A $\mathbb{Z}_2$ invariant for chiral and particle-hole symmetric topological chains

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We define a $\mathbb{Z}_2$-valued topological and gauge invariant associated to any 1-dimensional, translation-invariant topological insulator which satisfies either particle-hole symmetry or chiral symmetry. The invariant can be computed from the Berry phase associated to a suitable basis of Bloch functions which is compatible with the symmetries. We compute the invariant in the Su–Schrieffer–Heeger model for chiral symmetric insulators, and in the Kitaev model for particle-hole symmetric insulators. We show that in both cases the $\mathbb{Z}_2$ invariant predicts the existence of zero-energy boundary states for the corresponding truncated models.

I. INTRODUCTION

The field of topological insulators has attracted the attention of both the physics and mathematics community, due to their potential applications for solid state devices and quantum computation as well as their rich mathematical structure. A topological insulator is a solid described by a Hamilton operator, acting on an appropriate Hilbert space $\mathscr{H}$, whose spectrum is gapped; this allows to define the occupied energy levels as those below the spectral gap. For translation invariant systems, the classification of topological phases of matter is then tantamount to the classification of the vector bundles over momentum space spanned by these energy states; usually, their description is mediated by numerical topological invariants, which label the different phases. In particular, different scenarios arise if the system is constrained by certain pseudo-symmetries, which can enrich or trivialize the topology of the manifold of occupied states. From the physical point of view, the most interesting feature of these materials is that, when they are truncated, a non-trivial topology for the infinite system drives the existence of metallic (i.e. gapless) states which are spatially localized near the cut: this statement is the celebrated principle of *bulk-boundary correspondence* for topological insulators. For extended reviews of this rich research line, the reader is referred to Refs. 1, 3, and 7.

In this contribution, we will be concerned with systems which are 1-dimensional, display a discrete translational symmetry modelling the crystalline nature of the solid at hand, and where one of two further special types of (pseudo-)symmetries, namely *particle-hole* or *chiral* symmetry, is present. We adopt throughout the established terminology of "symmetries" when referring to the particle-hole or chiral operators, even if they anti-commute rather than commute with the Hamiltonian (see below)[17]; other points of view have been recently advocated[24]. The Hamiltonian of the quantum system acts on the one-particle Hilbert space of a 1-dimensional crystal (see below) and is assumed to be spectrally gapped (without loss of generality, with a spectral gap around zero energy), in order for the system to be classified as an insulator. The crystalline structure of configuration space is reflected at the level of the Hamiltonian by requiring that there is a family of translation operators T_λ, with λ in a lattice $\Gamma \subset \mathbb{R}$, such that $[H, T_\lambda] = 0$ for all $\lambda \in \Gamma$; for simplicity we will assume $\Gamma = \mathbb{Z}$ in what follows. By passing to the crystal-momentum representation via the Bloch–Floquet transform (see Section II), the Hamiltonian can then be fibered into a family of matrices $H(k)$, with $k \in \mathbb{R}/(2\pi\mathbb{Z}) \simeq S^1$ denoting the Bloch momentum spanning the Brillouin torus. The associated spectral projection $P_-(k)$ onto the negative energy levels (the "particles"), complemented by the orthogonal projection $P_+(k) = \mathbb{1} - P_-(k)$ onto positive energy levels (the "holes"), defines then a *vector bundle* over S^1, called the Bloch bundle[11,13]. It is the geometry of this bundle (or rather couple of bundles) that will be investigated in this paper; the reader should notice that, at this stage, both $P_-(k)$ and $P_+(k)$ define *topologically trivial* bundles, as Hermitian bundles over S^1.

Further symmetries of the Hamiltonian are specified by the existence of a unitary or anti-unitary operator S (in the case of chiral or particle-hole symmetries, respectively) such that $SH = -HS$. If, as is common in physical applications, one also requires that S acts only on internal degrees of freedom in the unit cell of the lattice, then these symmetries descend also to the Bloch–Floquet fibers $H(k)$ and $P(k)$ in a k-independent way. These further symmetries will allow us to detect a finer geometry in the "particle" and "hole" bundles, which will be quantified in the form of a *Berry phase*. We will show that this phase is quantized to an integer, and that its parity is a gauge invariant of the bundle. This will lead us to the definition of a $\mathbb{Z}_2$-valued gauge invariant of any chiral- or particle-hole-symmetric topological insulator, see Section IV (in particular Definition IV.9).

We will then compute this invariant in two prototypical models for these symmetry classes of topological insulators: the chiral-symmetric SSH model[21], presented in Section V, and the particle-hole-symmetric Kitaev chain[9], discussed in Section VI. In both models, we will also show how a non-trivial invariant predicts the presence of *zero-energy boundary states* when the 1-dimensional system is truncated to a half-lattice, in agreement with bulk-boundary correspondence: in particular, in the Kitaev model, these boundary states are predicted to behave as Majorana fermions, and would represent topologically robust states amenable for applications in quantum computation. We do not claim to have a general proof of the bulk-boundary correspon-

dence for our formulation of the bulk topological invariant, which at any rate can at most predict the parity of the number of zero-energy boundary states, and is not expected to yield a complete classification for chiral classes of topological insulators[4,15]. Indeed, the case of chiral-symmetric topological chains and their bulk-edge correspondence, formulated in terms of a $\mathbb{Z}$-valued (rather than $\mathbb{Z}_2$-valued) topological invariant, has been already mathematically investigated, even in models where disorder breaks translation invariance[5,15,19]. Nonetheless the evidence provided by these two paradigmatic models prompt us to the study of the link between our invariant and boundary states, which will be investigated in future work.

II. FIBER DECOMPOSITION AND SPECTRAL PROJECTIONS

A. Mathematical setting

We now pass to a more precise formulation of the models trated in this paper. We will discuss only so-called *tight-binding models*, and assume therefore that the configuration space of the quantum system is modelled after a 1-dimensional lattice, say $\mathbb{Z}$. Allowing for N further internal degrees of freedom per unit cell, possibly including a sub-lattice index, the one-particle Hilbert space will be therefore taken to be

$$\mathscr{H} = \ell^2(\mathbb{Z}) \otimes \mathbb{C}^N. \tag{1}$$

The restriction of our treatment to these models, which are nonetheless of common use in condensed matter physics, is justified as follows: as will be further detailed in Remark II.9, the presence of a chiral or particle-hole symmetry forces the spectrum of the Hamiltonian H to be symmetric around zero, namely $\mu \in \sigma(H) \Rightarrow -\mu \in \sigma(H)$. Since it is customary in quantum mechanics to assume a stability condition on the energy operator, namely that H is bounded from below, the previous condition implies that the Hamiltonian is bounded, and therefore precludes the use of continuum Schrödinger-type operators on $L^2(\mathbb{R})$; notice however that there have been however recent proposals[20] to obtain discrete models for chiral chains starting from Schrödinger operators on the line, under a suitable limit of deep potential wells. We therefore also exclude Dirac-type Hamiltonians (which can be particle-hole symmetric and unbounded both from above and from below) from our treatment. One could at any rate view the discrete models introduced below also as effective models, derived from one in the continuum via projection onto a gapped spectral subspace, under an adiabatic decoupling, consisting of some "conductance" and "valence" bands of the continuum model: provided these bands exhibit this chiral or particle-hole symmetry, the tight-binding approximation would yield a symmetric lattice model.

The first set of hypotheses on the model Hamiltonian deals with the crystalline structure of configuration space. Let us therefore denote by

$$T_\lambda : \mathscr{H} \to \mathscr{H}, \quad (T_\lambda \psi)_n := \psi_{n+\lambda}, \quad \psi = (\psi_n) \in \ell^2(\mathbb{Z}) \otimes \mathbb{C}^N$$

the translation operators.

Assumption II.1 (Translation-invariant insulator)**.** The Hamiltonian H acts on the Hilbert space $\mathscr{H}$ as in (1), and satisfies the following properties.

1. It is a bounded, self-adjoint operator on $\mathscr{H}$.

2. It is *translation-invariant*, namely $[T_\lambda, H] = 0$ for all $\lambda \in \mathbb{Z}$.

3. The spectrum of H has a gap around zero, namely there exists $g > 0$ such that $(-g, g) \cap \sigma(H) = \emptyset$.

It is easy to verify that the action of a translation-invariant self-adjoint operator H onto a vector $\psi = (\psi_n) \in \ell^2(\mathbb{Z}) \otimes \mathbb{C}^N$ is necessarily of the form

$$(H\psi)_n = A_0 \psi_n + \sum_{j \in \mathbb{N}^*} A_j \psi_{n+j} + A_j^* \psi_{n-j} \tag{2}$$

for an appropriate sequence of matrices $A_j \in M_N(\mathbb{C})$, $j \in \mathbb{N}$, with $A_0 = A_0^*$. Alternatively, if we denote by $\{e_n\}_{n \in \mathbb{Z}}$ the canonical basis of $\ell^2(\mathbb{Z})$ whose components are $(e_n)_m = \delta_{n,m}$ for $n, m \in \mathbb{Z}$, we can write

$$H(e_n \otimes v) = e_n \otimes A_0 v + \sum_{j \in \mathbb{N}^*} e_{n-j} \otimes A_j v + e_{n+j} \otimes A_j^* v, \quad n \in \mathbb{Z}, v \in \mathbb{C}^N, \tag{3}$$

and extend the definition of H from there by linearity. From a physical point of view A_j can be interpreted as a matrix-valued "hopping probability" for a particle to make a jump of j sites in the lattice. Boundedness of H implies some form of decay in the matrix norms $\|A_j\|$: to simplify the setting even further, we will be content to treat *finite-range operators*, and assume that

Assumption II.2 (Finite-range condition). With $A_j \in M_N(\mathbb{C})$ as above, there exists $R \in \mathbb{N}$ such that

$$A_j = 0 \quad \text{for} \quad j > R.$$

Such operators are sometimes called *band Jacobi operators* in the mathematics literature[22]. Assumptions II.1 and II.2 will be our standing hypotheses throughout this paper, and will not be recalled further.

Finally, the models of interest for this contribution satisfy either particle-hole or chiral symmetry, as specified in the following two Assumptions.

Assumption II.3 (Particle-Hole Symmetry, PHS). There exists an *anti-unitary* operator S_{PH} on $\mathcal{H} = \ell^2(\mathbb{Z}) \otimes \mathbb{C}^N$ such that

1. $S_{\text{PH}} = \mathbb{1}_{\ell^2(\mathbb{Z})} \otimes C$, where C is a anti-unitary matrix on $\mathbb{C}^N$ (namely, $C = UK$, where $U \in M_N(\mathbb{C})$ is a unitary matrix and K is a complex-conjugation operator on $\mathbb{C}^N$);

2. $S_{\text{PH}} H = -H S_{\text{PH}}$.

Assumption II.4 (Chiral Symmetry, CS). There exists a *unitary* operator S_{C} on $\mathcal{H} = \ell^2(\mathbb{Z}) \otimes \mathbb{C}^N$ such that

1. $S_{\text{C}} = \mathbb{1}_{\ell^2(\mathbb{Z})} \otimes S$, where S is a unitary matrix on $\mathbb{C}^N$;

2. $S_{\text{C}} H = -H S_{\text{C}}$.

A few comments on the definition of these symmetry operators are in order.

- Contrary to what is usually assumed in the literature on topological phases of matter[17], we do not need to assume anything concerning the squares of the symmetry operators S_{PH} and S_{C}. In view of representation-theoretic reasons, it is always the case that $S_{\text{C}}^2 = \mathbb{1}_{\mathcal{H}}$ while either $S_{\text{PH}}^2 = +\mathbb{1}_{\mathcal{H}}$ (*even* PHS) or $S_{\text{PH}}^2 = -\mathbb{1}_{\mathcal{H}}$ (*odd* PHS). These specifications will be immaterial for our discussion.

- The structure required on both symmetry operators, namely that they act trivially on the $\ell^2(\mathbb{Z})$-leg of the tensor product defining $\mathcal{H}$ in (1), may seem restrictive, but it is often satisfied in physical models of interest such as the ones presented in Sections V and VI. Notice that they imply in particular that also the symmetry operators are translation-invariant, namely $[S_*, T_\lambda] = 0$ for all $\lambda \in \mathbb{Z}$ and for $S_* \in \{S_{\text{PH}}, S_{\text{C}}\}$.

B. Bloch–Floquet representation

It is natural and convenient to exploit the translational symmetry of the operators considered in order to simplify their analysis. This can be done by using the theory of decomposable operators, see Ref. 16, Sec. XIII.16, and a vector-valued form of the Fourier series, called *Bloch–Floquet transform* in the context of condensed matter physics. We review this method in this Section for the finite-range, translation-invariant Hamiltonians described previously, commenting in particular on the interplay of the Bloch–Floquet transform with PHS and CS.

Denote as before by $\{e_n\}_{n \in \mathbb{Z}}$ the canonical basis of $\ell^2(\mathbb{Z})$. Set

$$\mathscr{F}: \ell^2(\mathbb{Z}) \otimes \mathbb{C}^N \to L^2(S^1; \mathbb{C}^N), \quad \mathscr{F}(e_n \otimes v) := \frac{e^{ink}}{\sqrt{2\pi}} v, \qquad n \in \mathbb{Z}, v \in \mathbb{C}^N.$$

This is clearly a bijective linear isometry because it sends an orthonormal basis to another orthonormal basis: $\mathscr{F}$ is then called the Bloch–Floquet (BF) transform. We then define

$$\widehat{H} := \mathscr{F} H \mathscr{F}^{-1}. \tag{4}$$

Analogously, if the PHS or CS Assumptions II.3 and II.4 hold, we can similarly define

$$\widehat{S_{\text{PH}}} = \mathscr{F} S_{\text{PH}} \mathscr{F}^{-1} \quad \text{and} \quad \widehat{S_{\text{C}}} = \mathscr{F} S_{\text{C}} \mathscr{F}^{-1}.$$

Assumptions II.3 and II.4 then imply at once that

$$\widehat{S_{\text{PH}}} \widehat{H} = -\widehat{H} \widehat{S_{\text{PH}}} \quad \text{or} \quad \widehat{S_{\text{C}}} \widehat{H} = -\widehat{H} \widehat{S_{\text{C}}}. \tag{5}$$

Lemma II.5. *The operator $\widehat{H}$ is decomposable in the sense of Ref. 16, Sec. XIII.16, namely there exists a family of self-adjoint matrices $H(k) \in M_N(\mathbb{C})$, called the* fiber operators, *such that*

$$\left(\widehat{H}u\right)(k) = H(k)u(k) \quad for \quad u \in L^2(S^1; \mathbb{C}^N). \tag{6}$$

With $\{A_j\}_{j\in\mathbb{N}}$ as in (2) or (3), the fiber operators are explicitly written in the following way:

$$H(k) = A_0 + \sum_{j=1}^{R} e^{-ijk} A_j + e^{ijk} A_j^*. \tag{7}$$

Proof. In the following, we identify for notational convenience

$$L^2(S^1; \mathbb{C}^N) \simeq L^2(S^1) \otimes \mathbb{C}^N.$$

For $n \in \mathbb{Z}$ and $v \in \mathbb{C}^N$, let us then compute, using (3),

$$
\begin{aligned}
\widehat{H}\left(\frac{e^{ink}}{\sqrt{2\pi}} \otimes v\right) &= \mathscr{F}\left[e_n \otimes A_0 v + \sum_{j=1}^{R} e_{n-j} \otimes A_j v + e_{n+j} \otimes A_j^* v\right] \\
&= \frac{e^{ink}}{\sqrt{2\pi}} \otimes A_0 v + \sum_{j=1}^{R} \frac{e^{i(n-j)k}}{\sqrt{2\pi}} \otimes A_j v + \frac{e^{i(n+j)k}}{\sqrt{2\pi}} \otimes A_j^* v \\
&= \left[A_0 + \sum_{j=1}^{R} e^{-ijk} A_j + e^{ijk} A_j^*\right]\left(\frac{e^{ink}}{\sqrt{2\pi}} \otimes v\right).
\end{aligned}
$$

Since the functions $\{e^{ink}/\sqrt{2\pi}\}_{n\in\mathbb{Z}}$ span $L^2(S^1)$ orthonormally, the conclusion follows by linearity. □

Remark II.6. The matrices $H(k)$ are 2π-periodic and *analytic* (in fact, entire) in the variable k, as each entry is a finite sum of complex exponential functions. Provided H is a bounded operator and the matrix norms of the A_j's decay sufficiently rapidly, the same holds true even if we relax the finite-range condition, Assumption II.2, by the Vitali–Porter theorem[18] (possibly restricting the analyticity domain to a strip of finite width around the real axis).

Lemma II.7. *If the PHS Assumption II.3 or the CS Assumption II.4 holds, then*

$$\left(\widehat{S_{\mathrm{PH}}}\,u\right)(k) = Cu(-k) \quad or \quad \left(\widehat{S_{\mathrm{C}}}\,u\right)(k) = Su(k), \qquad u \in L^2(S^1; \mathbb{C}^N),$$

where the (anti-)unitary operators $C, S\colon \mathbb{C}^N \to \mathbb{C}^N$ are as in the aforementioned Assumptions and act point-wise on $u \in L^2(S^1; \mathbb{C}^N)$.

Proof. As in the previous proof, by (anti-)linearity it suffices to compute the action of $\widehat{S_{\mathrm{PH}}}$ and $\widehat{S_{\mathrm{C}}}$ on functions $u(k)$ of the form $u(k) = e^{ink}/\sqrt{2\pi} \otimes v$, for $n \in \mathbb{Z}$ and $v \in \mathbb{C}^N$. We have then

$$\widehat{S_{\mathrm{PH}}}\left(\frac{e^{ink}}{\sqrt{2\pi}} \otimes v\right) = \mathscr{F}\left[S_{\mathrm{PH}}(e_n \otimes v)\right] = \mathscr{F}(e_n \otimes Cv) = \frac{e^{ink}}{\sqrt{2\pi}} \otimes Cv = C\left(\frac{e^{-ink}}{\sqrt{2\pi}} \otimes v\right)$$

as C is *anti*-linear.

Similarly we have

$$\widehat{S_{\mathrm{C}}}\left(\frac{e^{ink}}{\sqrt{2\pi}} \otimes v\right) = \mathscr{F}\left[S_{\mathrm{C}}(e_n \otimes v)\right] = \mathscr{F}(e_n \otimes Sv) = \frac{e^{ink}}{\sqrt{2\pi}} \otimes Sv = S\left(\frac{e^{ink}}{\sqrt{2\pi}} \otimes v\right)$$

as instead S is linear. □

Corollary II.8. *If the PHS Assumption II.3 holds, then the fiber operator $H(k)$ is anti-unitarily intertwined to the fiber operator $H(-k)$ by the relation*

$$CH(-k) = -H(k)C.$$

Similarly, if the CS Assumption II.4 holds, then the fiber operator $H(k)$ is unitarily intertwined to the fiber operator $H(k)$ by the relation

$$SH(k) = -H(k)S.$$

Proof. Both statements immediately follow by combining (5) and (6). □

Remark II.9. The above condition gives us useful information regarding the spectrum of the fiber operators $H(k)$ and therefore of the Hamiltonian H. Indeed, assume that $v \in \mathbb{C}^N$ is an eigenvector of $H(k)$ of eigenvalue E. Let the PHS Assumption II.3 hold. Then

$$H(-k)Cv = -CH(k)v = -C(Ev) = -\overline{E}Cv.$$

Due to the self-adjointness of $H(k)$, we have $E = \overline{E}$ and therefore Cv is an eigenvector of $H(-k)$ with opposite eigenvalue $-E$. Similarly, if instead the CS Assumption II.4 holds, then

$$H(k)Sv = -SH(k)v = -S(Ev) = -E\,Sv$$

and once again we find that Sv is an eigenvector for $H(k)$ with opposite eigenvalue $-E$.

From the theory of decomposable operators presented in Ref. 16, Theorems XIII.85-86, we know that the spectrum of $\widehat{H}$ (and therefore that of $H = \mathscr{F}^{-1}\widehat{H}\mathscr{F}$) is obtained as the union of the spectra of $H(k)$ for ranging $k \in S^1$. The above considerations allows us then to deduce that $\sigma(H)$ must be symmetric around $E = 0$. Moreover, in view of the insulator Assumption II.1, the spectral gap of H together with the analytic dependence of $H(k)$ and of its spectrum on $k \in S^1$ (see Remark II.6) imply that $0 \notin \sigma(H(k))$ for all $k \in S^1$. Thefore we have a clear separation of positive and negative energies also for the fibre operators $H(k)$.

Notice that the Bloch momentum $k = 0$ is fixed by the involution $k \mapsto -k$. Therefore, in view of what we just concluded, by the spectral theorem $\mathbb{C}^N$ has an orthonormal basis $v_1, \cdots, v_N$ consisting of eigenvectors the self-adjoint matrix $H(0)$, where the first vectors $v_1, \cdots, v_m$ have negative eigenvalues while the second vectors $v_{m+1}, \cdots, v_N$ have positive eigenvalues. The presence of C or S implies a the existence of a (anti-)linear bijection between the eigenspaces of $H(0)$ relative to negative and positive eigenvalues, and so $m = N - m$. Therefore, whenever Assumptions II.3 or II.4 hold, it will be assumed that the dimension of the fiber space $\mathbb{C}^N$ is a an even integer, $N = 2m$.

C. Spectral projections

The topological information of the insulator described by H, as we will detail later, is contained in the spectral projections of the fiber operators, which project over the vector subspace of $\mathbb{C}^N$ generated by its eigenvectors with negative eigenvalues. The collection of these subspaces leads to the definition of the *Bloch bundle*[11,13].

Since $H(k)$ depends analytically on k and is 2π-periodic, one would expect that their eigenvalues and eigenvectors do the same. This is partially true (compare Ref. 16, Theorem XIII.85-86), but problems can occur if different eigenvalues of $H(k)$ become degenerate at some $k_0 \in S^1$. What remains true even in this situation is that the *negative and positive eigenspaces* of $H(k)$ stay analytic and 2π-periodic with respect to k, thanks to the spectral gap. More precisely, consider a PHS or CS Hamiltonian H for which the considerations of the previous Subsection hold. Let $r > 0$ be such that $-2r$ is a lower bound for the spectrum of H, and therefore uniformly for the spectra of $H(k)$, $k \in S^1$. The *Riesz formula*[8]

$$P_-(k) := \frac{1}{2\pi i} \int_{\partial B_r(-r)} dz\,(z\mathbb{1} - H(k))^{-1}, \quad k \in S^1, \tag{8}$$

defines then an orthogonal projection, $P_-(k) = P_-(k)^* = P_-(k)^2$, on the subspace generated by the eigenvectors of $H(k)$ with negative eigenvalues. In the above, the integration is performed in the complex energy plane, along a circumference centered at $-r$ of radius r; the circle enclosed by this circumference only contains the negative eigenvalues of $H(k)$, where the resolvent function has its poles. The integral of a matrix should be understood as being performed entry-wise. By functional calculus, it is easily shown, e.g. in Ref. 14, Proposition 2.1, that $P_-(k)$ is as regular as $H(k)$, and shares with it the same periodicity properties with respect to k. Of course, the same holds for the spectral projection

$$P_+(k) := \mathbb{1} - P_-(k)$$

onto the eigenspace of $H(k)$ associated to positive eigenvalues.

Lemma II.10. *If either Assumption II.3 or II.4 hold, then*

$$CP_+(k) = P_-(-k)C \quad or \quad SP_+(k) = P_-(k)S. \tag{9}$$

Proof. The statement follows at once from Corollary II.8 and Remark II.9. □

III. PARALLEL TRANSPORT AND BLOCH BASES

We want to quantify the topological content of the spectral projections of the fiber operators $H(k)$ into a numerical invariant. This will be done in the next Section, starting from a moving basis for the fiber Hilbert space $\mathbb{C}^N$ tailored around the spectral subspace of the fiber operators $H(k)$. We therefore set the following

Definition III.1 (Bloch basis). Given a family of rank-m projections $P(k) \in M_N(\mathbb{C})$ which is 2π-periodic and at least C^1 in k, we will call a family of vectors $\{v_i(k)\}_{i \in \{1, \cdots, N\}} \subset \mathbb{C}^N$ a *Bloch basis associated to* $P(k)$ if it satisfies the following proprieties for every $k \in \mathbb{R}$.

- The collection $\{v_i(k)\}_{i \in \{1, \cdots, N\}}$ forms an orthonormal basis of $\mathbb{C}^N$.

- The vectors $\{v_i(k)\}_{i \in \{1,\ldots,m\}}$ span $\mathrm{Ran}\, P(k)$; consequently, the vectors $\{v_i(k)\}_{i \in \{m+1,\ldots,N\}}$ span $\ker P(k) = \mathrm{Ran}[\mathbb{1} - P(k)]$.

- Every $v_i(k)$ is 2π-periodic and as regular as $P(k)$ as a function of $k \in \mathbb{R}$.

Definition III.2 (Symmetric Bloch basis). Let $P_-(k)$ be as in (8) and $P_+(k) = \mathbb{1} - P_-(k)$. Assume that either Assumption II.3 or II.4 holds, so that $N = 2m$, $P_-(k)$ and $P_+(k)$ both have rank m, and (9) holds as well. Then a Bloch basis $\{v_i(k)\}_{i \in \{1, \cdots, N\}}$ associated to $P_-(k)$ will be called *particle-hole symmetric* if

$$C v_i(k) = v_{N-i+1}(-k) \quad \text{for all } i \in \{1, \ldots, m\}\ .$$

Similarly, the Bloch basis will be called *chiral symmetric* if

$$S v_i(k) = v_{N-i+1}(k) \quad \text{for all } i \in \{1, \ldots, m\}\ .$$

A. Parallel transport

For 1-dimensional systems, such as the ones at hand, it is possible to exhibit Bloch bases associated to the eigenprojections $P_-(k)$ via a tool from differential geometry called *parallel transport*. We will review this construction here, and show in particular how parallel transport behaves under PHS or CS.

Theorem III.3. *If $P(k) \in M_N(\mathbb{C})$ is a family of projections which is at least C^1 in k, then there exists a unique family of operators $T(k) \in M_N(\mathbb{C})$ that solves the Cauchy problem*

$$\begin{cases} T'(k) = [P'(k), P(k)]\, T(k), \\ T(0) = \mathbb{1}\,. \end{cases} \tag{10}$$

Here and in the following, the "prime" symbol $'$ denotes differentiation with respect to k. The family of operators $T(k)$ is at least as regular as $P(k)$ as a function of k. It further satisfies the following properties:

1. *Unitarity: Each $T(k)$ is unitary, $T(k)^* = T(k)^{-1}$.*

2. *Intertwining property:*

$$P(k)\, T(k) = T(k)\, P(0), \quad k \in \mathbb{R}. \tag{11}$$

If $P(k)$ is also 2π-periodic with respect to k, then $T(k)$ satisfies further the

3. *Telescopic property:*

$$T(k + 2\pi n) = T(k)\, T(2\pi)^n, \quad k \in \mathbb{R}, \quad n \in \mathbb{Z}. \tag{12}$$

We will call the family of unitaries $T(k)$ the parallel transport operators *associated to $P(k)$.*

Proof. Existence, uniqueness and regularity of the solution to the Cauchy problem (10) for every initial value T_0 follows from the standard theory of first-order linear differential equations (see e.g. Ref. 23, Section IV.14.VI).

a. Unitarity To prove that $T(k)$ is unitary, it suffices to notice that the (non-autonomous) generator of the differential equation is skew-adjoint:

$$\big[P'(k), P(k)\big]^* = -\big[P'(k), P(k)\big]\ .$$

b. Intertwining property The intertwining property (11) clearly holds at $k = 0$. To conclude that it holds for all $k \in \mathbb{R}$, one computes $[T(k)^* P(k) T(k)]'$ and shows that it vanishes. We have that

$$\frac{\mathrm{d}}{\mathrm{d}k} T(k)^* P(k) T(k) = T(k)^* \left\{ - \left[P'(k), P(k) \right] P(k) + P'(k) + P(k) \left[P'(k), P(k) \right] \right\} T(k).$$

The term in curly brackets vanishes, as one can verify with a straightforward algebraic computation using the identity $P(k) P'(k) P(k) = 0$ (following from differentiation of the relation $P(k) = P(k)^2$).

c. Telescopic property To prove (12), let us define $A(k) := T(k + 2\pi n)$ for fixed $n \in \mathbb{Z}$. By direct inspection, $A(k)$ solves the Cauchy problem (10) with $A(0) = T(2\pi n)$, as the family of projections $P(k)$ is 2π-periodic. The same is true for $B(k) := T(k) T(2\pi n)$, and by uniqueness it must hold that

$$T(k + 2\pi n) = T(k) T(2\pi n) \quad \text{for all } k \in \mathbb{R}, \ n \in \mathbb{Z}.$$

The above implies in particular

$$T(2\pi n) = T(2\pi)^n, \quad n \in \mathbb{Z}$$

from which (12) follows. □

Remark III.4. Uniqueness of the solution of the Cauchy problem in the statement of Theorem III.3 implies that the parallel transport operators associated to the families $P(k)$ and $Q(k) := \mathbb{1} - P(k)$ coincide, since they share the same generator of the linear differential equation:

$$\left[Q'(k), Q(k) \right] = \left[(\mathbb{1} - P(k))', \mathbb{1} - P(k) \right] = \left[P'(k), P(k) \right].$$

Lemma III.5. *Let $P_-(k)$ be the family of projections defined in (8), and denote by $T(k)$ the parallel transport unitaries associated to $P_-(k)$. Assume that either Assumption II.3 or II.4 holds. Then*

$$C T(k) = T(-k) C \quad \text{or} \quad S T(k) = T(k) S, \qquad k \in \mathbb{R}.$$

Proof. Under Assumption II.3, let us denote by $U(k) := C^{-1} T(-k) C$. Compute

$$U'(k) = -C^{-1} \left[P'_-(-k), P_-(-k) \right] T(-k) C = \left[-C^{-1} P'_-(-k) C, C^{-1} P_-(-k) C \right] C^{-1} T(-k) C$$
$$= \left[P'_+(k), P_+(k) \right] U(k)$$

where we used Lemma II.10 for the last equality. Since $U(0) = \mathbb{1}$ this means that $U(k)$ solves the Cauchy problem (10) for the parallel transport operators associated to $P_+(k) = \mathbb{1} - P_-(k)$. By Remark III.4 we conclude that $U(k) = T(k)$.

Arguing similarly under Assumption II.4, one can show that $V(k) := S^{-1} T(k) S$ and $T(k)$ solve the same Cauchy problem, and therefore coincide. □

B. Construction of symmetric Bloch bases

Using the parallel transport unitaries $T(k)$ we can try to construct a symmetric Bloch basis. If we fix an orthonormal basis $\{v_1(0), \cdots, v_{2m}(0)\} \subset \mathbb{C}^{2m}$ of eigenvectors of $H(0)$ such that the first half have negative eigenvalues while the second half have positive eigenvalues, we can define the family of vectors

$$\tilde{v}_i(k) := T(k) v_i(0), \quad k \in \mathbb{R}.$$

These vectors form an orthonormal basis of $\mathbb{C}^N$ that depends smoothly on k; moreover, in view of the intertwining property (11), we have that

$$P_-(k) \tilde{v}_i(k) = \begin{cases} \tilde{v}_i(k) & \text{if } i \leq m, \\ 0 & \text{if } i > m, \end{cases} \quad \text{while} \quad P_+(k) \tilde{v}_i(k) = \begin{cases} 0 & \text{if } i \leq m, \\ \tilde{v}_i(k), & \text{if } i > k. \end{cases}$$

Finally, if the model enjoys PHS or CS, then by Remark II.9 we can further choose the basis of eigenvectors of $H(0)$ in such a way that

$$C v_i(0) = v_{N-i+1}(0), \quad \text{or} \quad S v_i(0) = v_{N-i+1}(0). \tag{13}$$

Then, in view of Lemma III.5, we conclude that for $i \in \{1, \ldots, m\}$

$$C\tilde{v}_i(k) = CT(k)v_i(0) = T(-k)Cv_i(0) = T(-k)v_{N-i+1}(0) = \tilde{v}_{N-i+1}(-k),$$

or similarly

$$S\tilde{v}_i(k) = \tilde{v}_{N-i}(k).$$

This is almost enough to conclude that $\{\tilde{v}_i(k)\}_{i \in \{1, \ldots, N\}}$ is a symmetric Bloch basis, but unfortunately in general it will not be 2π-periodic since $T(2\pi) \neq T(0) = \mathbb{1}$. Therefore we need to adjust this construction.

Let us then focus on the unitary matrix $T(2\pi) \in M_N(\mathbb{C})$, called the *holonomy unitary*. By the spectral theorem, $T(2\pi)$ can be diagonalized by a unitary transformation V:

$$T(2\pi) = V^{-1} \begin{bmatrix} e^{i\phi_1} & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & e^{i\phi_N} \end{bmatrix} V, \quad \text{with} \quad V^{-1} = V^*, \quad \phi_i \in [0, 2\pi) \ \forall i \in \{1, \ldots, N\}.$$

With this choice of the phases for the eigenvalues of $T(2\pi)$, we let $X \in M_N(\mathbb{C})$ be the self-adjoint matrix

$$X = -i \ln T(2\pi) := V^{-1} \begin{bmatrix} \phi_1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \phi_N \end{bmatrix} V \tag{14}$$

so that $T(2\pi) = e^{iX}$. It is worth to notice that X and $T(2\pi)$ share the same eigenspaces.

Theorem III.6. *Let $P_-(k) \in M_N(\mathbb{C})$ be the rank-m projections defined in (8). Let also $\{v_1(0), \cdots, v_N(0)\} \subset \mathbb{C}^N$ be an orthonormal basis of eigenvectors of $H(0)$ such that $\{v_1(0), \cdots, v_m(0)\}$ span $\operatorname{Ran} P_-(0)$ while $\{v_{m+1}(0), \cdots, v_N(0)\}$ span $\ker P_-(0)$. Finally, denote by $T(k)$ the family of parallel transport unitaries associated to $P_-(k)$. Then the family of vectors*

$$v_i(k) := T(k) e^{-ikX/2\pi} v_i(0), \quad i \in \{1, \ldots, N\} \tag{15}$$

define a Bloch basis associated to $P_-(k)$ in the sense of Definition III.1.

If furthermore Assumption II.3 or II.4 holds, then the vectors defined in (15) form a symmetric Bloch basis associated to $P_-(k)$, in the sense of Definition III.2.

Proof. We split the proof in a few steps.

a. Spanning property   The vectors $\{v_i(k)\}_{i \in \{1, \ldots, N\}}$ are clearly orthonormal as they are obtained from the orthonormal basis of eigenvectors of $H(0)$ by means of unitary transformations. Let us check that the first m vectors span $\operatorname{Ran} P_-(k)$, so that the last $N - m$ will span $\operatorname{Ran} P_+(k)$. To this end, it suffices to notice that the intertwining property (11) of the parallel transport unitaries yields in particular

$$P_-(2\pi) T(2\pi) = P_-(0) T(2\pi) = T(2\pi) P_-(0)$$

in view of the 2π-periodicity of the family of projections. So $T(2\pi)$ commutes with $P_-(0)$, and as the matrix X in (14) is obtained from $T(2\pi)$ through functional calculus, so does X and therefore $e^{-ikX/2\pi}$ for all $k \in \mathbb{R}$. It then follows that the vectors $e^{-ikX/2\pi} v_i(0)$ for $i \in \{1, \ldots, m\}$ are orthonormal and in the range of $P_-(0)$, and are then mapped orthonormally by $T(k)$ to the range of $P_-(k)$ in view of the intertwining property again.

b. Regularity   Since $P_-(k)$ is analytic in k, $T(k)$ is as well by Theorem III.3. Also the matrix

$$e^{-ikX/2\pi} = V^{-1} \begin{bmatrix} e^{-ik\phi_1/2\pi} & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & e^{-ik\phi_N/2\pi} \end{bmatrix} V$$

depends analytically on k. We conclude that (15) defines an analytic $\mathbb{C}^N$-valued function of k.

c. Periodicity   To prove that $v_i(k)$ is 2π-periodic in k, we will exploit the telescopic property (12) of the parallel transport unitaries. We have indeed, for $k \in \mathbb{R}$ and $n \in \mathbb{Z}$,

$$v_i(k + 2\pi n) = T(k + 2\pi n) e^{-i(k + 2\pi n)X/2\pi} v_i(0) = T(k) T(2\pi)^n e^{-inX} e^{-ikX/2\pi} v_i(0)$$

$$= T(k) e^{-ikX/2\pi} v_i(0) = v_i(k),$$

since by definition $T(2\pi)^n = e^{inX}$.

d.   Symmetry   Under the CS hypothesis, we know from Lemma III.5 that S commutes with $T(k)$, so in particular it commutes with $T(2\pi)$ and by functional calculus with X and with $e^{-ikX/2\pi}$. Therefore it holds that

$$S v_i(k) = S T(k) e^{-ikX/2\pi} v_i(0) = T(k) e^{-ikX/2\pi} S v_i(0) = T(k) e^{-ikX/2\pi} v_{N-i+1}(0) = v_{N-i+1}(k)$$

as wanted.

Let us now assume the PHS hypothesis. Lemma III.5 and the telescopic property (12) together give that

$$CT(2\pi) = T(-2\pi)C = T(2\pi)^{-1}C \quad \Longleftrightarrow \quad C e^{iX} = e^{-iX} C$$

which by functional calculus implies for all $k \in \mathbb{R}$

$$C e^{-ikX/2\pi} = e^{ikX/2\pi} C.$$

Therefore it holds that

$$C v_i(k) = C T(k) e^{-ikX/2\pi} v_i(0) = T(-k) e^{ikX/2\pi} C v_i(0) = T(-k) e^{ikX/2\pi} v_{N-i+1}(0) = v_{N-i+1}(-k)$$

which concludes the proof. $\square$

IV.   BERRY PHASE AND THE $\mathbb{Z}_2$ INVARIANT

We are finally in position to extract the topological invariant out of any Bloch basis associated to the spectral projections $P_-(k)$ of the fiber Hamiltonians $H(k)$, which we know exist thanks to the results of the previous Section. The invariant will be formulated starting from the (*abelian*) *Berry phase* of the Bloch basis, whose definition we recall below.

Definition IV.1 (Berry phase). Let $P(k) \in M_N(\mathbb{C})$ be a 2π-periodic family of rank-m projections which is at least C^1 in k, and $\{v_i(k)\}_{i \in \{1,\cdots,N\}}$ be a Bloch basis associated to $P(k)$ in the sense of Definition III.1. The *Berry phase* of the Bloch basis is the following integral:

$$\frac{1}{2\pi i} \int_{S^1} dk \sum_{i=1}^{N} \langle v_i(k), v_i'(k) \rangle. \tag{16}$$

The same formula, in general, gives the holonomy phase of any moving basis (i.e. global frame) for the trivial bundle $S^1 \times \mathbb{C}^N$.

This Section will be devoted to proving some properties of the Berry phase defined above: it will be argued that it takes integer values, and that under PHS or CS the parity of this integer is a quantity which depends on the projections $P_-(k)$, and not on the choice of a Bloch basis compatible with the symmetries. This will lead to the formulation of the $\mathbb{Z}_2$ invariant.

A.   Properties of the Berry phase

Much of the following discussion will be based on the next result regarding homotopy classes of unitary-matrix-valued maps on the circle. This statement is well-known from algebraic topology, see e.g. Ref. 6, Proposition 13.11, but we provide a sketch of some aspects of the proof in Appendix A for the reader's convenience.

Theorem IV.2 (Winding number of unitary-matrix-valued maps). *Let $\pi_1(U(N))$ denote the group of (smooth) homotopy classes of (smooth) maps $S^1 \to U(N)$, with $U(N) := \{ U \in M_N(\mathbb{C}) : U^* = U^{-1} \}$, endowed with point-wise multiplication of maps as group operation. Then there is a group isomorphism*

$$\mathrm{wn} \colon \pi_1(U(N)) \xrightarrow{\sim} \mathbb{Z}, \qquad [U \colon S^1 \to U(N)] \mapsto \frac{1}{2\pi i} \int_{S^1} dk \, \mathrm{tr}\left(U(k)^* U'(k) \right). \tag{17}$$

The integer $\mathrm{wn}([U])$ *is called the* winding number *of (the homotopy class $[U]$ of) the map $U \colon S^1 \to U(N)$.*

We start by computing the Berry phase of the Bloch basis constructed in the previous Section.

Theorem IV.3. *Under the assumptions of Theorem III.6, we have that*

$$\frac{1}{2\pi i} \int_{S^1} dk \sum_{i=1}^{N} \langle v_i(k), v_i'(k) \rangle = -\frac{1}{2\pi} \, \mathrm{tr} X \quad \in \mathbb{Z}$$

where $\{v_i(k)\}_{i \in \{1,\dots,N\}}$ is as in (15) and X is as in (14). In particular, the Berry phase above is independent of the choice of $\{v_i(0)\}_{i \in \{1,\dots,N\}}$ as in the statement of Theorem III.6.

Proof. With the notation of Theorem III.6, let us define $W(k) := T(k)\,\mathrm{e}^{-\mathrm{i}kX/2\pi}$, so that $v_i(k) = W(k)\,v_i(0)$ for $i \in \{1,\ldots,N\}$. We can compute then

$$\frac{1}{2\pi\mathrm{i}} \int_{S^1} \mathrm{d}k \sum_{i=1}^{N} \langle v_i(k), v_i'(k)\rangle = \frac{1}{2\pi\mathrm{i}} \int_{S^1} \mathrm{d}k \sum_{i=1}^{N} \langle W(k)\,v_i(0), W'(k)\,v_i(0)\rangle = \frac{1}{2\pi\mathrm{i}} \int_{S^1} \mathrm{d}k \sum_{i=1}^{N} \langle v_i(0), W(k)^*\,W'(k)\,v_i(0)\rangle$$

$$= \frac{1}{2\pi\mathrm{i}} \int_{S^1} \mathrm{d}k \; \mathrm{tr}\left(W(k)^*\,W'(k)\right)$$

owing to the fact that $\{v_i(0)\}_{i\in\{1,\ldots,N\}}$ is an orthonormal basis of $\mathbb{C}^N$. In view of Theorem IV.2, this allows to conclude that

$$\frac{1}{2\pi\mathrm{i}} \int_{S^1} \mathrm{d}k \sum_{i=1}^{N} \langle v_i(k), v_i'(k)\rangle = \mathrm{wn}([W]) \in \mathbb{Z}.$$

To prove the equality claimed in the statement, we compute then

$$W'(k) = \frac{\mathrm{d}}{\mathrm{d}k}\left(T(k)\,\mathrm{e}^{-\mathrm{i}kX/2\pi}\right) = T'(k)\,\mathrm{e}^{-\mathrm{i}kX/2\pi} + T(k)\,\mathrm{e}^{-\mathrm{i}kX/2\pi}\,\frac{X}{2\pi\mathrm{i}} = [P_-'(k), P_-(k)]\,W(k) + W(k)\,\frac{X}{2\pi\mathrm{i}}$$

and therefore

$$W(k)^*\,W'(k) = W(k)^*\,[P_-'(k), P_-(k)]\,W(k) + \frac{X}{2\pi\mathrm{i}}.$$

Consequently

$$\mathrm{tr}\left(W(k)^*\,W'(k)\right) = \mathrm{tr}\left(W(k)^*\,[P_-'(k), P_-(k)]\,W(k)\right) + \frac{1}{2\pi\mathrm{i}}\,\mathrm{tr}\,X = \mathrm{tr}\left([P_-'(k), P_-(k)]\right) + \frac{1}{2\pi\mathrm{i}}\,\mathrm{tr}\,X$$

due to the invariance of the trace under the unitary conjugation by $W(k)$. Now, the first summand on the right-hand side of the above vanishes because commutators are traceless, and we conclude that

$$\mathrm{wn}([W]) = \frac{1}{2\pi\mathrm{i}} \int_{S^1} \mathrm{d}k \; \mathrm{tr}\left(W(k)^*\,W'(k)\right) = \frac{1}{(2\pi\mathrm{i})^2}\,\mathrm{tr}\,X \int_{S^1} \mathrm{d}k = -\frac{1}{2\pi}\,\mathrm{tr}\,X$$

as claimed.

Finally $\mathrm{tr}\,X$ does not depend on the choice of the basis $\{v_i(0)\}_{i\in\{1,\ldots,N\}}$ for $\mathbb{C}^N$, so neither does the Berry phase of the Bloch basis $\{v_i(k)\}_{i\in\{1,\ldots,N\}}$. $\qquad\square$

Remark IV.4. Since $T(2\pi) = \mathrm{e}^{\mathrm{i}X}$ and $\mathrm{tr}(X) = 2\pi n$ for $n = -\mathrm{wn}([W]) \in \mathbb{Z}$, it must be that $\det T(2\pi) = \mathrm{e}^{\mathrm{i}\,\mathrm{tr}\,X} = \mathrm{e}^{2\pi\mathrm{i}n} = 1$. So, while the parallel transport unitaries $T(k)$ are not 2π-periodic in k in general (compare (12)), the determinant map $k \mapsto \det T(k)$ is, and therefore has a well defined winding number in view of Proposition A.2, which can be alternatively used to compute (up to a sign) the Berry phase of the Bloch basis in (15).

The next result will tell us that, when a change of Bloch basis is performed (also called a *change of Bloch gauge*), the Berry phase changes by an integer. In combination with the previous result, we can conclude that Berry phases are always integer-valued.

Theorem IV.5. *Let* $\{v_i(k)\}_{i\in\{1,\ldots,N\}}$ *be is as in (15) and let* $\{u_i(k)\}_{i\in\{1,\ldots,N\}}$ *be any Bloch basis associated to* $P_-(k)$, *in the sense of Definiton III.1. Define the change-of-basis matrix* $G(k)$, *called* Bloch gauge, *such that* $u_i(k) = G(k)\,v_i(k)$ *for all* $i \in \{1,\ldots,N\}$. *Then* $G(k)$ *is unitary,* 2π-*periodic and as regular in k as the Bloch bases. Moreover*

$$\frac{1}{2\pi\mathrm{i}} \int_{S^1} \mathrm{d}k \sum_{i=1}^{N} \langle u_i(k), u_i'(k)\rangle = \frac{1}{2\pi\mathrm{i}} \int_{S^1} \mathrm{d}k \sum_{i=1}^{N} \langle v_i(k), v_i'(k)\rangle + \mathrm{wn}([G]) \quad \in \mathbb{Z}$$

where $\mathrm{wn}([G])$ *denotes the winding number of the map* $G \colon S^1 \to U(N)$.

Proof. For each $k \in \mathbb{R}$, the matrix $G(k)$ is unitary, as it maps one orthonormal basis into another. Moreover, in the 2π-periodic and regular orthonormal basis $\{v_i(k)\}_{i\in\{1,\ldots,N\}}$ for $\mathbb{C}^N$, the Bloch gauge $G(k)$ has entries

$$\langle v_j(k), G(k)\,v_i(k)\rangle = \langle v_j(k), u_i(k)\rangle, \quad i,j \in \{1,\ldots,N\},$$

and therefore it is itself 2π-periodic and regular, as wanted.

We can then compute

$$
\begin{aligned}
\frac{1}{2\pi i} \int_{S^1} dk \sum_{i=1}^{N} \langle u_i(k), u_i'(k) \rangle &= \frac{1}{2\pi i} \int_{S^1} dk \sum_{i=1}^{N} \langle G(k) v_i(k), \partial_k \left(G(k) v_i(k) \right) \rangle \\
&= \frac{1}{2\pi i} \int_{S^1} dk \sum_{i=1}^{N} \langle G(k) v_i(k), G(k) v_i'(k) \rangle + \frac{1}{2\pi i} \int_{S^1} dk \sum_{i=1}^{N} \langle G(k) v_i(k), G'(k) v_i(k) \rangle \\
&= \frac{1}{2\pi i} \int_{S^1} dk \sum_{i=1}^{N} \langle v_i(k), v_i'(k) \rangle + \frac{1}{2\pi i} \int_{S^1} dk \sum_{i=1}^{N} \langle v_i(k), G(k)^* G'(k) v_i(k) \rangle \\
&= \frac{1}{2\pi i} \int_{S^1} dk \sum_{i=1}^{N} \langle v_i(k), v_i'(k) \rangle + \frac{1}{2\pi i} \int_{S^1} dk \, \mathrm{tr} \left(G(k)^* G'(k) \right) \\
&= \frac{1}{2\pi i} \int_{S^1} dk \sum_{i=1}^{N} \langle v_i(k), v_i'(k) \rangle + \mathrm{wn}([G]),
\end{aligned}
$$

as claimed.   □

Remark IV.6. By definition, a Bloch basis $\{u_i(k)\}_{i \in \{1,\dots,N\}}$ associated to $P_-(k)$ has the first m vectors in $\mathrm{Ran}\, P_-(k)$ and the last $N - m$ in $\mathrm{Ran}\, P_+(k)$, where as usual $P_+(k) = \mathbb{1} - P_-(k)$. Therefore, the Bloch gauge $G(k)$ which maps the Bloch basis $\{v_i(k)\}_{i \in \{1,\dots,N\}}$ in (15) to $\{u_i(k)\}_{i \in \{1,\dots,N\}}$ has a block-diagonal form in the decomposition $\mathbb{C}^N = \mathrm{Ran}\, P_-(k) \oplus \mathrm{Ran}\, P_+(k)$, i.e.

$$
G(k) = \begin{bmatrix} G_-(k) & 0 \\ 0 & G_+(k) \end{bmatrix} \tag{18}
$$

where $G_\pm(k) = P_\pm(k) G(k) P_\pm(k)$ seen as a linear operator on $\mathrm{Ran}\, P_\pm(k)$. In particular

$$
u_i(k) = \begin{cases} G_-(k) v_i(k) & \text{if } i \in \{1,\dots,m\}, \\ G_+(k) v_i(k) & \text{if } i \in \{m+1,\dots,N\}. \end{cases}
$$

B.   Symmetric Berry phases

We now turn to the investigation of how PHS and CS affect the value of Berry phases.

Proposition IV.7. *Let Assumption II.3 or II.4 hold. Let $\{v_i(k)\}_{i \in \{1,\dots,N\}}$ be is as in (15) and let $\{u_i(k)\}_{i \in \{1,\dots,N\}}$ be any symmetric Bloch basis associated to $P_-(k)$, in the sense of Definiton III.2. Finally, let $G(k)$ be the Bloch gauge defined in Theorem IV.5. Then*

$$
\mathrm{wn}([G]) \in 2\mathbb{Z}.
$$

Proof. We will use the block decomposition of $G(k)$ from (18). As usual we will denote by m the rank of $P_-(k)$, so that in particular $N = 2m$.

   a.   CS   Under Assumption II.4, we have that

$$
v_{N-i+1}(k) = S v_i(k) \quad \text{and} \quad u_{N-i+1}(k) = S u_i(k) \quad \text{for } i \in \{1,\dots,m\}.
$$

We have also, for $i \in \{1,\dots,m\}$,

$$
G_+(k) S v_i(k) = G_+(k) v_{N-i+1}(k) = u_{N-i+1}(k) = S u_i(k) = S G_-(k) v_i(k).
$$

Since $\{v_i(k)\}_{i \in \{1,\dots,m\}}$ span $\mathrm{Ran}\, P_-(k)$ orthonormally, we conclude that

$$
G_+(k) P_+(k) S = G_+(k) S P_-(k) = S G_-(k) P_-(k).
$$

Since $G_\pm(k) = P_\pm(k) G(k) P_\pm(k)$ by definition, we conclude from the above that

$$
P_+(k) G(k) P_+(k) S = S P_-(k) G(k) P_-(k)
$$

and therefore

$$\det G(k) = \det G_-(k) \cdot \det G_+(k) = \left(\det G_-(k) \right)^2.$$

(In the above, it should be noted that $\det G$ is the determinant of a linear operator on $\mathbb{C}^N = \mathbb{C}^{2m}$, while $\det G_\pm$ are determinants of linear operators on $\operatorname{Ran} P_\pm(k) \simeq \mathbb{C}^m$.) In view of the results of Appendix A, the winding number $\operatorname{wn}([G])$ can be computed as the winding $w(\det G)$ of the map $\det G \colon S^1 \to S^1$, and additivity of this winding number (Proposition A.2) yields

$$\operatorname{wn}([G]) = 2 \operatorname{wn}([G_-]) \in 2\mathbb{Z}.$$

b. **PHS** Under Assumption II.3, we have this time

$$G_+(-k) C v_i(k) = G_+(-k) v_{N-i+1}(-k) = u_{N-i+1}(-k) = C u_i(k) = C G_-(k) v_i(k)$$

for $i \in \{1, \ldots, m\}$, and therefore

$$P_+(-k) G(-k) P_+(-k) C = C P_-(k) G(k) P_-(k).$$

By antilinearity of C, the above implies that

$$\det G_+(-k) = \overline{\det G_-(k)} = \det G_-(k)^* = \det G_-(k)^{-1}$$

and in view of Remark A.3

$$w(\det G_+) = -w(\det G_+ \circ \iota) = -w(\det G_-^{-1}) = w(\det G_-)$$

where $\iota(k) := -k$. As before, this identity allows to deduce that $\operatorname{wn}([G]) = \operatorname{wn}([G_-]) + \operatorname{wn}([G_+]) = 2 \operatorname{wn}([G_-]) \in 2\mathbb{Z}$, which concludes the proof. $\hspace{2em}$ $\square$

Corollary IV.8. *Under the assumptions of Proposition IV.7, the* mod 2 *equivalence class*

$$\left[\frac{1}{2\pi i} \int_{S^1} dk \sum_{i=1}^{2m} \langle u_i(k), u_i'(k) \rangle \right] = \left[\frac{1}{\pi i} \int_{S^1} dk \sum_{i=1}^{m} \langle u_i(k), u_i'(k) \rangle \right] \quad \in \mathbb{Z}_2$$

does not depend on the choice of a symmetric Bloch basis $\{u_i(k)\}_{i \in \{1, \ldots, N\}}$ *associated to* $P_-(k)$.

Proof. The independence of the mod 2 reduction of the Berry phase from the Bloch basis is a direct consequence of Theorem IV.5 and Proposition IV.7, so we only need to prove the rewriting of the Berry phase claimed in the statement.

c. **CS** Under Assumption II.4 it suffices to notice that for a chiral symmetric Bloch basis $\{u_i(k)\}_{i \in \{1, \ldots, N\}}$

$$\langle u_{N-i+1}(k), u_{N-i+1}'(k) \rangle = \langle S u_i(k), S u_i'(k) \rangle = \langle u_i(k), u_i'(k) \rangle, \quad i \in \{1, \ldots, m\},$$

and therefore

$$\sum_{i=1}^{2m} \langle u_i(k), u_i'(k) \rangle = 2 \sum_{i=1}^{m} \langle u_i(k), u_i'(k) \rangle.$$

d. **PHS** This time, under Assumption II.3, we have that for a particle-hole symmetric Bloch basis

$$u_{N-i+1}(-k) = C u_i(k) \quad \Longrightarrow \quad -u_{N-i+1}'(-k) = C u_i'(k), \quad i \in \{1, \ldots, m\},$$

and therefore

$$\langle u_{N-i+1}(-k), u_{N-i+1}'(-k) \rangle = -\langle C u_i(k), C u_i'(k) \rangle = -\overline{\langle u_i(k), u_i'(k) \rangle}, \quad i \in \{1, \ldots, m\},$$

due to the antilinearity of C. Now, the normalization $\langle u_i(k), u_i(k) \rangle \equiv 1$ implies that $\langle u_i(k), u_i'(k) \rangle$ is a purely imaginary number, which yields

$$\langle u_{N-i+1}(-k), u_{N-i+1}'(-k) \rangle = \langle u_i(k), u_i'(k) \rangle, \quad i \in \{1, \ldots, m\}.$$

Notice now that, by changing variables to $\kappa = -k$, we can rewrite

$$\int_0^{2\pi} \mathrm{d}k \sum_{j=m+1}^{2m} \langle u_j(k), u_j'(k) \rangle = -\int_0^{-2\pi} \mathrm{d}\kappa \sum_{j=m+1}^{2m} \langle u_j(-\kappa), u_j'(-\kappa) \rangle$$

$$= \int_{-2\pi}^0 \mathrm{d}\kappa \sum_{i=1}^m \langle u_i(\kappa), u_i'(\kappa) \rangle = \int_0^{2\pi} \mathrm{d}\kappa \sum_{i=1}^m \langle u_i(\kappa), u_i'(\kappa) \rangle \,,$$

where in the last equality we shifted the integration interval thanks to the 2π-periodicity of the Bloch basis. As before, this allows to conclude that

$$\frac{1}{2\pi \mathrm{i}} \int_{S^1} \mathrm{d}k \sum_{i=1}^{2m} \langle u_i(k), u_i'(k) \rangle = \frac{1}{\pi \mathrm{i}} \int_{S^1} \mathrm{d}k \sum_{i=1}^m \langle u_i(k), u_i'(k) \rangle$$

as wanted.   □

C. The $\mathbb{Z}_2$ invariant

The above result finally puts in the position to set the following

Definition IV.9 (The $\mathbb{Z}_2$ invariant)**.** Let H be a finite-range Hamiltonian on $\ell^2(\mathbb{Z}) \otimes \mathbb{C}^N$ modeling a translation-invariant insulator, see Assumptions II.1 and II.2. Assume also that H is either particle-hole symmetric or chiral symmetric, in the sense of Assumption II.3 or II.4 respectively. Then the quantity

$$I_{\mathrm{PHC}}(H) := \frac{1}{\pi \mathrm{i}} \int_{S^1} \mathrm{d}k \sum_{i=1}^m \langle u_i(k), u_i'(k) \rangle \mod 2 \quad \in \mathbb{Z}_2 \tag{19}$$

is a gauge invariant of the spectral projection of H onto the negative energy eigenspace. Here $\{u_i(k)\}_{i \in 1, \dots, N}$ is any symmetric Bloch basis, in the sense of Definition III.2.

The above definition of our $\mathbb{Z}_2$ invariant I_{PHC} is formulated in terms of a symmetric basis for the spectral projections $P_-(k)$ corresponding to negative eigenvalues of the fiber Hamiltonians; the symmetry dictates how the corresponding basis for $P_+(k) = \mathbb{1} - P_-(k)$ should be defined. This could make the numerical computation of the invariant in specific models more accessible.

The next result states that $I_{\mathrm{PHC}}(H)$ is also invariant under continuous deformations, i.e. homotopies, of the model, and therefore qualifies as a "topological invariant".

Theorem IV.10 (Topological invariance of I_{PHC})**.** *Assume that H_t, $t \in [0,1]$, is a continuous family of bounded operators in $\ell^2(\mathbb{Z}) \otimes \mathbb{C}^N$ with the properties described in Definition IV.9. Assume that the spectral gap of H_t stays open for all $t \in [0,1]$. Then*

$$I_{\mathrm{PHC}}(H_0) = I_{\mathrm{PHC}}(H_1) \,.$$

Proof. The homotopy $t \mapsto H_t$ induces a corresponding homotopy $t \mapsto P_-(k;t)$ between the spectral projections of the fiber operators $H_t(k)$, which remains continuous due to the fact that the gap remains open. Since both $k \in S^1$ and $t \in [0,1]$ range over compact sets, by uniform continuity there exists $\delta > 0$ such that

$$\sup_{k \in S^1} \|P_-(k;t) - P_-(k;s)\| < 1 \quad \text{if} \quad |t-s| < \delta \,.$$

Let us use the short-hand notation $P_t(k) := P_-(k;t)$ and $P_s(k) := P_-(k;s)$ in the following. The above implies the existence of a *Kato–Nagy unitary* (see Ref. 8, Chapter I, Section 4.6)

$$U_{t,s}(k) := \left[\mathbb{1} - (P_t(k) - P_s(k))^2\right]^{-1/2} [P_t(k) P_s(k) + (\mathbb{1} - P_t(k)) (\mathbb{1} - P_s(k))]$$

such that

$$P_t(k) U_{t,s}(k) = U_{t,s}(k) P_s(k) \,.$$

From the above explicit expression for the Kato–Nagy unitary, it is clear that it is as regular in k as the projections, jointly continuous in t and s, and commutes with C or S if the models are particle-hole symmetric or chiral symmetric, respectively.

Let us fix for example $s = 0$, and let $\{u_i(k;0)\}_{i \in \{1,\ldots,N\}}$ be a symmetric Bloch basis associated to $P_-(k;0)$. By the above properties of the Kato–Nagy unitary, the collection of vectors

$$u_i(k;t) := U_{t,0}(k)\, u_i(k;0), \quad i \in \{1,\ldots,N\},$$

defines a symmetric Bloch basis associated to $P_-(k;t)$, as long as $|t| < \delta$. Arguing as in the proof of Proposition IV.7, one can check that the Berry phase of the Bloch basis $\{u_i(k;t)\}_{i \in \{1,\ldots,N\}}$ has the same parity of the one of the Bloch basis $\{u_i(k;0)\}_{i \in \{1,\ldots,N\}}$, which defines the invariant $I_{\mathrm{PHC}}(H_0)$. This implies that $I_{\mathrm{PHC}}(H_t)$ is constant on the interval $[0,\delta)$. Partitioning the interval $[0,1]$ into a sequence of intervals of length $\delta/2$ and iterating this argument yields the conclusion of the proof. □

Remark IV.11. It is important to stress that, in the above statement, the symmetry (be it chiral or particle-hole) is required to be *unbroken* along the whole homotopy $t \mapsto H_t$, on top of the assumption that the continuous deformation of H_0 to H_1 does not close the spectral gap. Indeed, one could connect also Hamiltonians which are in different topological phases (meaning that they have different values of I_{PHC}) without closing the gap, but breaking the symmetry along the deformation. The authors of Ref. 20, for example, provide a deformation of (continuum models for) a "topological" chiral chain to a "trivial" one which keeps the spectral gap open, but do not claim that the deformation also leaves the chiral symmetry unbroken.

V. SSH MODEL

The Su–Schrieffer–Heeger (SSH) model, introduced in Ref. 21 to model a molecular chain of polyacetylene, is often considered as a prototypical example of a chiral-symmetric topological insulator. The Hamiltonian $H_{\mathrm{SSH}} \equiv H_{\mathrm{SSH}}(\delta)$ acts on the Hilbert space $\mathscr{H} = \ell^2(\mathbb{Z}) \otimes \mathbb{C}^2$ as

$$(H_{\mathrm{SSH}}\psi)_n = A_1\,\psi_{n+1} + A_0\,\psi_n + A_1^*\,\psi_{n-1}, \quad \psi \in \ell^2(\mathbb{Z}) \otimes \mathbb{C}^2,$$

where

$$A_1 = \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}, \quad A_0 \equiv A_0(\delta) = \begin{bmatrix} 0 & \delta \\ \delta & 0 \end{bmatrix}, \quad \text{with} \quad \delta \in \mathbb{R}.$$

The SSH Hamiltonian thus fits Assumptions II.1 and II.2, provided we exclude some values of the parameter δ which lead to gapless spectrum. To this end, we apply Lemma II.5 to obtain the fiber operators

$$H_{\mathrm{SSH}}(k) = A_0 + \mathrm{e}^{-ik}A_1 + \mathrm{e}^{ik}A_1^* = \begin{bmatrix} 0 & \delta + \mathrm{e}^{ik} \\ \delta + \mathrm{e}^{-ik} & 0 \end{bmatrix}$$

with eigenvalues (*Bloch bands*)

$$E_\pm(k) := \pm\sqrt{(\delta + \cos k)^2 + (\sin k)^2}. \tag{20}$$

The SSH model represents an insulator if and only if $E_\pm(k) \neq 0$ for all $k \in \mathbb{R}$, that is, if $\delta \notin \{-1,1\}$.

Moreover, it is easily verified that this model verifies the CS hypothesis (or, more appropriately, a sublattice symmetry hypothesis), Assumption II.4, with respect to the CS operator $S_{\mathrm{C}} = \mathbb{1}_{\ell^2(\mathbb{Z})} \otimes S$ with $S = \sigma_3$, the third Pauli matrix, i.e.

$$S \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} x \\ -y \end{bmatrix}.$$

The SSH model is thus amenable to our analysis conducted in the previous Sections: as we will see, the parameter δ can be used to toggle topological and non-topological phases.

A. The $\mathbb{Z}_2$ invariant for the SSH model

In order to compute the invariant $I_{\mathrm{PHC}}(\delta) \equiv I_{\mathrm{PHC}}(H_{SSH}(\delta))$ in (19), let us pick a smooth and periodic eigenvector for $H_{SSH}(k)$ with negative eigenvalue. To this end, let us denote $z(k) := \delta + \mathrm{e}^{ik}$, so that in particular $E_\pm(k) = \pm|z(k)|$ and $z(k) \neq 0$ as long as the Hamiltonian is an insulator. Solving the eigenvalue equation $H(k)\,u(k) = E_-(k)\,u(k)$ yields the normalized eigenvector

$$u(k) = \frac{1}{\sqrt{2}} \begin{bmatrix} -1 \\ \sqrt{\dfrac{z(k)}{\overline{z(k)}}} \end{bmatrix}$$

from which we find, with a straightforward computation,

$$\langle u(k), u'(k) \rangle = \frac{1}{4} \frac{\overline{z'(k)} z(k) - \overline{z(k)} z'(k)}{\overline{z(k)} z(k)} = -\frac{i}{2} \operatorname{Im} \frac{z'(k)}{z(k)}.$$

Therefore the $\mathbb{Z}_2$ invariant can be computed as

$$I_{\text{PHC}}(\delta) = \frac{1}{\pi i} \int_{S^1} dk \, \langle u(k), u'(k) \rangle \bmod 2 = -\frac{1}{2\pi} \int_{S^1} dk \operatorname{Im} \frac{z'(k)}{z(k)} \bmod 2$$

$$= \operatorname{Re} \left[-\frac{1}{2\pi i} \int_{S^1} dk \frac{z'(k)}{z(k)} \right] \bmod 2.$$

By the Cauchy integral formula, the integral above computes the winding number around the origin of the curve γ in the complex plane obtained as the image of $k \mapsto z(k) = \delta + e^{ik}$, namely a circle of unit radius centered around $\delta \in \mathbb{R} \subset \mathbb{C}$. This winding number is an integer, and therefore the real part in right-hand side of the above identity is redundant: in particular, the curve γ winds around the origin once if $\delta \in (-1, 1)$ or zero times otherwise. (Notice that γ passes through $0 \in \mathbb{C}$ if $\delta = \pm 1$, which are excluded values if we want the spectral gap to be open.) We conclude that

$$I_{\text{PCH}}(\delta) = \begin{cases} 1 & \text{if } \delta \in (-1, 1), \\ 0 & \text{if } \delta \in \mathbb{R} \setminus [-1, 1]. \end{cases}$$

Incidentally, let us observe that the integer winding number of $k \mapsto z(k)$ coincides with the "bulk" topological invariant associated to 2-band chiral chains in Refs. 5 and 19.

B. Boundary modes for the SSH model

When a topological insulator is cut along some edge, the *bulk-boundary correspondence* predicts the appearance of new modes which fill the spectral gap of the bulk Hamiltonian and are spatially localized around the cut. We investigate this situation here for the SSH model, and verify that localized boundary modes to appear exactly for the values of the parameter δ for which $I_{\text{PCH}} \neq 0 \in \mathbb{Z}_2$. For a general proof of a bulk-edge correspondence in (disordered) chiral chains, we refer the reader to Ref. 5.

Let us define a truncated version of the SSH Hamiltonian as follows: it will be given by the operator $H_{\text{SSH}}^\sharp$ acting on $\mathcal{H}^\sharp := \ell^2(\mathbb{N}) \otimes \mathbb{C}^2$ as

$$(H_{\text{SSH}}^\sharp \psi)_n := (H_{\text{SSH}} \psi)_n \quad \text{if } n > 0, \quad \text{and}$$

$$(H_{\text{SSH}}^\sharp \psi)_0 := A_1 \psi_1 + A_0 \psi_0, \quad \psi \in \ell^2(\mathbb{N}) \otimes \mathbb{C}^2.$$

The truncated Hamiltonian imposes a Dirichlet condition on H_{SSH} which sets $\psi_n = 0$ for negative n. This boundary condition does not change the essential spectrum of H_{SSH}, which remains given by the two bands obtained as images of the functions defined in (20), but pure point spectrum may appear in the bulk gap. We therefore look for zero-energy modes of $H_{\text{SSH}}^\sharp$, namely for a vector $\psi = ([x_n, y_n]^\text{T}) \in \mathcal{H}^\sharp$, $\psi \neq 0$, such that $H_{\text{SSH}}^\sharp \psi = 0$. Explicitly, this reads

$$\begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} x_{n+1} \\ y_{n+1} \end{bmatrix} + \begin{bmatrix} 0 & \delta \\ \delta & 0 \end{bmatrix} \begin{bmatrix} x_n \\ y_n \end{bmatrix} + \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} x_{n-1} \\ y_{n-1} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \quad \text{if } n > 0, \quad \text{and}$$

$$\begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} x_1 \\ y_1 \end{bmatrix} + \begin{bmatrix} 0 & \delta \\ \delta & 0 \end{bmatrix} \begin{bmatrix} x_0 \\ y_0 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}.$$

This yields the recursion rule

$$\begin{cases} \delta x_0 = -x_1, \\ \delta y_0 = 0, \\ x_{n+1} = -\delta x_n & \text{if } n > 0, \\ \delta y_n = -y_{n-1} & \text{if } n > 0. \end{cases}$$

This obviously means that $x_n = (-\delta)^n x_0$ and $y_n \equiv 0$. In order for the resulting vector ψ to be square-summable in the index $n \in \mathbb{N}$, we therefore have to require

$$\|\psi\|_{\mathcal{H}^\sharp}^2 = \sum_{n \in \mathbb{N}} |x_n|^2 + |y_n|^2 = \sum_{n \in \mathbb{N}} |\delta|^{2n} < \infty \quad \Longleftrightarrow \quad |\delta| < 1.$$

This range for δ coincides exactly with the values of the parameter in which the $\mathbb{Z}_2$ invariant $I_{\text{PHC}}(\delta)$ is non-trivial.

VI. KITAEV CHAIN

The Kitaev chain was introduced in Ref. 9 as a model for a topological superconductor. In the notation introduced in Section II the Hamiltonian $H_{\mathrm{Kit}} \equiv H_{\mathrm{Kit}}(\mu, \delta)$ acts on the Hilbert space $\mathscr{H} = \ell^2(\mathbb{Z}) \otimes \mathbb{C}^2$ as

$$(H_{\mathrm{Kit}} \psi)_n = A_1 \psi_{n+1} + A_0 \psi_n + A_1^* \psi_{n-1}$$

where

$$A_1 \equiv A_1(\delta) = \begin{bmatrix} 0 & 1+\delta \\ 1-\delta & 0 \end{bmatrix}, \quad A_0 \equiv A_0(\mu) = \begin{bmatrix} 0 & \mu \\ \mu & 0 \end{bmatrix}, \quad \text{with} \quad \delta, \mu \in \mathbb{R}.$$

To check that this models an insulator, we compute the fiber operators as prescribed by Lemma II.5 and obtain

$$H_{\mathrm{Kit}}(k) = \begin{bmatrix} 0 & (1+\delta)\,\mathrm{e}^{-\mathrm{i}k} + \mu + (1-\delta)\,\mathrm{e}^{\mathrm{i}k} \\ (1-\delta)\,\mathrm{e}^{-\mathrm{i}k} + \mu + (1+\delta)\,\mathrm{e}^{\mathrm{i}k} & 0 \end{bmatrix},$$

which in turn yields the Bloch bands

$$E_\pm(k) := \pm\sqrt{(\mu + 2\cos k)^2 + (2\delta \sin k)^2}\,.$$

Therefore, the Kitaev Hamiltonian is gapped if and only if $E_\pm(k) \neq 0$ for every $k \in \mathbb{R}$: this leads to exclude the set of parameters μ, δ given by

$$\eta := \left\{ (\mu, \delta) \in \mathbb{R}^2 : |\mu| < 2 \text{ and } \delta = 0 \quad \text{or} \quad |\mu| = 2 \text{ and } \delta \in \mathbb{R} \right\}.$$

If $(\mu, \delta) \in \mathbb{R}^2 \setminus \eta$, the Kitaev Hamiltonian H_{Kit} thus verifies both Assumptions II.1 and II.2. Moreover, this model verifies the PHS hypothesis II.3 with respect to the operator $S_{\mathrm{PH}} = \mathbb{1}_{\ell^2(\mathbb{Z})} \otimes C$ with

$$C \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} \bar{x} \\ -\bar{y} \end{bmatrix}.$$

The Kitaev chain also satisfies the CS from the previous Section on the SSH model, but it is often considered paradigmatic for its anti-unitary particle-hole symmetry.

A. The $\mathbb{Z}_2$ invariant for the Kitaev chain

The invariant

$$I_{\mathrm{PHC}}(\mu, \delta) \equiv I_{\mathrm{PHC}}(H_{\mathrm{Kit}}(\mu, \delta)) \in \mathbb{Z}_2$$

can be computed following the same lines of the argument for the SSH model, starting this time from the function

$$z(k) := (1+\delta)\,\mathrm{e}^{-\mathrm{i}k} + \mu + (1-\delta)\,\mathrm{e}^{\mathrm{i}k} = \mu + 2\cos k - 2\mathrm{i}\delta \sin k, \quad k \in \mathbb{R}.$$

Its image $\gamma \subset \mathbb{C}$ describes an ellipse centered around $\mu \in \mathbb{R}$ with semi-axes 2 and 2δ; its orientation is dictated by the sign of $\delta \in \mathbb{R}$. As before $I_{\mathrm{PHC}}(\mu, \delta) \in \mathbb{Z}_2$ computes the parity of the winding number of this curve around the origin in $\mathbb{C}$, and therefore we conclude that

$$I_{\mathrm{PHC}}(\mu, \delta) = \begin{cases} 1 & \text{if } |\mu| < 2 \text{ and } \delta \neq 0, \\ 0 & \text{otherwise in } \mathbb{R}^2 \setminus \eta. \end{cases} \tag{21}$$

B. Boundary modes for the Kitaev chain

As we did for the SSH model, we now pass to the investigation of zero-energy boundary modes for a truncated Kitaev chain. These modes are predicted to behave as Majorana particles, and their topological nature makes them amenable for applications in quantum computing as robust qubits.

The truncated operator $H_{\text{Kit}}^{\sharp}$ acts on $\mathscr{H}^{\sharp} = \ell^2(\mathbb{N}) \otimes \mathbb{C}^2$ as

$$(H_{\text{Kit}}^{\sharp} \psi)_n := (H_{\text{Kit}} \psi)_n \quad \text{if } n > 0, \quad \text{and}$$
$$(H_{\text{Kit}}^{\sharp} \psi)_0 := A_1 \psi_1 + A_0 \psi_0, \quad \psi \in \ell^2(\mathbb{N}) \otimes \mathbb{C}^2.$$

This means that a vector $\psi = ([x_n, y_n]^{\text{T}}) \in \mathscr{H}^{\sharp}$, $\psi \neq 0$, such that $H_{\text{Kit}}^{\sharp} \psi = 0$ satisfies

$$\begin{bmatrix} 0 & 1+\delta \\ 1-\delta & 0 \end{bmatrix} \begin{bmatrix} x_{n+1} \\ y_{n+1} \end{bmatrix} + \begin{bmatrix} 0 & \mu \\ \mu & 0 \end{bmatrix} \begin{bmatrix} x_n \\ y_n \end{bmatrix} + \begin{bmatrix} 0 & 1-\delta \\ 1+\delta & 0 \end{bmatrix} \begin{bmatrix} x_{n-1} \\ y_{n-1} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \quad \text{if } n > 0, \quad \text{and}$$

$$\begin{bmatrix} 0 & 1+\delta \\ 1-\delta & 0 \end{bmatrix} \begin{bmatrix} x_1 \\ y_1 \end{bmatrix} + \begin{bmatrix} 0 & \mu \\ \mu & 0 \end{bmatrix} \begin{bmatrix} x_0 \\ y_0 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix},$$

leading this time to the decoupled recursion rules

$$\begin{cases} (1-\delta)x_1 + \mu x_0 = 0, \\ (1-\delta)x_{n+1} + \mu x_n + (1+\delta)x_{n-1} = 0 & \text{if } n > 0, \end{cases} \tag{22}$$

and

$$\begin{cases} (1+\delta)y_1 + \mu y_0 = 0, \\ (1+\delta)y_{n+1} + \mu y_n + (1-\delta)y_{n-1} = 0 & \text{if } n > 0. \end{cases} \tag{23}$$

Remark VI.1. Notice that one is obtained from the other by the exchange of $\delta \leftrightarrow -\delta$: in particular, if the "particle" $\psi = ([x_n(\mu, \delta), 0]^{\text{T}}) \in \mathscr{H}^{\sharp}$ is a solution for the first recurrence relation, then the "hole" $\psi = ([0, x_n(\mu, -\delta)]^{\text{T}}) \in \mathscr{H}^{\sharp}$ is a solution for the second recurrence equation, and viceversa.

    a.   The case $\delta = \pm 1$ The situation is simpler when $\delta = \pm 1$: indeed, if $\delta = 1$ the relation (23) reduces to

$$\begin{cases} 2y_1 + \mu y_0 = 0, \\ 2y_{n+1} + \mu y_n = 0 & \text{if } n > 0, \end{cases}$$

which is of the form already encountered in the SSH model. In particular, the solution $y_n = (-\mu/2)^n y_0$ is square-summable if and only if $|\mu| < 2$. Notice that $I_{\text{PHC}}(\mu, 1)$ is non-trivial exactly in this range of parameters. Similar considerations hold for (23) starting from $\delta = -1$.

    b.   The characteristic equation   From now one we will suppose $\delta \neq \pm 1$. Moreover, in view of Remark VI.1, it will be enough to restrict the range of parameters to $(\mathbb{R}^2 \setminus \eta) \cap \{\delta \geq 0, \delta \neq 1\}$ and solve the system (23). Under these assumptions, the latter can be recast as

$$\begin{cases} y_{n+1} + \dfrac{\mu}{1+\delta} y_n + \dfrac{1-\delta}{1+\delta} y_{n-1} = 0 & \text{for } n \in \mathbb{N}, \\ y_{-1} = 0, \quad y_0 \neq 0 \end{cases} \tag{24}$$

(the condition on y_0 is to exclude the trivial solution $y_n \equiv 0$ and hence $\psi = 0 \in \mathscr{H}^{\sharp}$ which cannot define an eigenvector for $H_{\text{Kit}}^{\sharp}$). The theory of homogeneous linear difference equations with constant coefficients[2] prompts to consider the *characteristic equation*

$$\lambda^2 + \frac{\mu}{1+\delta} \lambda + \frac{1-\delta}{1+\delta} = 0. \tag{25}$$

If $\lambda_+ \neq \lambda_-$ are the distinct roots of the above equation, then the general solution of (24) is given by

$$y_n = a\lambda_+^n + b\lambda_-^n,$$

while if $\lambda_+ = \lambda_- = \lambda$ solutions are of the form

$$y_n = (a+bn)\lambda^n.$$

In both cases, a, b are constants chosen to fit the initial conditions for the recursion: in particular they cannot be simultaneously zero if we want a non-trivial solution. The above solutions can be easily verified by plugging in the recurrence relation an *ansatz* of the form $y_n = \lambda^n$.

Let us consider first the case $\lambda_+ = \lambda_- = \lambda$. In order to have that $\psi = ([0, y_n]^T)$ is square-summable, we need to impose that

$$\|\psi\|^2_{\mathcal{H}^{\sharp}} = \sum_{n \in \mathbb{N}} |y_n|^2 = \sum_{n \in \mathbb{N}} |a + bn|^2 |\lambda|^{2n} < \infty.$$

The behaviour of the series on the right-hand side is dictated by its geometric part, and hence it converges if and only if $|\lambda| < 1$. In the case $\lambda_+ \neq \lambda_-$, we appeal to the following

Lemma VI.2. *Given $a, b \in \mathbb{C}$, the series*

$$\sum_{n \in \mathbb{N}} |a\lambda_+^n + b\lambda_-^n|^2$$

converges if and only if $|\lambda_+| < 1$ and $|\lambda_-| < 1$.

Proof. The statement is clearly true if either $\lambda_+ = 0$ or $\lambda_- = 0$, or if $a = 0$ or $b = 0$. Hence let us assume that $a \neq 0 \neq b$ and, without loss of generality, that $|\lambda_+| > |\lambda_-| > 0$. If $|\lambda_+| > 1$ then

$$|a\lambda_+^n + b\lambda_-^n|^2 = |\lambda_+|^{2n} \left| a + b \left(\frac{\lambda_-}{\lambda_+}\right)^n \right|^2 \longrightarrow \infty \quad \text{for } n \to \infty$$

so the series cannot converge. Viceversa, if both λ_+ and λ_- are smaller than 1 in absolute value, we can write

$$\sum_{n \in \mathbb{N}} |a\lambda_+^n + b\lambda_-^n|^2 = \sum_{n \in \mathbb{N}} |a|^2 |\lambda_+|^{2n} + |b|^2 |\lambda_-|^{2n} + 2\,\mathrm{Re}\left[\overline{a}b\left(\overline{\lambda_+}\lambda_-\right)^n\right]$$

which is a sum of geometric series whose ratios are complex numbers with modulus smaller than 1, so they converge. $\qquad\square$

With the above considerations at hand, we are led to investigate the roots of the characteristic equation (25), namely

$$\lambda_{\pm} := \frac{1}{2}\left[-\frac{\mu}{1+\delta} \pm \sqrt{\frac{\mu^2 - 4(1-\delta)(1+\delta)}{(1+\delta)^2}}\right] = \frac{1}{2}\left[-\frac{\mu}{1+\delta} \pm \sqrt{\frac{\mu^2 - 4 + 4\delta^2}{(1+\delta)^2}}\right]$$

and to study when they are both smaller than 1 in absolute value.

c. Coinciding roots of the characteristic equation If $\lambda_+ = \lambda_- = -\mu/2(1+\delta)$, then observing that we are restricting to $\delta \geq 0$ we have that

$$\left|-\frac{\mu}{2(1+\delta)}\right| < 1 \quad \Longleftrightarrow \quad |\mu| < \min_{\delta \geq 0} |2(1+\delta)| = 2.$$

d. Complex roots of the characteristic equation If $\mu^2 + 4\delta^2 < 4$, the characteristic equation has two distinct complex roots

$$\lambda_{\pm} = \frac{1}{2}\left[-\frac{\mu}{1+\delta} \pm i\sqrt{\frac{4 - 4\delta^2 - \mu^2}{(1+\delta)^2}}\right].$$

Since $|\lambda| < 1$ if and only if $|\lambda|^2 < 1$, we can bound

$$|\lambda_+|^2 = |\lambda_-|^2 = \frac{1}{4}\left[\frac{\mu^2}{(1+\delta)^2} + \frac{4 - 4\delta^2 - \mu^2}{(1+\delta)^2}\right] = \frac{1 - \delta^2}{(1+\delta)^2} = 1 - \frac{2\delta}{1+\delta} < 1$$

for all $\delta > 0$. If $\delta = 0$, the relation $\mu^2 + 4\delta^2 < 4$ forces $|\mu| < 2$: but the region $\{|\mu| < 2 \text{ and } \delta = 0\}$ in parameter space lies in η, and is therefore excluded from our analysis. We conclude that once again square-integrable solutions of the recurrence relation (24) exists if $\mu^2 + 4\delta^2 < 4$ for all $\delta > 0$, that is, for $|\mu| < 2$.

e. Real roots of the characteristic equation Finally, when $\mu^2 + 4\delta^2 > 4$ the characteristic equation has two distinct real roots

$$\lambda_{\pm} = \frac{1}{2}\left[-\frac{\mu}{1+\delta} \pm \sqrt{\frac{\mu^2 - 4 + 4\delta^2}{(1+\delta)^2}}\right].$$

We are led this time to solve the system

$$\begin{cases} \dfrac{\mu^2}{4(1+\delta)^2} + \dfrac{\mu^2 + 4\delta^2 - 4}{4(1+\delta)^2} - \dfrac{\mu}{1+\delta}\sqrt{\dfrac{\mu^2 + 4\delta^2 - 4}{4(1+\delta)^2}} < 1 \\[3mm] \dfrac{\mu^2}{4(1+\delta)^2} + \dfrac{\mu^2 + 4\delta^2 - 4}{4(1+\delta)^2} + \dfrac{\mu}{1+\delta}\sqrt{\dfrac{\mu^2 + 4\delta^2 - 4}{4(1+\delta)^2}} < 1 \end{cases}$$

which after a lengthy but straightforward computation is shown to be equivalent to $|\mu| < 2$.

f. Conclusions In conclusion, if we combine all the previous results we obtain that, if $\delta \geq 0$ (and, in view of Remark VI.1, also if $\delta \leq 0$), there is a zero-energy boundary state for the truncated Kitaev chain if and only if $|\mu| < 2$. Comparing with (21), we conclude that as in the SSH model the presence of boundary states occurs exactly for those values of the physical parameters μ, δ for which the $\mathbb{Z}_2$ invariant is non-trivial.

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DATA AVAILABILITY STATEMENT

Data sharing is not applicable to this article as no new data were created or analyzed in this study.

Appendix A: Winding numbers for unitary matrices

This Appendix is devoted to give some insights into the proof of Theorem IV.2; more details can be found e.g. in Ref. 12, Section III. The statement that $U(N)$-valued maps on S^1 are characterized by their winding number up to homotopy can be essentially reduced to the analogous fact for $N = 1$, namely that maps $S^1 \to U(1) \simeq S^1$ are described by the way they wind around the origin in the complex plane. The reduction step is based on the following

Proposition A.1. *If $U \colon \mathbb{R} \to U(N)$ is at least C^1, then*

$$\frac{\partial_k \det U(k)}{\det U(k)} = \mathrm{tr}\left(U(k)^* U'(k)\right).$$

Proof. Since $U(k)$ is unitary we have $U(k)U(k)^* = \mathbb{1}$, and using the fact that $\det(\mathbb{1}+H) = 1 + \mathrm{tr}(H) + \mathscr{O}(\|H\|^2)$ we can compute

$$\partial_k \det U(k) = \lim_{h\to 0} \frac{\det U(k+h) - \det U(k)}{h} = \det U(k) \cdot \lim_{h\to 0} \frac{\det\left(\mathbb{1} - U(k)^* U(k) + U(k)^* U(k+h)\right) - 1}{h}$$

$$= \det U(k) \cdot \lim_{h\to 0} \frac{\mathrm{tr}\left(U(k)^* U(k+h) - U(k)^* U(k)\right)}{h} = \det U(k) \cdot \mathrm{tr}\left\{ U(k)^* \cdot \left[\lim_{h\to 0} \frac{U(k+h) - U(k)}{h} \right] \right\}$$

$$= \det U(k) \cdot \mathrm{tr}\left(U(k)^* U'(k)\right). \qquad \square$$

The above result immediately gives that $\mathrm{wn}([U])$ defined in (17) can be computed as

$$\mathrm{wn}([U]) = \frac{1}{2\pi\mathrm{i}} \int_{S^1} \mathrm{d}k \, \frac{\partial_k \det U(k)}{\det U(k)}.$$

We thus shift our focus on the function $u := \det U \colon S^1 \to U(1) \simeq S^1$.

Proposition A.2. *Let $f, g \colon S^1 \to S^1$ be two differentiable maps. The integral*

$$w(f) := \frac{1}{2\pi\mathrm{i}} \int_{S^1} \mathrm{d}k \, \frac{f'(k)}{f(k)}$$

is integer-valued, and depends only on the homotopy class of f: it is called the winding number *of f. Moreover, the winding number of the product is the sum of the two winding numbers:*

$$w(f \cdot g) = w(f) + w(g).$$

Proof. The image of $f\colon S^1 \to S^1$ can be seen as a rectifiable and closed curve $\gamma \subset \mathbb{C}$. By the Cauchy integral formula

$$\int_{S^1} dk \frac{f'(k)}{f(k)} = \int_{\gamma} dz \frac{1}{z} = 2\pi i \operatorname{Ind}_\gamma(0)$$

where $\operatorname{Ind}_\gamma(0)$ computes the winding number of the curve γ around the origin in $\mathbb{C}$. As is well known, this quantity is integer-valued.

If $f_s \colon S^1 \to S^1$, $s \in [0,1]$, is a smooth homotopy between two maps f_0 and f_1, then

$$\frac{d}{ds} \int_{S^1} dk \frac{f_s'(k)}{f_s(k)} = \int_{S^1} dk \frac{\partial_s \partial_k f_s(k) f_s(k) - \partial_k f_s(k) \partial_s f_s(k)}{f_s(k)^2} = \int_{S^1} dk\, \partial_k \left(\frac{\partial_s f_s(k)}{f_s(k)} \right) = 0$$

and therefore $w(f)$ is constant along the homotopy class of f.

Finally, to show the additive property of the winding number, it suffices to compute

$$w(f \cdot g) = \frac{1}{2\pi i} \int_{S^1} dk \frac{\partial_k (fg)(k)}{f(k)g(k)} = \frac{1}{2\pi i} \int_{S^1} dk \frac{\partial_k f(k)}{f(k)} + \frac{1}{2\pi i} \int_{S^1} dk \frac{\partial_k g(k)}{g(k)} dk = w(f) + w(g). \qquad \square$$

Remark A.3. Let $\iota\colon S^1 \to S^1$ be the involution $k \mapsto -k$. For $f\colon S^1 \to S^1$, we then have

$$w(f \circ \iota) = -w(f).$$

Indeed, we can compute $(f \circ \iota)'(k) = -f'(-k)$ and therefore

$$2\pi i\, w(f \circ \iota) = -\int_0^{2\pi} dk \frac{f'(-k)}{f(-k)} = \int_0^{-2\pi} d\kappa \frac{f'(\kappa)}{f(\kappa)} = -\int_{-2\pi}^0 d\kappa \frac{f'(\kappa)}{f(\kappa)} = -\int_0^{2\pi} d\kappa \frac{f'(\kappa)}{f(\kappa)} = -2\pi i\, w(f)$$

where in the second equality we used the substitution $\kappa = \iota(k) = -k$ (from which $d\kappa = -dk$) and in the second-to-last equality we shifted the integration interval by periodicity of f.

Proposition A.4. *The map*

$$\pi_1\left(S^1\right) \to \mathbb{Z}, \quad [f] \mapsto \frac{1}{2\pi i} \int_{S^1} dk \frac{f'(k)}{f(k)}$$

is a bijection.

Proof. See e.g. Ref. 10, Chapter 1, Section 5 or Ref. 12, pages 7-8. $\qquad \square$

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