e.g. Refs. [46–50]. In particular, novel topological phases and excitations can appear [51–55]. Another direction is to consider a non-Hermitian chain or defect, which can also host non-trivial and stable topological modes [56]. As in the case of infinite-range couplings, the emergence of non-Hermitian topological phases implies the extension of the ten-fold way classification for Hermitian Hamiltonians [57–58] and the modification of the bulk-edge correspondence [59].

Acknowledgments: Research partially supported by grants E21,17R, DGIID-DGA and PGC2018-095328-B-100, MINECO (Spain). FA acknowledges support from Brazilian Ministries MEC and MCTIC, from Simons Foundation (Grant Number 884966, AF), and from ERC under Consolidator Grant Number 771536 (NEMO), and acknowledges the warm hospitality and support of Departamento de Física Teórica, Universidad de Zaragoza, during several stages of this work.

[1] M. Asorey, *Space, matter and topology*, Nature Phys. 12, 616 (2016), arXiv:1607.00666 [cond-mat.mes-hall]

[2] X.-L. Qi, S.-C. Zhang, *Topological insulators and superconductors*, Rev. Mod. Phys. 83, 1057 (2011), arXiv:1008.2026 [cond-mat.mes-hall]

[3] M. Z. Hasan, C. L. Kane, *Colloquium: Topological insulators*, Rev. Mod. Phys. 82, 3045 (2010), arXiv:1002.3895 [cond-mat.mes-hall]
[4] A. Bernevig, T. L. Hughes, *Topological Insulators and Topological Superconductors*, Princeton: Princeton University Press, 2013

[5] A. Kitaev, *Unpaired Majorana fermions in quantum wires*, Phys.-Usp. 44, 131 (2001), arXiv:cond-mat/0010440 [cond-mat.mes-hall]

[6] L. P. Rokhinson, X. Liu, J. K. Furdyna, *Observation of the fractional ac Josephson effect: the signature of Majorana particles*, Nature Phys. 8, 795 (2012), arXiv:1204.4212 [cond-mat.mes-hall]

[7] A. Das, Y. Ronen, Y. Most, Y. Oreg, M. Heiblum, H. Shtrikman, *Evidence of Majorana fermions in an Al-InAs nanowire topological superconductor*, Nature Phys. 8, 887 (2012), arXiv:1205.7073 [cond-mat.mes-hall]

[8] V. Mourik, K. Zuo, S. M. Frolov, S. R. Plissard, E. P. A. M. Bakkers, L. P. Kouwenhoven, *Signatures of Majorana fermions in hybrid superconductor-semiconductor nanowire devices*, Science 336, 1003 (2012), arXiv:1204.2792 [cond-mat.mes-hall]

[9] S. Nadj-Perge, I. K. Drozdov, J. Li, H. Chen, S. Jeon, J. Seo, A. H. MacDonald, A. Bernevig, A. Yazdani, *Observation of Majorana Fermions in Ferromagnetic Atomic Chains on a Superconductor*, Science 346, 602 (2014), arXiv:1410.0682 [cond-mat.mes-hall]

[10] S. Das Sarma, H. Pan, *Disorder-induced zero-bias peaks in Majorana nanowires*, Phys. Rev. B 103, 195158 (2021), arXiv:2103.05628 [cond-mat.mes-hall]

[11] A. Kitaev, *Fault-tolerant quantum computation by anyons*, Ann. Phys. 303, 2 (2003), arXiv:quant-ph/9707021

[12] J. K. Pachos, *Introduction to Topological Quantum Computation*, Cambridge University Press, 2012

[13] S. Das Sarma, M. Freedman, C. Nayak, *Majorana Zero Modes and Topological Quantum Computation*, npj Quantum Information 1, 15001 (2015), arXiv:1501.02813 [cond-mat.str-el]

[14] A. Altland, M. R. Zirnbauer, *Nonstandard symmetry classes in mesoscopic normal-superconducting hybrid structures*, Phys. Rev. B 55, 1142 (1997), arXiv:cond-mat/9602137

[15] A. Kitaev, *Periodic table for topological insulators and superconductors*, AIP Conf. Proc. 1134, 22 (2009), arXiv:0901.2686 [cond-mat.mes-hall]

[16] S. Ryu, A. P. Schnyder, A. Furusaki, A. W. W. Ludwig, *Topological insulators and superconductors: tenfold way and dimensional hierarchy*, New J. Phys. 12, 065010 (2010),
[17] S. Ryu, Y. Hatsugai, Topological Origin of Zero-Energy Edge States in Particle-Hole Symmetric Systems, Phys. Rev. Lett. 89, 077002 (2002), arXiv:cond-mat/0112197 [cond-mat.supr-con]

[18] M. Henkel, A. Patkós, M. Schlotmann, The Ising quantum chain with defects. The exact solution, Nucl. Phys. B 314, 609 (1989)

[19] U. Grimm, The quantum Ising chain with a generalized defect, Nucl. Phys. B 340, 633 (1990), arXiv:hep-th/0310089

[20] V. Eisler, I. Peschel, Solution of the fermionic entanglement problem with interface defects, Ann. Phys. 522, 679 (2010), arXiv:1005.2144 [cond-mat.stat-mech]

[21] B. Bertini, M. Fagotti, Determination of the Nonequilibrium Steady State Emerging from a Defect, Phys. Rev. Lett. 117, 130402 (2016), arXiv:1604.04276 [cond-mat.stat-mech]

[22] A. Alase, E. Cobanera, G. Ortiz, L. Viola, Exact Solution of Quadratic Fermionic Hamiltonians for Arbitrary Boundary Conditions, Phys. Rev. Lett. 117, 076804 (2016), arXiv:1601.05486 [cond-mat.supr-con]

[23] E. Cobanera, A. Alase, G. Ortiz, L. Viola, Generalization of Bloch’s theorem for arbitrary boundary conditions: Interfaces and topological surface band structure, Phys. Rev. B 98, 245423 (2018), arXiv:1808.07555 [cond-mat.stat-mech]

[24] J. S. Calderón-García, A. F. Reyes-Lega, Majorana Fermions and Orthogonal Complex Structures, Mod. Phys. Lett. A 33, 1840001 (2018), arXiv:1712.05069 [cond-mat.str-el]

[25] M. N. Najafi, M. A. Rajabpour, Formation probabilities and statistics of observables as defect problems in free fermions and quantum spin chains, Phys. Rev. B 101, 165415 (2020), arXiv:1911.04595 [cond-mat.stat-mech]

[26] F. Ares, J. G. Esteve, F. Falceto, A. Usón, Complex behavior of the density in composite quantum systems, Phys. Rev. B 102, 165121 (2020), arXiv:2004.06813 [cond-mat.stat-mech]

[27] D. J. Thouless, Quantization of particle transport, Phys. Rev. B 27, 6083 (1983)

[28] J. K. Asbóth, L. Oroszlány, A. Pályi, A Short Course on Topological Insulators: Band-structure topology and edge states in one and two dimensions, Lecture Notes in Physics, 919 (2016), arXiv:1509.02295 [cond-mat.mes-hall]

[29] Y. E. Kraus, Y. Lahini, Z. Ringel, M. Verbin, O. Zilberberg, Topological States and Adiabatic Pumping in Quasicrystals, Phys. Rev. Lett. 109, 106402 (2012), arXiv:1109.5983
[cond-mat.mes-hall]

[30] M. Lohse, C. Schweizer, O. Zilberberg, M. Aidelsburger, I. Bloch, *A Thouless Quantum Pump with Ultracold Bosonic Atoms in an Optical Superlattice*, Nature Phys. 12, 350 (2016), arXiv:1507.02225 [cond-mat.quant-gas]

[31] S. Nakajima, T. Tomita, S. Taie, T. Ichinose, H. Ozawa, L. Wang, M. Troyer, Y. Takahashi, *Topological Thouless Pumping of Ultracold Fermions*, Nature Phys. 12, 296 (2016), arXiv:1507.02223 [cond-mat.quant-gas]

[32] O. Zilberberg, S. Huang, J. Guglielmon, M. Wang, K. Chen, Y. E. Kraus, M. C. Rechtsman, *Photonic topological pumping through the edges of a dynamical four-dimensional quantum Hall system*, Nature 553, 59 (2018), arXiv:1705.08361 [quant-ph]

[33] Y. Kuno, Y. Hatsugai, *Interaction Induced Topological Charge Pump*, Phys. Rev. Research 2, 042024 (2020), arXiv:2007.11215 [cond-mat.quant-gas]

[34] J. C. Y. Teo, C. L. Kane, *Topological Defects and Gapless Modes in Insulators and Superconductors*, Phys. Rev. B 82, 115120 (2010), arXiv:1006.0690 [cond-mat.mes-hall]

[35] A. Keselman, L. Fu, A. Stern, E. Berg, *Inducing time reversal invariant topological superconductivity and fermion parity pumping in quantum wires*, Phys. Rev. Lett. 111, 116402 (2013), arXiv:1305.4948 [cond-mat.str-el]

[36] E. Lieb, T. Schultz, D. Mattis, *Two soluble models of an antiferromagnetic chain*, Ann. Phys. 16, 407 (1961)

[37] A. Uhlmann, *Anti- (Conjugate) Linearity*, Sci. China Phys. Mech. Astron. 59, 630301 (2016), arXiv:1507.06545 [quant-ph]

[38] R. F. Streater, A. S. Wightman, *PCT, Spin and Statistics, and All That*, Princeton Landmarks in Mathematics and Physics (2001)

[39] A. R. Its, B.-Q. Jin, V. E. Korepin, *Entanglement in XY Spin Chain*, J. Phys. A: Math. Gen. 38, 2975 (2005), arXiv:quant-ph/0409027

[40] A. R. Its, F. Mezzadri, M. Y. Mo, *Entanglement entropy in quantum spin chains with finite range interaction*, Commun. Math. Phys. 284, 117 (2008), arXiv:0708.0161 [math-ph]

[41] F. Ares, J. G. Esteve, F. Falceto, A. R. de Queiroz, *On the Möbius transformation in the entanglement entropy of fermionic chains*, J. Stat. Mech. (2016) 043106, arXiv:1511.02382 [math-ph]

[42] F. Ares, J. G. Esteve, F. Falceto, A. R. de Queiroz, *Entanglement entropy and Möbius tran-
formations for critical fermionic chains}, J. Stat. Mech. (2017) 063104, arXiv:1612.07319 [quant-ph]

[43] A. Kitaev, J. Preskill, Topological entanglement entropy, Phys. Rev. Lett. 96, 110404 (2005), arXiv:hep-th/0510092

[44] M. Levin, X.-G. Wen, Detecting topological order in a ground state wave function, Phys. Rev. Lett. 96, 110405 (2006), arXiv:cond-mat/0510613 [cond-mat.str-el]

[45] D. Vodola, L. Lepori, E. Ercolessi, A. V. Gorshkov, G. Pupillo, Kitaev Chains with Long-Range Pairing, Phys. Rev. Lett. 113, 156402 (2014), arXiv:1405.5440 [cond-mat.str-el]

[46] D. Vodola, L. Lepori, E. Ercolessi, G. Pupillo, Long-range Ising and Kitaev models: Phases, correlations and edge modes, New J. Phys. 18, 015001 (2016), arXiv:1508.00820 [cond-mat.str-el]

[47] M. Van Regemortel, D. Sels, M. Wouters, Information propagation and equilibration in long-range Kitaev chains, Phys. Rev. A 93, 032311 (2016), arXiv:1511.05459 [cond-mat.stat-mech]

[48] L. Lepori, A. Trombettoni, D. Vodola, Singular dynamics and emergence of nonlocality in long-range quantum models, J. Stat. Mech. 033102 (2017), arXiv:1607.05358 [cond-mat.str-el]

[49] F. Ares, J. G. Esteve, F. Falceto, A. R. de Queiroz, Entanglement entropy in the long-range Kitaev chain, Phys. Rev. A 97, 062301 (2018), arXiv:1801.07043 [quant-ph]

[50] F. Ares, J. G. Esteve, F. Falceto, Z. Zimboras, Sublogarithmic behaviour of the entanglement entropy in fermionic chains, J. Stat. Mech. (2019) 093105, arXiv:1902.07540 [cond-mat.stat-mech]

[51] O. Viyuela, D. Vodola, G. Pupillo, M. A. Martin-Delgado, Topological Massive Dirac Edge Modes and Long-Range Superconducting Hamiltonians, Phys. Rev. B 94, 125121 (2016), arXiv:1511.05018 [cond-mat.str-el]

[52] A. Alecce, L. Dell’Anna, Extended Kitaev chain with longer-range hopping and pairing, Phys. Rev. B 95, 195160 (2017), arXiv:1703.10086 [cond-mat.str-el]

[53] L. Lepori, L. Dell’Anna, Long-range topological insulators and weakened bulk-boundary correspondence, New J. Phys. 19, 103030 (2017), arXiv:1612.08155 [cond-mat.str-el]

[54] O. Viyuela, L. Fu, M. A. Martin-Delgado, Chiral Topological Superconductors Enhanced by Long-Range Interactions, Phys. Rev. Lett. 120, 017001 (2018), arXiv:1707.02326 [cond-
[55] S. B. Jäger, L. Dell’Anna, G. Morigi, *Edge states of the long-range Kitaev chain: an analytical study*, Phys. Rev. B 102, 035152 (2020), arXiv:2006.00092 [cond-mat.str-el]

[56] V. M. Martinez Alvarez, J. E. Barrios Vargas, M. Berdakin, L. E. F. Foa Torres, *Topological states of non-Hermitian systems*, Eur. Phys. J. Spec. Top. 227, 1295 (2018), arXiv:1805.08200 [cond-mat.mes-hall]

[57] S. Lieu, *Topological phases in the non-Hermitian Su-Schrieffer-Heeger model*, Phys. Rev. B 97, 045106 (2018), arXiv:1709.03788 [cond-mat.mes-hall]

[58] K. Kawabata, K. Shiozaki, M. Ueda, M. Sato, *Symmetry and Topology in Non-Hermitian Physics*, Phys. Rev. X 9, 041015 (2019), arXiv:1812.09133 [cond-mat.mes-hall]

[59] F. K. Kunst, E. Edvardsson, J. C. Budich, E. J. Bergholtz, *Biorthogonal Bulk-Boundary Correspondence in Non-Hermitian Systems*, Phys. Rev. Lett. 121, 026808 (2018), arXiv:1805.06492 [cond-mat.mes-hall]