Z₂ INVARIANTS OF TOPOLOGICAL INSULATORS AS GEOMETRIC OBSTRUCTIONS

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ABSTRACT. We consider a gapped periodic quantum system with time-reversal symmetry of fermionic (or odd) type, i.e. the time-reversal operator squares to −1. We investigate the existence of periodic and time-reversal invariant Bloch frames in dimensions 2 and 3. In 2d, the obstruction to the existence of such a frame is shown to be encoded in a Z₂-valued topological invariant, which can be computed by a simple algorithm. We prove that the latter agrees with the Fu-Kane index. In 3d, instead, four Z₂ invariants emerge from the construction, again related to the Fu-Kane-Mele indices. When no topological obstruction is present, we provide a constructive algorithm yielding explicitly a periodic and time-reversal invariant Bloch frame. The result is formulated in an abstract setting, so that it applies both to discrete models and to continuous ones.

KEYWORDS. Topological insulators, time-reversal symmetry, Kane-Mele model, Z₂ invariants, Bloch frames.

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1. INTRODUCTION

In the recent past, the solid state physics community has developed an increasing interest in phenomena having topological and geometric origin. The first occurrence of systems displaying different quantum phases which can be labelled by topological indices can be traced back at least to the seminal paper by Thouless, Kohmoto, Nightingale and den Nijs [TKNN], in the context of the Integer Quantum Hall Effect. The first topological invariants to make their appearance in the condensed matter literature were thus Chern numbers: two distinct insulating quantum phases, which cannot be deformed one into the other by means of continuous (adiabatic) transformations without closing the gap between energy bands, are indexed by different integers (see [Gr] and references therein). These topological invariants are related to an observable quantity, namely to the transverse (Hall) conductivity of the system under consideration [TKNN, Gr]; the fact that the topological invariant is an integer explains why the observable is quantized. Beyond the realm of Quantum Hall systems, similar non-trivial topological phases appear whenever time-reversal symmetry is broken, even in absence of external magnetic fields, as early foreseen by Haldane [Hal]. Since this pioneering observation, the field of Chern insulators flourished [SPFKS, Ch, FC].

More recently, a new class of materials has been first theorized and then experimentally realized, where instead interesting topological quantum phases arise while preserving time-reversal symmetry: these materials are the so-called time-reversal symmetric (TRS) topological insulators (see [An, HK] for recent reviews). The peculiarity of these materials is that different quantum phases are labelled by integers modulo 2; from a phenomenological point of view, these indices are connected to the presence of spin edge currents responsible for the Quantum Spin Hall Effect [KM1, KM2]. It is crucial for the display of these currents that time-reversal symmetry is of fermionic (or odd) type, that is, the time-reversal operator $\Theta$ is such that $\Theta^2 = -1$.

In a milestone paper [KM1], Kane and Mele consider a tight-binding model governing the dynamics of an electron in a 2-dimensional honeycomb lattice subject to nearest- and next-to-nearest-neighbour hoppings, similarly to what happens in the Haldane model [Hal], with the addition of further terms, including time-reversal invariant spin-orbit interaction. This prototype model is used to propose a $\mathbb{Z}_2$ index to label the topological phases of 2d TRS topological insulators, and to predict
the presence of observable currents in Quantum Spin Hall systems. An alternative formulation for this $\mathbb{Z}_2$ index is then provided by Fu and Kane in [FK], where the authors also argue that such index measures the obstruction to the existence of a continuous periodic Bloch frame which is moreover compatible with time-reversal symmetry. Similar indices appear also in 3-dimensional systems [FKM].

Since the proposals by Fu, Kane and Mele, there has been an intense activity in the community aimed at the explicit construction of smooth symmetric Bloch frames, in order to connect the possible topological obstructions to the $\mathbb{Z}_2$ indices [SV3], and to study the localization of Wannier functions in TRS topological insulators [SV1, SV2]. However, while the geometric origin of the integer-valued topological invariants is well-established (as was mentioned above, they represent Chern numbers of the Bloch bundle, in the terminology of [Pa]), the situation is less clear for the $\mathbb{Z}_2$-valued indices of TRS topological insulators. Many interpretations of the $\mathbb{Z}_2$ indices have been given, using homotopic or $K$-theoretic classifications [AZ, MB, Ki, RSFL], $C^*$-algebraic approaches [Pr1, Pr2, Sch], the bulk-edge correspondence [ASV, GP], monodromy arguments [Pr3], or gauge-theoretic methods [FW]. However, we believe that a clear and simple topological explanation of how they arise from the symmetries of the system is still missing in the literature.

In this paper, we provide a geometric characterization of these $\mathbb{Z}_2$ indices as topological obstructions to the existence of continuous periodic and time-reversal symmetric Bloch frames, thus substantiating the claim in [FK] on mathematical grounds. We consider a gapped periodic quantum system in presence of fermionic time-reversal symmetry (compare Assumption 1), and we investigate whether there exists a global continuous Bloch frame which is both periodic and time-reversal symmetric. While in 1$d$ this always exists, a topological obstruction may arise in 2$d$. We show in Section 3 that such obstruction is encoded in a $\mathbb{Z}_2$ index $\delta$, which is moreover a topological invariant of the system, with respect to those continuous deformations which preserve the symmetries. We prove that $\delta \in \mathbb{Z}_2$ agrees with the Fu-Kane index $\Delta \in \mathbb{Z}_2$ [FK], thus providing a proof that the latter is a topological invariant (Sections 4 and 5). Lastly, in Section 6 we investigate the same problem in 3$d$, yielding to the definition of four $\mathbb{Z}_2$-valued topological obstructions, which are compared with the indices proposed by Fu, Kane and Mele in [FKM]. In all cases where there is no topological obstruction (i.e. the $\mathbb{Z}_2$ topological invariants vanish), we also provide an explicit algorithm to construct a global smooth Bloch frame which is periodic and time-reversal symmetric (see also Appendix A).

The main advantage of our method is that, being geometric in nature, it is based only on the fundamental symmetries of the Hamiltonian modeling the system, namely invariance by lattice translations (i.e. periodicity) and fermionic time-reversal symmetry. No further assumptions on the Hamiltonian and its gaps are needed in our approach, thus making it model-independent; in particular, it applies both to continuous and to tight-binding models, and both to the 2-dimensional and
3-dimensional setting. To the best of our knowledge, our method appears to be the first obstruction-theoretic characterization of the $\mathbb{Z}_2$ invariants in the pioneering field of 3-dimensional TRS topological insulators. The method proposed here encompasses all models studied by the community, in particular the Fu-Kane-Mele models in 2d and 3d [KM], [EK], [FKM]. More general tight-binding models in 2-dimensions were considered e.g. in [ASV] and [GP], where an equivalence between the edge and the bulk index for TRS topological insulators is proved: our general result applies also to the time-reversal invariant bundles (in the terminology of [GP]) considered there, up to an identification of the coordinates on the basis torus.

Another strong point in our approach is that the construction is algorithmic in nature, and gives also a way to compute the $\mathbb{Z}_2$ invariants in a given system (see formulae (3.16) and (5.4)). This makes our proposal well-suited for numerical implementation, which may be particularly appealing to the computational physics community [SV1], [SV3].

We are confident that the methodology proposed in this paper will contribute in the clarification of the geometric origin of $\mathbb{Z}_2$ invariants in TRS topological insulators, and that the constructive algorithm may be used to compute these invariants in real materials to discern the presence of interesting quantum phases.

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2. Setting and main results

2.1. Statement of the problem and main results. We consider a gapped periodic quantum system with fermionic time-reversal symmetry, and we focus on the family of spectral eigenprojectors up to the gap, in Bloch-Floquet representation. In most of the applications, these projectors read

\[ P(k) = \sum_{n \in \text{occ}} |u_n(k)\rangle \langle u_n(k)|, \quad k \in \mathbb{R}^d, \tag{2.1} \]

where \( u_n(k) \) are the periodic parts of the Bloch functions, and the sum runs over all occupied bands.

Abstracting from specific models, we let \( \mathcal{H} \) be a separable Hilbert space with scalar product \( \langle \cdot, \cdot \rangle \), \( \mathcal{B}(\mathcal{H}) \) denote the algebra of bounded linear operators on \( \mathcal{H} \), and \( \mathcal{U}(\mathcal{H}) \) the group of unitary operators on \( \mathcal{H} \). We also consider a maximal lattice \( \Lambda = \text{Span}_\mathbb{Z} \{e_1, \ldots, e_d\} \simeq \mathbb{Z}^d \subset \mathbb{R}^d \): in applications, \( \Lambda \) is the dual lattice to the periodicity Bravais lattice \( \Gamma \) in position space. The object of our study will be a family of orthogonal projectors \( \{P(k)\}_{k \in \mathbb{R}^d} \subset \mathcal{B}(\mathcal{H}), P(k)^* = P(k) = P(k)^2 \), satisfying the following

**Assumption 1.** The family of orthogonal projectors \( \{P(k)\}_{k \in \mathbb{R}^d} \) enjoys the following properties:

1. **smoothness:** the map \( \mathbb{R}^d \ni k \mapsto P(k) \in \mathcal{B}(\mathcal{H}) \) is \( C^\infty \)-smooth;
2. **\( \tau \)-covariance:** the map \( k \mapsto P(k) \) is covariant with respect to a unitary representation \( \tau: \Lambda \to \mathcal{U}(\mathcal{H}) \) of the lattice \( \Lambda \) on the Hilbert space \( \mathcal{H} \), i.e.
   \[ P(k + \lambda) = \tau(\lambda)P(k)\tau(\lambda)^{-1}, \quad \text{for all } k \in \mathbb{R}^d, \forall \lambda \in \Lambda; \]
3. **time-reversal symmetry:** the map \( k \mapsto P(k) \) is time-reversal symmetric, i.e. there exists an antiunitary operator \( \Theta: \mathcal{H} \to \mathcal{H} \), called the time-reversal operator, such that
   \[ \Theta^2 = -1_\mathcal{H} \quad \text{and} \quad P(-k) = \Theta P(k)\Theta^{-1}. \]

Moreover, the unitary representation \( \tau: \Lambda \to \mathcal{U}(\mathcal{H}) \) and the time-reversal operator \( \Theta: \mathcal{H} \to \mathcal{H} \) satisfy

4. **\( \Theta \tau(\lambda) = \tau(\lambda)^{-1}\Theta \)** for all \( \lambda \in \Lambda \).

\[ \diamond \]

Assumption 1 is satisfied by the spectral eigenprojectors of most Hamiltonians modelling gapped periodic quantum systems, in presence of fermionic time-reversal symmetry. Provided the Fermi energy lies in a spectral gap, the map \( k \mapsto P(k) \)

\[^{1}\text{This means that } \tau(0) = 1_\mathcal{H} \text{ and } \tau(\lambda_1 + \lambda_2) = \tau(\lambda_1)\tau(\lambda_2) \text{ for all } \lambda_1, \lambda_2 \in \Lambda. \text{ It follows in particular that } \tau(\lambda)^{-1} = \tau(\lambda^*) = \tau(-\lambda) \text{ for all } \lambda \in \Lambda. \]

\[^{2}\text{Recall that a surjective antilinear operator } \Theta: \mathcal{H} \to \mathcal{H} \text{ is called } \text{antiunitary} \text{ if } (\Theta \psi_1, \Theta \psi_2) = \langle \psi_2, \psi_1 \rangle \text{ for all } \psi_1, \psi_2 \in \mathcal{H}. \]
defined in (2.1) will be smooth (compare (P_1)), while \( \tau \)-covariance and (fermionic) time-reversal symmetry (properties (P_2) and (P_{3,-})) are inherited from the corresponding symmetries of the Hamiltonian. In particular, several well-established models satisfy the previous Assumption, including the eigenprojectors for the tight-binding Hamiltonians proposed by Fu, Kane and Mele in [KM_1, FK, FKM], as well as in many continuous models. Finally, Assumption 1 is satisfied also in the tight-binding models studied in [GP]: the family of projectors is associated to the vector bundle used by Graf and Porta to define a bulk index, under a suitable identification of the variables \((k_1, k_2)\) with the variables \((k, z)\) appearing in [GP].

For a family of projectors satisfying Assumption 1 it follows from (P_1) that the rank \( m \) of the projectors \( P(k) \) is constant in \( k \). We will assume that \( m < +\infty \); property (P_{3,-}) then gives that \( m \) must be even. Indeed, the formula \((\phi, \psi) := \langle \Theta \phi, \psi \rangle\) for \( \phi, \psi \in \mathcal{H} \) defines a bilinear, skew-symmetric, non-degenerate form on \( \mathcal{H} \); its restriction to \( \text{Ran} \ P(0) \subset \mathcal{H} \) (which is an invariant subspace for the action of \( \Theta \) in view of (P_{3,-})) is then a symplectic form, and a symplectic vector space is necessarily even-dimensional.

The goal of our analysis will be to characterize the possible obstructions to the existence of a continuous symmetric Bloch frame for the family \( \{P(k)\}_{k \in \mathbb{R}^d} \), which we define now.

**Definition 1 ((Symmetric) Bloch frame).** Let \( \{P(k)\}_{k \in \mathbb{R}^d} \) be a family of projectors satisfying Assumption 1 and let also \( \Omega \) be a region in \( \mathbb{R}^d \). A Bloch frame for \( \{P(k)\}_{k \in \mathbb{R}^d} \) on \( \Omega \) is a collection of maps \( \Omega \ni k \mapsto \phi_a(k) \in \mathcal{H}, \ a \in \{1, \ldots, m\} \), such that for all \( k \in \Omega \) the set \( \Phi(k) := \{\phi_1(k), \ldots, \phi_m(k)\} \) is an orthonormal basis spanning \( \text{Ran} \ P(k) \). When \( \Omega = \mathbb{R}^d \), the Bloch frame is said to be global. A Bloch frame is called

(F_0) **continuous** if all functions \( \phi_a : \Omega \to \mathcal{H}, a \in \{1, \ldots, m\} \), are continuous;

(F_1) **smooth** if all functions \( \phi_a : \Omega \to \mathcal{H}, a \in \{1, \ldots, m\} \), are \( C^\infty \)-smooth.

We also say that a global Bloch frame is

(F_2) \( \tau \)-equivariant if

\[
\phi_a(k + \lambda) = \tau(\lambda) \phi_a(k) \quad \text{for all } k \in \mathbb{R}^d, \lambda \in \Lambda, a \in \{1, \ldots, m\};
\]

(F_3) time-reversal invariant if

\[
\phi_b(-k) = \sum_{a=1}^{m} \Theta \phi_a(k) \varepsilon_{ab} \quad \text{for all } k \in \mathbb{R}^d, b \in \{1, \ldots, m\}
\]

for some unitary and skew-symmetric matrix \( \varepsilon = (\varepsilon_{ab})_{1 \leq a,b \leq m} \in U(\mathbb{C}^m), \varepsilon_{ab} = -\varepsilon_{ba} \).

(3) The coordinates \((k_1, \ldots, k_d)\) are expressed in terms of a basis \( \{e_1, \ldots, e_d\} \subset \mathbb{R}^d \) generating the lattice \( \Lambda \) as \( \Lambda = \text{Span}_\mathbb{Z} \{e_1, \ldots, e_d\} \).
A global Bloch frame which is both $\tau$-equivariant and time-reversal invariant is called \textbf{symmetric}.

We are now in position to state our goal: we seek the answer to the following
\begin{center}
\textbf{Question (Q$_d$).} Let $d \leq 3$. Given a family of projectors $\{P(k)\}_{k \in \mathbb{R}^d}$ satisfying Assumption 1 above, is it possible to find a global symmetric Bloch frame for $\{P(k)\}_{k \in \mathbb{R}^d}$, which varies continuously in $k$, i.e. a global Bloch frame satisfying $(F_0)$, $(F_2)$ and $(F_3)$?
\end{center}

We will address this issue via an algorithmic approach. We will show that the existence of such a global continuous symmetric Bloch frame is in general \textbf{topologically obstructed}. Explicitly, the main results of this paper are the following.

\textbf{Theorem 1 (Answer to (Q$_1$)).} Let $d = 1$, and let $\{P(k)\}_{k \in \mathbb{R}}$ be a family of projectors satisfying Assumption 1. Then there exists a global continuous symmetric Bloch frame for $\{P(k)\}_{k \in \mathbb{R}}$, in the sense of Definition 1. Moreover, such Bloch frame can be explicitly constructed.

The proof of Theorem 1 is contained in Section 3.3 (see Remark 4).

\textbf{Theorem 2 (Answer to (Q$_2$)).} Let $d = 2$, and let $\{P(k)\}_{k \in \mathbb{R}^2}$ be a family of projectors satisfying Assumption 1. Then there exists a global continuous symmetric Bloch frame for $\{P(k)\}_{k \in \mathbb{R}^2}$, in the sense of Definition 1, if and only if
\begin{equation}
\delta(P) = 0 \in \mathbb{Z}_2,
\end{equation}
where $\delta(P)$ is defined in (3.16). Moreover, if (2.2) holds, then such Bloch frame can be explicitly constructed.

The proof of Theorem 2, leading to the definition of the $\mathbb{Z}_2$ index $\delta(P)$, is the object of Section 3. Moreover, in Section 3.6 we prove that $\delta(P)$ is actually a \textbf{topological invariant} of the family of projectors (Proposition 4), which agrees with the Fu-Kane index (Theorem 5).

\textbf{Theorem 3 (Answer to (Q$_3$)).} Let $d = 3$, and let $\{P(k)\}_{k \in \mathbb{R}^3}$ be a family of projectors satisfying Assumption 1. Then there exists a global continuous symmetric Bloch frame for $\{P(k)\}_{k \in \mathbb{R}^3}$, in the sense of Definition 1, if and only if
\begin{equation}
\delta_{1,0}(P) = \delta_{1,+}(P) = \delta_{2,+}(P) = \delta_{3,+}(P) = 0 \in \mathbb{Z}_2,
\end{equation}
where $\delta_{1,0}(P)$, $\delta_{1,+}(P)$, $\delta_{2,+}(P)$ and $\delta_{3,+}(P)$ are defined in (6.1). Moreover, if (2.3) holds, then such Bloch frame can be explicitly constructed.

The proof of Theorem 3 leading to the definition of the four $\mathbb{Z}_2$ invariants $\delta_{1,0}(P), \delta_{1,+}(P), \delta_{2,+}(P)$ and $\delta_{3,+}(P)$, is the object of Section 6.

\textbf{Remark 1 (Smooth Bloch frames).} Since the family of projectors $\{P(k)\}_{k \in \mathbb{R}^d}$ satisfies the smoothness assumption $[P_1]$ one may ask whether global \textbf{smooth} symmetric Bloch frames exist for $\{P(k)\}_{k \in \mathbb{R}^d}$, i.e. global Bloch frames satisfying $(F_1)$.
We show in Appendix A that, whenever a global continuous symmetric Bloch frame exists, then one can also find an arbitrarily close frame which is also smooth.

2.2. Properties of the reshuffling matrix $\varepsilon$ and geometric reinterpretation.

We introduce some further notation. Let $\text{Fr}(m, \mathcal{H})$ denote the set of $m$-frames, namely $m$-tuples of orthonormal vectors in $\mathcal{H}$. If $\Phi = \{\phi_1, \ldots, \phi_m\}$ is an $m$-frame, then we can obtain a new frame in $\text{Fr}(m, \mathcal{H})$ by means of a unitary matrix $M \in \mathcal{U}(\mathbb{C}^m)$, setting

$$(\Phi \bowtie M)_b := \sum_{a=1}^{m} \phi_a M_{ab}.$$  

This defines a free right action $\bowtie$ of $\mathcal{U}(\mathbb{C}^m)$ on $\text{Fr}(m, \mathcal{H})$.

Moreover, we can extend the action of the unitary $\tau(\lambda) \in \mathcal{U}(\mathcal{H})$, $\lambda \in \Lambda$, and of the time-reversal operator $\Theta : \mathcal{H} \to \mathcal{H}$ to $m$-frames, by setting

$$(\tau_\lambda \Phi)_a := \tau(\lambda) \phi_a \quad \text{and} \quad (\Theta \Phi)_a := \Theta \phi_a \quad \text{for} \quad \Phi = \{\phi_1, \ldots, \phi_m\} \in \text{Fr}(m, \mathcal{H}).$$

The unitary $\tau_\lambda$ commutes with the $\mathcal{U}(\mathbb{C}^m)$-action, i.e.

$$\tau_\lambda (\Phi \bowtie M) = (\tau_\lambda \Phi) \bowtie M, \quad \text{for all} \quad \Phi \in \text{Fr}(m, \mathcal{H}), M \in \mathcal{U}(\mathbb{C}^m),$$

because $\tau(\lambda)$ is a linear operator on $\mathcal{H}$. Notice instead that, by the antilinearity of $\Theta$, one has

$$\Theta (\Phi \bowtie M) = (\Theta \Phi) \bowtie M, \quad \text{for all} \quad \Phi \in \text{Fr}(m, \mathcal{H}), M \in \mathcal{U}(\mathbb{C}^m).$$

We can recast properties $(F_2)$ and $(F_3)$ for a global Bloch frame in this notation as

$$(F'_2) \quad \Phi(k + \lambda) = \tau_\lambda \Phi(k), \quad \text{for all} \quad k \in \mathbb{R}^d$$

and

$$(F'_3) \quad \Phi(-k) = \Theta \Phi(k) \bowtie \varepsilon, \quad \text{for all} \quad k \in \mathbb{R}^d.$$  

Remark 2 (Compatibility conditions on $\varepsilon$). Observe that, by antunitarity of $\Theta$, we have that for all $\phi \in \mathcal{H}$

$$(2.4) \quad \langle \Theta \phi, \phi \rangle = \langle \Theta^2 \phi, \phi \rangle = -\langle \Theta \phi, \phi \rangle$$

and hence $\langle \Theta \phi, \phi \rangle = 0$; the vectors $\phi$ and $\Theta \phi$ are always orthogonal. This motivates the presence of the “reshuffling” unitary matrix $\varepsilon$ in $(F_3)$, the naïve definition of time-reversal symmetric Bloch frame, namely $\phi_a(-k) = \Theta \phi_a(k)$, would be incompatible with the fact that the vectors $\{\phi_a(k)\}_{a=1,\ldots,m}$ form a basis for $\text{Ran} \ P(k)$ for example at $k = 0$. Notice, however, that if property $(P_{3,-})$ is replaced by

$$(P_{3,+}) \quad \Theta^2 = 1_\mathcal{H} \quad \text{and} \quad P(-k) = \Theta P(k)\Theta^{-1},$$

$\varepsilon$ This terminology means that $\Phi \bowtie 1 = \Phi$, $(\Phi \bowtie M_1) \bowtie M_2 = \Phi \bowtie (M_1 M_2)$ and that if $\Phi \bowtie M_1 = \Phi \bowtie M_2$ then $M_1 = M_2$, for all $\Phi \in \text{Fr}(m, \mathcal{H})$ and $M_1, M_2 \in \mathcal{U}(\mathbb{C}^m)$.
then (2.4) does not hold anymore, and one can indeed impose the compatibility of a Bloch frame $\Phi$ with the time-reversal operator by requiring that $\Phi(-k) = \Theta \Phi(k)$. Indeed, one can show [FMP] that under this modified assumption there is no topological obstruction to the existence of a global smooth symmetric Bloch frame for all $d \leq 3$.

We have thus argued why the presence of the reshuffling matrix $\varepsilon$ in condition \([F_3]\) is necessary. The further assumption of skew-symmetry on $\varepsilon$ is motivated as follows. Assume that $\Phi = \{\Phi(k)\}_{k \in \mathbb{R}^d}$ is a time-reversal invariant Bloch frame. Consider Equation (F′4) with $k$ and $-k$ exchanged, and act on the right with $\varepsilon^{-1}$ to both sides, to obtain
\[
\Phi(k) \triangleleft \varepsilon^{-1} = \Theta \Phi(-k).
\]
Substituting again the expression in (F′4) for $\Phi(-k)$ on the right-hand side of the above equality, one obtains
\[
\Phi(k) \triangleleft \varepsilon^{-1} = \Theta (\Theta \Phi(k) \triangleleft \varepsilon) = (\Theta^2 \Phi(k)) \triangleleft \varepsilon = \Phi(k) \triangleleft (-\varepsilon)
\]
and hence we deduce that $\varepsilon^{-1} = -\varepsilon$. On the other hand, by unitarity $\varepsilon^{-1} = \varepsilon^T$ and hence $\varepsilon^T = -\varepsilon$. So $\varepsilon$ must be not only unitary, but also skew-symmetric. In particular $\varepsilon \varepsilon = -\mathbf{1}$.

Notice that, according to [Hua, Theorem 7], the matrix $\varepsilon$, being unitary and skew-symmetric, can be put in the form
\[
\begin{pmatrix}
0 & 1 \\
-1 & 0
\end{pmatrix} \oplus \cdots \oplus 
\begin{pmatrix}
0 & 1 \\
-1 & 0
\end{pmatrix}
\]
in a suitable orthonormal basis. Hence, up to a reordering of such basis, there is no loss of generality in assuming that $\varepsilon$ is in the standard symplectic form (2.5)
\[
\varepsilon = \begin{pmatrix}
0 & \mathbb{1}_n \\
-\mathbb{1}_n & 0
\end{pmatrix}
\]
where $n = m/2$ (remember that $m$ is even). We will make use of this fact later on.

**Remark 3 (Geometric reinterpretation).** Let us recast the above definitions in a more geometric language. Given a smooth and $\tau$-covariant family of projectors $\{P(k)\}_{k \in \mathbb{R}^d}$ one can construct a vector bundle $\mathcal{P} \to \mathbb{T}^d$, called the Bloch bundle, having the (Brillouin) $d$-torus $\mathbb{T}^d := \mathbb{R}^d/\Lambda$ as base space, and whose fibre over the point $k \in \mathbb{T}^d$ is the vector space $\text{Ran} P(k)$ (see [Pa, Section 2.1] for details). The main result in [Pa] (see also [MP]) is that, if $d \leq 3$ and if $\{P(k)\}_{k \in \mathbb{R}^d}$ is also time-reversal symmetric, then the Bloch bundle $\mathcal{P} \to \mathbb{T}^d$ is trivial, in the category of $C^\infty$-smooth vector bundles. This is equivalent to the existence of a global $\tau$-equivariant Bloch frame: this can be seen as a section of the frame bundle $\text{Fr}(\mathcal{P}) \to \mathbb{T}^d$.

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(5) The presence of a “symplectic” condition may seem unnatural in the context of complex Hilbert spaces. A more abstract viewpoint, based on quiver-theoretic techniques, can indeed motivate the appearance of the standard symplectic matrix [CFMP].
\( \mathbb{T}^d \), which is the principal \( \mathcal{U}(\mathbb{C}^m) \)-bundle whose fibre over the point \( k \in \mathbb{T}^d \) is the set of orthonormal frames in \( \text{Ran} \, P(k) \).

The time-reversal operator \( \Theta \) induces by restriction a (non-vertical) automorphism of \( P \), i.e. a morphism

\[
\begin{array}{ccc}
\mathcal{P} & \xrightarrow{\widehat{\Theta}} & \mathcal{P} \\
\downarrow & & \downarrow \\
\mathbb{T}^d & \xrightarrow{\theta} & \mathbb{T}^d
\end{array}
\]

where \( \theta : \mathbb{T}^d \rightarrow \mathbb{T}^d \) denotes the involution \( \theta(k) = -k \). This means that a vector in the fibre \( \text{Ran} \, P(k) \) is mapped via \( \widehat{\Theta} \) into a vector in the fibre \( \text{Ran} \, P(-k) \). The morphism \( \widehat{\Theta} : \mathcal{P} \rightarrow \mathcal{P} \) still satisfies \( \widehat{\Theta}^2 = -1 \), i.e. it squares to the vertical automorphism of \( P \) acting fibrewise by multiplication by \(-1\). ∎
3. Construction of a symmetric Bloch frame in 2d

In this Section, we tackle Question (Q_d) stated in Section 2.1 for \( d = 2 \).

3.1. Effective unit cell, vertices and edges. Consider the unit cell

\[
\mathbb{B} := \left\{ k = \sum_{j=1}^{2} k_j e_j \in \mathbb{R}^2 : -\frac{1}{2} \leq k_i \leq \frac{1}{2}, \ i = 1, 2 \right\}.
\]

Points in \( \mathbb{B} \) give representatives for the quotient Brillouin torus \( \mathbb{T}^2 = \mathbb{R}^2 / \Lambda \), i.e. any point \( k \in \mathbb{R}^2 \) can be written (in an a.e.-unique way) as \( k = k' + \lambda \), with \( k' \in \mathbb{B} \) and \( \lambda \in \Lambda \).

Properties \([P_2]\) and \([P_{3,-}\)] for a family of projections reflect the relevant symmetries of \( \mathbb{R}^2 \): the already mentioned inversion symmetry \( \theta(k) = -k \) and the translation symmetries \( t_\lambda(k) = k + \lambda \), for \( \lambda \in \Lambda \). These transformations satisfy the commutation relation \( \theta t_\lambda = t_{-\lambda} \theta \) (compare the analogue property \([P_4]\) at the level of operators on \( \mathcal{H} \)). Consequently, they form a subgroup of the affine group \( \text{Aut}(\mathbb{R}^2) \), consisting of the set \( \{t_\lambda, \theta t_\lambda\}_{\lambda \in \Lambda} \). Periodicity (or rather, \( \tau \)-covariance) for families of projectors and, correspondingly, Bloch frames allows one to focus one’s attention to points \( k \in \mathbb{B} \). Implementing also the inversion or time-reversal symmetry restricts further the set of points to be considered to the effective unit cell

\[
\mathbb{B}_{\text{eff}} := \{ k = (k_1, k_2) \in \mathbb{B} : k_1 \geq 0 \}.
\]

A more precise statement is contained in Proposition \([\dagger]\). Let us first introduce some further terminology. We define the vertices of the effective unit cell to be the points \( k_\lambda \in \mathbb{B}_{\text{eff}} \) which are fixed by the transformation \( t_\lambda \theta \). One immediately realizes that

\[
t_\lambda \theta(k_\lambda) = k_\lambda \iff k_\lambda = \frac{1}{2} \lambda,
\]

i.e. vertices have half-integer components in the basis \( \{e_1, e_2\} \). Thus, the effective unit cell contains exactly six vertices, all of which fall on its boundary, namely

\[
v_1 = (0, 0), \quad v_2 = (0, -\frac{1}{2}), \quad v_3 = \left( \frac{1}{2}, -\frac{1}{2} \right),
\]

\[
v_4 = \left( \frac{1}{2}, 0 \right), \quad v_5 = \left( \frac{1}{2}, \frac{1}{2} \right), \quad v_6 = \left( 0, \frac{1}{2} \right).
\]

We also introduce the oriented edges \( E_i \), joining two consecutive vertices \( v_i \) and \( v_{i+1} \) (the index \( i \) must be taken modulo 6).

The following extension result allows us to reduce the problem of the existence of a global continuous symmetric Bloch frame to that of a Bloch frame defined only on the effective unit cell \( \mathbb{B}_{\text{eff}} \), satisfying further conditions on its boundary.
Figure 1. The effective unit cell (shaded area), its vertices and its edges. We use adapted coordinates \((k_1, k_2)\) such that \(k = k_1 e_1 + k_2 e_2\).

**Proposition 1.** Let \(\{P(k)\}_{k \in \mathbb{R}^2}\) be a family of orthogonal projectors satisfying Assumption [4]. Assume that there exists a global continuous symmetric Bloch frame \(\Phi = \{\Phi(k)\}_{k \in \mathbb{R}^2}\) for \(\{P(k)\}_{k \in \mathbb{R}^2}\). Then \(\Phi\) satisfies the vertex conditions

\[
\Phi(k_\lambda) = \tau_\lambda \Theta \Phi(k_\lambda) \triangleleft \varepsilon, \quad k_\lambda \in \{v_1, \ldots, v_6\}
\]

and the edge symmetries

\[
\Phi(\theta(k)) = \Theta \Phi(k) \triangleleft \varepsilon \quad \text{for } k \in E_1 \cup E_6,
\]
\[
\Phi(e_2(k)) = \tau_{e_2} \Phi(k) \quad \text{for } k \in E_2,
\]
\[
\Phi(t_{-e_1}(k)) = \tau_{-e_1} \Theta \Phi(k) \triangleleft \varepsilon \quad \text{for } k \in E_3 \cup E_4,
\]
\[
\Phi(t_{-e_2}(k)) = \tau_{-e_2} \Phi(k) \quad \text{for } k \in E_5.
\]

Conversely, let \(\Phi_{\text{eff}} = \{\Phi_{\text{eff}}(k)\}_{k \in \mathbb{B}_{\text{eff}}}\) be a continuous Bloch frame for \(\{P(k)\}_{k \in \mathbb{R}^2}\), defined on the effective unit cell \(\mathbb{B}_{\text{eff}}\) and satisfying the vertex conditions (V) and the edge symmetries (E). Then there exists a global continuous symmetric Bloch frame \(\Phi\) whose restriction to \(\mathbb{B}_{\text{eff}}\) coincides with \(\Phi_{\text{eff}}\).

**Proof.** Let \(\Phi\) be a global Bloch frame as in the statement of the Proposition. Then conditions [4]' and [4]' imply that at the six vertices

\[
\Phi(k_\lambda) = \Phi(t_{\lambda} \theta(k_\lambda)) = \tau_\lambda \Phi(\theta(k_\lambda)) = \tau_\lambda \Theta \Phi(k_\lambda) \triangleleft \varepsilon,
\]
that is, Φ satisfies the vertex conditions \((\mathbb{V})\). The edge symmetries \((\mathbb{E})\) can be checked similarly, again by making use of \((\mathbb{F}'_3)\) and \((\mathbb{F}'_4)\).

Conversely, assume that a continuous Bloch frame \(\Phi_{\text{eff}}\) is given on \(\mathcal{B}_{\text{eff}}\), and satisfies \((\mathbb{V})\) and \((\mathbb{E})\). We extend the definition of \(\Phi_{\text{eff}}\) to the unit cell \(\mathcal{B}\) by setting

\[
\Phi_{\text{uc}}(k) := \begin{cases} 
\Phi_{\text{eff}}(k) & \text{if } k \in \mathcal{B}_{\text{eff}}, \\
\Theta \Phi_{\text{eff}}(\theta(k)) \triangleleft \varepsilon & \text{if } k \in \mathcal{B} \setminus \mathcal{B}_{\text{eff}}.
\end{cases}
\]

The definition of \(\Phi_{\text{uc}}\) can in turn be extended to \(\mathbb{R}^2\) by setting

\[
\Phi(k) := \tau_{\lambda} \Phi_{\text{uc}}(k') \quad \text{if } k = k' + \lambda \text{ with } k' \in \mathcal{B}, \lambda \in \Lambda.
\]

The vertex conditions and the edge symmetries ensure that the above defines a global continuous Bloch frame; moreover, by construction Φ is also symmetric, in the sense of Definition 1.

In view of Proposition 1, our strategy to examine Question (Q_2) will be to consider a continuous Bloch frame \(\Psi\) defined over the effective unit cell \(\mathcal{B}_{\text{eff}}\) (whose existence is guaranteed by the fact that \(\mathcal{B}_{\text{eff}}\) is contractible and no further symmetry is required), and try to modify it in order to obtain a new family of frames \(\Phi\), which is defined on the effective unit cell and satisfies also the vertex conditions and the edge symmetries; these allow the above extension procedure to yield a global continuous symmetric Bloch frame. Notice that, since both are orthonormal frames in \(\text{Ran}\ P(k)\), the given Bloch frame \(\Psi(k)\) and the unknown symmetric Bloch frame \(\Phi(k)\) differ by the action of a unitary matrix \(U(k)\):

\[
(3.2) \quad \Phi(k) = \Psi(k) \triangleleft U(k), \quad U(k) \in \mathcal{U}(\mathbb{C}^m).
\]

Thus, we can equivalently treat the family \(\mathcal{B}_{\text{eff}} \ni k \mapsto U(k) \in \mathcal{U}(\mathbb{C}^m)\) as our unknown.

### 3.2. Solving the vertex conditions

Let \(k_{\lambda}\) be one of the six vertices in \(\mathbb{Z}_2\). If \(\Phi\) is a symmetric Bloch frame, then, by Proposition 1, \(\Phi(k_{\lambda})\) satisfies the vertex condition \(\mathbb{V}\), stating the equality between the two frames \(\Phi(k_{\lambda})\) and \(\tau_{\lambda} \Theta \Phi(k_{\lambda}) \triangleleft \varepsilon\).

For a general Bloch frame \(\Psi\), instead, \(\Psi(k_{\lambda})\) and \(\tau_{\lambda} \Theta \Psi(k_{\lambda}) \triangleleft \varepsilon\) may very well be different. Nonetheless, they are both orthonormal frames in \(\text{Ran}\ P(k_{\lambda})\), so there exists a unique unitary matrix \(U_{\text{obs}}(k_{\lambda}) \in \mathcal{U}(\mathbb{C}^m)\) such that

\[
(3.3) \quad \Psi(k_{\lambda}) \triangleleft U_{\text{obs}}(k_{\lambda}) = \tau_{\lambda} \Theta \Psi(k_{\lambda}) \triangleleft \varepsilon.
\]

The obstruction unitary \(U_{\text{obs}}(k_{\lambda})\) must satisfy a compatibility condition. In fact, by applying \(\tau_{\lambda} \Theta\) to both sides of \((3.3)\) we obtain that

\[
\tau_{\lambda} \Theta (\Psi(k_{\lambda}) \triangleleft U_{\text{obs}}(k_{\lambda})) = \tau_{\lambda} \Theta (\tau_{\lambda} \Theta \Psi(k_{\lambda}) \triangleleft \varepsilon) = \\
= \tau_{\lambda} \Theta \tau_{\lambda} \Theta \Psi(k_{\lambda}) \triangleleft \varepsilon = \\
= \tau_{\lambda} \tau_{-\lambda} \Theta^2 \Psi(k_{\lambda}) \triangleleft \varepsilon = \\
= \Psi(k_{\lambda}) \triangleleft (-\varepsilon)
\]
where in the second-to-last equality we used the commutation relation \([\mathcal{P}_4]\). On the other hand, the left-hand side of this equality is also given by
\[
\tau_\lambda \Theta (\Psi(k_\lambda) \triangleleft U_{\text{obs}}(k_\lambda)) = \tau_\lambda \Theta \Psi(k_\lambda) \triangleleft U_{\text{obs}}(k_\lambda) = \\
= (\Psi(k_\lambda) \triangleleft (U_{\text{obs}}(k_\lambda) \varepsilon^{-1})) \triangleleft U_{\text{obs}}(k_\lambda) = \\
= \Psi(k_\lambda) \triangleleft (U_{\text{obs}}(k_\lambda) \varepsilon^{-1} U_{\text{obs}}(k_\lambda))
\]
where in the second equality we used the relation which is obtained acting on the right with \(\varepsilon^{-1}\) on both sides of (3.3). By the freeness of the action of \(\mathcal{U}(\mathbb{C}^m)\) on frames and the fact that \(\varepsilon^{-1} = -\varepsilon\) by Remark \(2\) we deduce that
\[
U_{\text{obs}}(k_\lambda) \varepsilon U_{\text{obs}}(k_\lambda) = \varepsilon, \quad \text{i.e.} \quad U_{\text{obs}}(k_\lambda)^T \varepsilon = \varepsilon U_{\text{obs}}(k_\lambda)
\]
where we have used the fact that \(U_{\text{obs}}(k_\lambda)^{-1} = U_{\text{obs}}(k_\lambda)^T\) by unitarity.

Now, notice that the given Bloch frame \(\Psi(k)\) and the unknown symmetric Bloch frame \(\Phi(k)\), satisfying the vertex condition \((\mathbb{W})\), differ by the action of a unitary matrix \(U(k)\), as in (3.2). We want to relate the obstruction unitary \(U_{\text{obs}}(k_\lambda)\) to the unknown \(U(k_\lambda)\). In order to do so, we rewrite \((\mathbb{W})\) as
\[
\Psi(k_\lambda) \triangleleft U(k_\lambda) = \Phi(k_\lambda) = \tau_\lambda \Theta \Phi(k_\lambda) \triangleleft \varepsilon = \\
= \tau_\lambda \Theta (\Psi(k_\lambda) \triangleleft U(k_\lambda)) \triangleleft \varepsilon = \\
= \tau_\lambda (\Theta \Psi(k_\lambda) \triangleleft U(k_\lambda)) \triangleleft \varepsilon = \\
= \tau_\lambda \Theta \Psi(k_\lambda) \triangleleft (U(k_\lambda) \varepsilon) = \\
= (\Psi(k_\lambda) \triangleleft (U_{\text{obs}}(k_\lambda) \varepsilon^{-1})) \triangleleft (U(k_\lambda) \varepsilon) = \\
= \Psi(k_\lambda) \triangleleft (U_{\text{obs}}(k_\lambda) \varepsilon^{-1} U(k_\lambda) \varepsilon).
\]
Again by the freeness of the \(\mathcal{U}(\mathbb{C}^m)\)-action, we conclude that
\[
U(k_\lambda) = U_{\text{obs}}(k_\lambda) \varepsilon^{-1} U(k_\lambda) \varepsilon, \quad \text{i.e.} \quad U_{\text{obs}}(k_\lambda) = U(k_\lambda) \varepsilon^{-1} U(k_\lambda)^T \varepsilon.
\]

The next Lemma establishes the equivalence between the two conditions (3.4) and (3.5).

**Lemma 1.** Let \(\varepsilon \in \mathcal{U}(\mathbb{C}^m) \cap \Lambda^2 \mathbb{C}^m\) be a unitary and skew-symmetric matrix. The following conditions on a unitary matrix \(V \in \mathcal{U}(\mathbb{C}^m)\) are equivalent:

(a) \(V\) is such that \(V^T \varepsilon = \varepsilon V\);

(b) there exists a matrix \(U \in \mathcal{U}(\mathbb{C}^m)\) such that \(V = U \varepsilon^{-1} U^T \varepsilon\).

**Proof.**

**Step 1:** (b) \(\Rightarrow\) (a). Suppose \(V = U \varepsilon^{-1} U^T \varepsilon\). Then
\[
V^T \varepsilon = \varepsilon^T U (\varepsilon^{-1})^T U^T \varepsilon = (-\varepsilon) U (-\varepsilon^{-1}) U^T \varepsilon = \varepsilon U \varepsilon^{-1} U^T \varepsilon = \varepsilon V,
\]

**Step 2:** (a) \(\Rightarrow\) (b). Every unitary matrix can be diagonalized by means of a unitary transformation. Hence there exist a unitary matrix \(W \in \mathcal{U}(\mathbb{C}^m)\) and a diagonal matrix \(\Lambda = \text{diag}(\lambda_1, \ldots, \lambda_m)\) such that
\[
V = WE^{i\Lambda}W^*.
\]
where the collection \( \{ e^{i\lambda_1}, \ldots, e^{i\lambda_m} \} \) forms the spectrum of \( V \). The condition \( V^T \epsilon = \epsilon V \) is then equivalent to

\[
\prod \epsilon W^A W^T \epsilon = \epsilon W e^{iA} W^* \quad \iff \quad e^{iA} W^T \epsilon W = W^T \epsilon W e^{iA},
\]

i.e. the matrix \( A := W^T \epsilon W \) commutes with the diagonal matrix \( e^{iA} \).

According to [Hua, Lemma in §6], for every unitary matrix \( Z \) there exists a unitary matrix \( Y \) such that \( Y^2 = Z \) and that \( YB = BY \) whenever \( ZB = BZ \). We can apply this fact in the case where \( Z = e^{iA} \) is diagonal, and give an explicit form of \( Y \): Normalize the arguments \( \lambda_i \) of the eigenvalues of \( V \) so that \( \lambda_i \in [0, 2\pi) \), and define \( Y := e^{iA/2} = \text{diag}(e^{i\lambda_1/2}, \ldots, e^{i\lambda_m/2}) \).

We claim now that the matrix

\[
U := We^{iA/2}W^*
\]

(which is clearly unitary, as it is a product of unitary matrices) satisfies condition \((b)\) in the statement of the Lemma. Indeed, upon multiplying by \( WW^* = 1 \), we get that

\[
U \epsilon^{-1} U^T \epsilon = We^{iA/2}W^* \epsilon^{-1} W e^{iA/2} W^T \epsilon WW^* = W e^{iA/2} A^{-1} e^{iA/2} A W^* = W e^{iA} W^* = V.
\]

This concludes the proof of the Lemma.

The above result allows us to solve the vertex condition, or equivalently the equation \((3.5)\) for \( U(k\lambda) \), by applying Lemma 1 to \( V = U_{\text{obs}}(k\lambda) \) and \( U = U(k\lambda) \).

3.3. Extending to the edges. To extend the definition of the symmetric Bloch frame \( \Phi(k) \) (or equivalently of the matrix \( U(k) \) appearing in \((3.2)\)) also for \( k \) on the edges \( E_i \) which constitute the boundary \( \partial \mathbb{B}_{\text{eff}} \), we use the path-connectedness of the group \( \mathcal{U}(\mathbb{C}^m) \). Indeed, the latter fact implies that we can choose a continuous path \((6)\) \( W_i : [0, 1/2] \to \mathcal{U}(\mathbb{C}^m) \) such that \( W_i(0) = U(v_i) \) and \( W_i(1/2) = U(v_{i+1}) \), where \( v_i \) and \( v_{i+1} \) are the end-points of the edge \( E_i \). Now set

\[
\tilde{U}(k) := \begin{cases} 
W_1(-k_2) & \text{if } k \in E_1, \\
W_2(k_1) & \text{if } k \in E_2, \\
W_3(k_2 + 1/2) & \text{if } k \in E_3.
\end{cases}
\]

\[(6)\] Explicitly, a continuous path of unitaries \( W : [0, 1/2] \to \mathcal{U}(\mathbb{C}^m) \) connecting two unitary matrices \( U_1 \) and \( U_2 \) can be constructed as follows. Diagonalize \( U_1^{-1} U_2 = PD P^* \), where \( D = \text{diag}(e^{i\beta_1}, \ldots, e^{i\beta_m}) \) and \( P \in \mathcal{U}(\mathbb{C}^m) \). For \( t \in [0, 1/2] \) set

\[
W(t) = U_1 D_1 P^*, \quad \text{where} \quad D_1 := \text{diag}(e^{2\beta_1 t}, \ldots, e^{2\beta_m t}).
\]

One easily realizes that \( W(0) = U_1 \), \( W(1/2) = U_2 \) and \( W(t) \) depends continuously on \( t \), as required.
In this way we obtain a continuous map \( \hat{U} : E_1 \cup E_2 \cup E_3 \rightarrow U(\mathbb{C}^m) \). Let \( \hat{\Phi}(k) := \Psi(k) \langle \hat{U}(k) \) for \( k \in E_1 \cup E_2 \cup E_3 \); we extend this frame to a \( \tau \)-equivariant, time-reversal invariant frame on \( \partial \mathbb{B}_{\text{eff}} \) by setting

\[
\hat{\Phi}(k) := \begin{cases} 
\tilde{\Phi}(k) & \text{if } k \in E_1 \cup E_2 \cup E_3, \\
\tau_{e_1} \tilde{\Phi}(\theta t_{-e_1}(k)) \circ \varepsilon & \text{if } k \in E_4, \\
\tau_{e_2} \tilde{\Phi}(t_{-e_2}(k)) & \text{if } k \in E_5, \\
\Theta \tilde{\Phi}(\theta(k)) \circ \varepsilon & \text{if } k \in E_6.
\end{cases}
\]

By construction, \( \hat{\Phi}(k) \) satisfies all the edge symmetries for a symmetric Bloch frame \( \Phi \) listed in \([\mathbb{F}]\), as one can immediately check.

**Remark 4 (Proof of Theorem \([\mathbb{F}]\)).** The above argument also shows that, when \( d = 1 \), global continuous symmetric Bloch frames for a family of projectors \( \{P(k)\}_{k \in \mathbb{R}} \) satisfying Assumption \([\mathbb{F}]\) can always be constructed. Indeed, the edge \( E_1 \cup E_6 \) can be regarded as a 1-dimensional unit cell \( \mathbb{B}^{(1)} \), and the edge symmetries on it coincide exactly with properties \([\mathbb{F}_2]\) and \([\mathbb{F}_3]\). Thus, by forcing \( \tau \)-equivariance, one can extend the definition of the frame continuously on the whole \( \mathbb{R} \), as in the proof of Proposition \([\mathbb{F}]\). Hence, this proves Theorem \([\mathbb{F}]\). \(\diamondsuit\)

3.4. Extending to the face: a \( \mathbb{Z}_2 \) obstruction. In order to see whether it is possible to extend the frame \( \tilde{\Phi} \) to a continuous symmetric Bloch frame \( \Phi \) defined on the whole effective unit cell \( \mathbb{B}_{\text{eff}} \), we first introduce the unitary map \( \hat{U}(k) \) which maps the input frame \( \Psi(k) \) to the frame \( \hat{\Phi}(k) \), i.e. such that

\[
\hat{\Phi}(k) = \Psi(k) \langle \hat{U}(k), \quad k \in \partial \mathbb{B}_{\text{eff}}
\]

(compare \([3.2]\)). This defines a continuous map \( \hat{U} : \partial \mathbb{B}_{\text{eff}} \rightarrow U(\mathbb{C}^m) \); we are interested in finding a continuous extension \( U : \mathbb{B}_{\text{eff}} \rightarrow U(\mathbb{C}^m) \) of \( \hat{U} \) to the effective unit cell.

From a topological viewpoint, \( \partial \mathbb{B}_{\text{eff}} \) is homeomorphic to a circle \( S^1 \). It is well-known \([\text{DNF}]\) Thm. 17.3.1] that, if \( X \) is a topological space, then a continuous map \( f : S^1 \rightarrow X \) defines an element in the fundamental group \( \pi_1(X) \) by taking its homotopy class \([f]\). Moreover, \( f \) extends to a continuous map \( F : D^2 \rightarrow X \), where \( D^2 \) is the 2-dimensional disc enclosed by the circle \( S^1 \), if and only if \([f] \in \pi_1(X) \) is the trivial element. In our case, the space \( X \) is the group \( U(\mathbb{C}^m) \), and it is also well-known \([\text{Hus}]\) Ch. 8, Sec. 12] that the exact sequence of groups

\[
1 \longrightarrow \mathbb{R}U(\mathbb{C}^m) \longrightarrow U(\mathbb{C}^m) \xrightarrow{\text{det}} U(1) \longrightarrow 1
\]

induces an isomorphism \( \pi_1(U(\mathbb{C}^m)) \simeq \pi_1(U(1)) \). On the other hand, the degree homomorphism \([\text{DNF}]\) §13.4(b)]

\[
\deg : \pi_1(U(1)) \simeq \mathbb{Z}, \quad [\varphi : S^1 \rightarrow U(1)] \mapsto \frac{1}{2\pi i} \oint_{S^1} dz \partial_z \log \varphi(z)
\]
establishes an isomorphism of groups $\pi_1(U(1)) \simeq \mathbb{Z}$. We conclude that a continuous map $f : \partial B_{\text{eff}} \to U(\mathbb{C}^m)$ can be continuously extended to $F : B_{\text{eff}} \to U(\mathbb{C}^m)$ if and only if $\text{deg}([\det f]) \in \mathbb{Z}$ is zero.

In our case, we want to extend the continuous map $U : \partial B_{\text{eff}} \to U(C_m)$ to the whole effective unit cell $B_{\text{eff}}$. However, rather than checking whether $\text{deg}([\det \hat{U}])$ vanishes, it is sufficient to find a unitary-matrix-valued map that “unwinds” the determinant of $\hat{U}(k)$, while preserving the relevant symmetries on Bloch frames. More precisely, the following result holds.

**Proposition 2.** Let $\Phi$ be the Bloch frame defined on $\partial B_{\text{eff}}$ that appears in (3.7), satisfying the vertex conditions $[\text{V}]$ and the edge symmetries $[\text{E}]$. Assume that there exists a continuous map $X : \partial B_{\text{eff}} \to U(C_m)$ such that

- $(X_1)$ $\text{deg}([\det X]) = -\text{deg}([\det \hat{U}])$, and
- $(X_2)$ also the frame $\Phi \triangleleft X$ satisfies $[\text{V}]$ and $[\text{E}]$.

Then there exists a global continuous symmetric Bloch frame $\Phi$ that extends $\hat{\Phi} \triangleleft X$ to the whole $\mathbb{R}^2$.

Conversely, if $\Phi$ is a global continuous symmetric Bloch frame, then its restriction to $\partial B_{\text{eff}}$ differs from $\hat{\Phi}$ by the action of a unitary-matrix-valued continuous map $X$, satisfying $(X_1)$ and $(X_2)$ above.

**Proof.** If a map $X$ as in the statement of the Proposition exists, then the map $U := \hat{U}X : \partial B_{\text{eff}} \to U(\mathbb{C}^m)$ satisfies $\text{deg}([\det U]) = 0$ (because $\text{deg}$ is a group homomorphism), and hence extends continuously to $U_{\text{eff}} : B_{\text{eff}} \to U(\mathbb{C}^m)$. This allows to define a continuous symmetric Bloch frame $\Phi_{\text{eff}}(k) := \Psi(k) \triangleleft U_{\text{eff}}(k)$ on the whole effective unit cell $B_{\text{eff}}$, and by Proposition 1 such definition can be then extended continuously to $\mathbb{R}^2$ to obtain the desired global continuous symmetric Bloch frame $\Phi$.

Conversely, if a global continuous symmetric Bloch frame $\Phi$ exists, then its restriction $\Phi_{\text{eff}}$ to the boundary of the effective unit cell satisfies $\Phi_{\text{eff}}(k) = \Psi(k) \triangleleft U_{\text{eff}}(k)$ for some unitary matrix $U_{\text{eff}}(k) \in U(\mathbb{C}^m)$, and moreover $\text{deg}([\det U_{\text{eff}}]) = 0$ because $U_{\text{eff}} : \partial B_{\text{eff}} \to U(\mathbb{C}^m)$ extends to the whole effective unit cell. From (3.7) we deduce that $\Phi_{\text{eff}}(k) = \hat{\Phi}(k) \triangleleft (\hat{U}(k)^{-1}U_{\text{eff}}(k))$; the unitary matrix $X(k) := \hat{U}(k)^{-1}U_{\text{eff}}(k)$ then satisfies $\text{deg}([\det X]) = -\text{deg}([\det \hat{U}])$, and, when restricted to $\partial B_{\text{eff}}$, both $\Phi_{\text{eff}}$ and $\hat{\Phi}$ have the same symmetries, namely $[\text{V}]$ and $[\text{E}]$.

Proposition 2 reduces the question of existence of a global continuous symmetric Bloch frame to that of existence of a continuous map $X : \partial B_{\text{eff}} \to U(\mathbb{C}^m)$ satisfying conditions $[X_1]$ and $[X_2]$. We begin by imposing condition $[X_2]$ on $X$, and then check its compatibility with $[X_1]$.

We spell out explicitly what it means for the Bloch frame $\hat{\Phi} \triangleleft X$ to satisfy the edge symmetries $[\text{E}]$, provided that $\hat{\Phi}$ satisfies them. For $k = (0, k_2) \in E_1 \cup E_6$, we
obtain that
\[
\hat{\Phi}(0, -k_2) \triangleleft X(0, -k_2) = \Theta \left( \hat{\Phi}(0, k_2) \triangleleft X(0, k_2) \right) \triangleleft \varepsilon
\]
\[
\downarrow
\]
\[
(\Theta \hat{\Phi}(0, k_2) \triangleleft \varepsilon) \triangleleft X(0, -k_2) = (\Theta \hat{\Phi}(0, k_2) \triangleleft \overline{X}(0, k_2)) \triangleleft \varepsilon
\]
\[
\downarrow
\]
\[
\Theta \hat{\Phi}(0, k_2) \triangleleft (\varepsilon X(0, -k_2)) = \Theta \hat{\Phi}(0, k_2) \triangleleft (\overline{X}(0, k_2) \varepsilon)
\],
by which we deduce that
\[
(3.9) \quad \varepsilon X(0, -k_2) = \overline{X}(0, k_2) \varepsilon, \quad k_2 \in [-1/2, 1/2].
\]
Similarly, for \( k = (1/2, k_2) \in E_3 \cup E_4 \), we obtain
\[
\hat{\Phi}(1/2, -k_2) \triangleleft X(1/2, -k_2) = \tau_{e_1} \Theta \left( \hat{\Phi}(1/2, k_2) \triangleleft X(1/2, k_2) \right) \triangleleft \varepsilon
\]
\[
\downarrow
\]
\[
(\tau_{e_1} \Theta \hat{\Phi}(1/2, k_2) \triangleleft \varepsilon) \triangleleft X(1/2, -k_2) = (\tau_{e_1} \Theta \hat{\Phi}(1/2, k_2) \triangleleft \overline{X}(1/2, k_2)) \triangleleft \varepsilon
\]
\[
\downarrow
\]
\[
\tau_{e_1} \Theta \hat{\Phi}(1/2, k_2) \triangleleft (\varepsilon X(1/2, -k_2)) = \tau_{e_1} \Theta \hat{\Phi}(1/2, k_2) \triangleleft (\overline{X}(1/2, k_2) \varepsilon)
\],
by which we deduce that
\[
(3.10) \quad \varepsilon X(1/2, -k_2) = \overline{X}(1/2, k_2) \varepsilon, \quad k_2 \in [-1/2, 1/2].
\]
Finally, the conditions \([E]\) for \( k \in E_2 \) and \( k \in E_5 \) are clearly the inverse one of each other, so we can treat both at once. For \( k = (k_1, 1/2) \in E_5 \), we obtain that
\[
\hat{\Phi}(k_1, -1/2) \triangleleft X(k_1, -1/2) = \tau_{-e_2} \left( \hat{\Phi}(k_1, 1/2) \triangleleft X(k_1, 1/2) \right)
\]
\[
\downarrow
\]
\[
(\tau_{-e_2} \hat{\Phi}(k_1, 1/2)) \triangleleft X(k_1, -1/2) = (\tau_{-e_2} \hat{\Phi}(k_1, 1/2)) \triangleleft X(k_1, 1/2)
\]
by which we deduce that
\[
(3.11) \quad X(k_1, -1/2) = X(k_1, 1/2), \quad k_1 \in [0, 1/2].
\]
Thus we have shown that condition \([X_2]\) on \( X \) is equivalent to the relations \((3.9), (3.10)\) and \((3.11)\). Notice that these contain also the relations satisfied by \( X(k) \) at the vertices \( k = k_\lambda \), which could be obtained by imposing that the frame \( \hat{\Phi} \triangleleft X \) satisfies the vertex conditions \([V]\) whenever \( \hat{\Phi} \) does. Explicitly, these relations on \( X(k_\lambda) \) read
\[
(3.12) \quad \varepsilon X(k_\lambda) = \overline{X}(k_\lambda) \varepsilon, \quad i.e. \quad X(k_\lambda)^\top \varepsilon X(k_\lambda) = \varepsilon.
\]
This relation has interesting consequences. Indeed, in view of Remark \([2]\) we may assume that \( \varepsilon \) is in the standard symplectic form \((2.6)\). Then \((3.12)\) implies that
the matrices $X(k_{\lambda})$ belong to the symplectic group $\text{Sp}(2n, \mathbb{C})$. As such, they must be unimodular, i.e.

$$\det X(k_{\lambda}) = 1.$$ 

(3.13)

We now proceed in establishing how the properties on $X$ we have deduced from $(X_2)$ influence the possible values that the degree of the map $\xi := \det X : \partial B_{\text{eff}} \to U(1)$ can attain. We use the formula in (3.8) to evaluate such degree. The integral on the boundary $\partial B_{\text{eff}}$ of the effective unit cell splits as the sum of the integrals over the oriented edges $E_1, \ldots, E_6$:

$$\deg([\xi]) = \frac{1}{2\pi i} \int_{\partial B_{\text{eff}}} dz \partial z \log \det X(z) = \sum_{i=1}^{6} \frac{1}{2\pi i} \int_{E_i} dz \partial z \log \det X(z).$$

Our first observation is that all the summands on the right-hand side of the above equality are integers. Indeed, from (3.13) we deduce that all maps $\xi_i := \det X|_{E_i} : E_i \to U(1)$, $i = 1, \ldots, 6$, are indeed periodic, and hence have well-defined degrees: these are evaluated exactly by the integrals appearing in the above sum. We will denote by $S^1_i$ the edge $E_i$ with its endpoints identified: we have thus established that

$$\deg([\xi]) = \sum_{i=1}^{6} \frac{1}{2\pi i} \int_{S^1_i} dz \partial z \log \det X(z) = \sum_{i=1}^{6} \deg([\xi_i]).$$

(3.14)

From Equation (3.11), the integrals over $E_2$ and $E_5$ compensate each other, because the integrands are the same but the orientations of the two edges are opposite. We thus focus our attention on the integrals over $S^1_3$ and $S^1_4$ (respectively on $S^1_3$ and $S^1_4$). From Equations (3.9) and (3.10), we deduce that if $k_* \in \{0, 1/2\}$ then

$$X(k_*, k_2) = \varepsilon X(k_*, -k_2) \varepsilon^{-1}$$

which implies in particular that

$$(\det X(k_*, k_2))^{-1} = \overline{\det X(k_*, k_2)} = \det \left( \varepsilon X(k_*, -k_2) \varepsilon^{-1} \right) = \det X(k_*, -k_2)$$

(the first equality follows from the fact that $\det X(k_*, k_2) \in U(1)$). Thus, calling $z = -k_2$ the coordinate on $S^1_3$ and $S^1_6$ (so that the two circles are oriented positively with respect to $z$), we can rewrite the above equality for $k_* = 0$ as

$$\xi_6(z) = \overline{\xi_1(-z)}$$

so that

$$\deg([\xi_6]) = -\deg([\overline{\xi_1}]) \quad \text{(because evaluation at $(-z)$ changes the orientation of $S^1_1$)}$$

$$= \deg([\xi_1]) \quad \text{(because if $\varphi : S^1 \to U(1)$ then $\deg([\varphi]) = -\deg([\overline{\varphi}])$)}.$$

Similarly, for $k_* = 1/2$ we get (using this time the coordinate $z = k_2$ on $S^1_3$ and $S^1_4$)

$$\deg([\xi_4]) = \deg([\xi_3]).$$
Plugging both the equalities that we just obtained in (3.14), we conclude that

\[(3.15) \quad \deg([\xi]) = 2(\deg([\xi_1]) + \deg[\xi_3]) \in 2 \cdot \mathbb{Z}.\]

We have thus proved the following

**Proposition 3.** Let \(X : \partial \mathbb{B}_{\text{eff}} \to U(\mathbb{C}^n)\) satisfy condition \([X_2]\) as in the statement of Proposition 2. Then the degree of its determinant is even:

\[\deg([\det X]) \in 2 \cdot \mathbb{Z}.\]

By the above Proposition, we deduce the following \(\mathbb{Z}_2\) classification for symmetric families of projectors in 2 dimensions.

**Theorem 4.** Let \(\{P(k)\}_{k \in \mathbb{R}^2}\) be a family of orthogonal projectors satisfying Assumption 1. Let \(\hat{U} : \partial \mathbb{B}_{\text{eff}} \to U(\mathbb{C}^m)\) be defined as in (3.7). Then there exists a global continuous symmetric Bloch frame \(\Phi\) for \(\{P(k)\}_{k \in \mathbb{R}^2}\), in the sense of Definition 1, if and only if

\[\deg([\det \hat{U}]) \equiv 0 \mod 2.\]

**Proof.** By Proposition 2, we know that the existence of a global continuous symmetric Bloch frame is equivalent to that of a continuous map \(X : \partial \mathbb{B}_{\text{eff}} \to U(\mathbb{C}^m)\) satisfying conditions \(X_1\) and \(X_2\), as in the statement of the Proposition, so that in particular it should have \(\deg([\det X]) = -\deg([\det \hat{U}])\). In view of Proposition 3, condition \([X_2]\) cannot hold in the case where \(\deg([\det \hat{U}])\) is odd.

In the case in which \(\deg([\det \hat{U}])\) is even, instead, it just remains to exhibit a map \(X : \partial \mathbb{B}_{\text{eff}} \to U(\mathbb{C}^m)\) satisfying (3.9), (3.10) and (3.11), and such that

\[\deg([\det X]) = -\deg([\det \hat{U}]) = -2s, \quad s \in \mathbb{Z}.\]

In the basis where \(\varepsilon\) is of the form (2.5), define

\[X(k) := \begin{cases} \text{diag} \left( e^{-2\pi i s(k_2+1/2)}, e^{-2\pi i s(k_2+1/2)}, 1, \ldots, 1 \right) & \text{if } k \in E_3 \cup E_4, \\ 1 & \text{otherwise}. \end{cases}\]

One checks at once that \(X(k)\) satisfies (3.9), (3.10) and (3.11) – which are equivalent to \([X_2]\) as shown before –, and defines a continuous map \(X : \partial \mathbb{B}_{\text{eff}} \to U(\mathbb{C}^m)\). Since \(X\) is constant on \(E_1\), formula (3.15) for the degree of the determinant of \(X(k)\) simplifies to

\[\deg([\det X]) = 2 \left( \frac{1}{2\pi i} \oint_{S^2_3} dz \partial_z \log \det X(z) \right) = 2 \left( \frac{1}{2\pi i} \int_{-1/2}^0 dk_2 \partial_{k_2} \log \det X(1/2, k_2) \right).\]

Since \(\det X(1/2, k_2) = e^{-4\pi i s k_2}\), one immediately computes \(\deg([\det X]) = -2s\), as wanted. \(\square\)
The index

\[ \delta(P) := \deg([\det \hat{U}]) \mod 2 \]

is thus the \( \mathbb{Z}_2 \) topological invariant (see Section 3.6 below) of the family of projectors \( \{P(k)\}_{k \in \mathbb{R}^2} \), satisfying Assumption 1, which encodes the obstruction to the existence of a global continuous symmetric Bloch frame. One of our main results, Theorem 2, is then reduced to Theorem 4.

3.5. **Well-posedness of the definition of \( \delta \).** In the construction of the previous Subsection, leading to the definition (3.16) of the \( \mathbb{Z}_2 \) index \( \delta \), a number of choices has to be performed, namely the input frame \( \Psi \) and the interpolation \( \langle \hat{U} \rangle_{E_1 \cup E_2 \cup E_3} \) (compare Section 3.3). This Subsection is devoted to showing that the value of the index \( \delta(P) \in \mathbb{Z}_2 \) is independent of such choices, and thus is really associated with the bare family of projectors \( \{P(k)\}_{k \in \mathbb{R}^2} \). Moreover, the index \( \delta \) is also independent of the choice of a basis \( \{e_1, e_2\} \) for the lattice \( \Lambda \), as will be manifest from the equivalent formulation (5.2) of the invariant we will provide in Section 5.

3.5.1. **Gauge independence of \( \delta \).** As a first step, we will prove that the \( \mathbb{Z}_2 \) index \( \delta \) is independent of the choice of the input Bloch frame \( \Psi \).

Indeed, assume that another Bloch frame \( \Psi_{\text{new}} \) is chosen: the two frames will be related by a unitary gauge transformation, say

\[ \Psi_{\text{new}}(k) = \Psi(k) \triangleleft G(k), \quad G(k) \in \mathcal{U}(\mathbb{C}^m), \quad k \in \mathbb{B}_{\text{eff}}. \]

These two frames will produce, via the procedure illustrated above, two symmetric Bloch frames defined on \( \partial \mathbb{B}_{\text{eff}} \), namely

\[ \Phi(k) = \Psi(k) \triangleleft \hat{U}(k) \quad \text{and} \quad \Phi_{\text{new}}(k) = \Psi_{\text{new}}(k) \triangleleft \hat{U}_{\text{new}}(k), \quad k \in \partial \mathbb{B}_{\text{eff}}. \]

From (3.17) we can rewrite the second equality as

\[ \Phi_{\text{new}}(k) = \Psi(k) \triangleleft \left( G(k) \hat{U}_{\text{new}}(k) \right), \quad k \in \partial \mathbb{B}_{\text{eff}}. \]

The two frames \( \Phi \) and \( \Phi_{\text{new}} \) both satisfy the vertex conditions (\( \nabla \)) and the edge symmetries (\( \square \)), hence the matrix \( X(k) := \left( G(k) \hat{U}_{\text{new}}(k) \right)^{-1} \hat{U}(k) \), which transforms \( \Phi_{\text{new}} \) into \( \Phi \), enjoys condition (\( \chi_2 \)) from Proposition 2. Applying Proposition 3 we deduce that

\[ \deg([\det \hat{U}]) \equiv \deg([\det (G \hat{U}_{\text{new}})]) \mod 2. \]

Observe that, since the degree is a group homomorphism,

\[ \deg([\det (G \hat{U}_{\text{new}})]) = \deg([\det \hat{U}_{\text{new}}]) + \deg([\det G]). \]

The matrix \( G(k) \) is by hypothesis defined and continuous on the whole effective unit cell: this implies that the degree of its determinant along the boundary of \( \mathbb{B}_{\text{eff}} \) vanishes, because its restriction to \( \partial \mathbb{B}_{\text{eff}} \) extends continuously to the interior of \( \mathbb{B}_{\text{eff}} \).
Thus we conclude that \(\text{deg}(\det(G\tilde{U}_{\text{new}})) = \text{deg}(\det\tilde{U}_{\text{new}}))\); plugging this in (3.18) we conclude that
\[
\delta = \text{deg}(\det\tilde{U}) \equiv \text{deg}(\det\tilde{U}_{\text{new}}) = \delta_{\text{new}} \mod 2,
\]
as we wanted.

3.5.2. Invariance under edge extension. Recall that, after solving the vertex conditions and finding the value \(U(k_\lambda) = \tilde{U}(k_\lambda)\) at the vertices \(k_\lambda\), we interpolated those – using the path-connectedness of the group \(U(C^m)\) – to obtain the definition of \(\tilde{U}(k)\) first for \(k \in E_1 \cup E_2 \cup E_3\), and then, imposing the edge symmetries, extended it to the whole \(\partial B_{\text{eff}}\) (see Sections 3.2 and 3.3). We now study how a change in this interpolation affects the value of \(\text{deg}(\det\tilde{U})\).

Assume that a different interpolation \(\tilde{U}_{\text{new}}(k)\) has been chosen on \(E_1 \cup E_2 \cup E_3\), leading to a different unitary-matrix-valued map \(\tilde{U}_{\text{new}}: \partial B_{\text{eff}} \to U(C^m)\). Starting from the input frame \(\Psi\), we thus obtain two different Bloch frames:
\[
\hat{\Phi}(k) = \Psi(k) \triangleleft \tilde{U}(k) \quad \text{and} \quad \hat{\Phi}_{\text{new}}(k) = \Psi(k) \triangleleft \tilde{U}_{\text{new}}(k), \quad k \in \partial B_{\text{eff}}.
\]
From the above equalities, we deduce at once that \(\hat{\Phi}(k) = \hat{\Phi}_{\text{new}}(k) \triangleleft X(k)\), where \(X(k) := \tilde{U}_{\text{new}}(k)^{-1}\tilde{U}(k)\). We now follow the same line of argument as in the previous Subsection. Since both \(\hat{\Phi}\) and \(\hat{\Phi}_{\text{new}}\) satisfy the vertex conditions (V) and the edge symmetries (E) by construction, the matrix-valued map \(X: \partial B_{\text{eff}} \to U(C^m)\) just defined enjoys condition \((X_2)\) as in the statement of Proposition 2. It follows now by Proposition 3 that the degree \(\text{deg}(\det X)\) is even. Since the degree defines a group homomorphism, this means that
\[
\text{deg}(\det X) = \text{deg}(\det\tilde{U}) - \text{deg}(\det\tilde{U}_{\text{new}}) \equiv 0 \mod 2
\]
or equivalently
\[
\delta = \text{deg}(\det\tilde{U}) \equiv \text{deg}(\det\tilde{U}_{\text{new}}) = \delta_{\text{new}} \mod 2,
\]
as claimed.

3.6. Topological invariance of \(\delta\). The aim of this Subsection is to prove that the definition (3.16) of the \(\mathbb{Z}_2\) index \(\delta(P)\) actually provides a topological invariant of the family of projectors \(\{P(k)\}_{k \in \mathbb{R}^2}\), with respect to those continuous deformation preserving the relevant symmetries specified in Assumption 1. More formally, the following result holds.

**Proposition 4.** Let \(\{P_0(k)\}_{k \in \mathbb{R}^2}\) and \(\{P_1(k)\}_{k \in \mathbb{R}^2}\) be two families of projectors satisfying Assumption 1. Assume that there exists a homotopy \(\{P_t(k)\}_{k \in \mathbb{R}^2}, t \in [0, 1]\), between \(\{P_0(k)\}_{k \in \mathbb{R}^2}\) and \(\{P_1(k)\}_{k \in \mathbb{R}^2}\), such that \(\{P_t(k)\}_{k \in \mathbb{R}^2}\) satisfies Assumption 1 for all \(t \in [0, 1]\). Then
\[
\delta(P_0) = \delta(P_1) \in \mathbb{Z}_2.
\]
Proof. The function \((t, k) \mapsto P_t(k)\) is a continuous function on the compact set \([0, 1] \times B_{\text{eff}},\) and hence is uniformly continuous. Thus, there exists \(\mu > 0\) such that
\[
\|P_t(k) - P_t(\tilde{k})\|_{B(\mathcal{H})} < 1 \quad \text{if} \quad \max\left\{|k - \tilde{k}|, |t - \tilde{t}|\right\} < \mu.
\]
In particular, choosing \(t_0 < \mu,\) we have that
\[
(3.19) \quad \|P_t(k) - P_0(k)\|_{B(\mathcal{H})} < 1 \quad \text{if} \quad t \in [0, t_0], \quad \text{uniformly in} \quad k \in B_{\text{eff}}.
\]
We will show that \(\delta(P_0) = \delta(P_{t_0}).\) Iterating this construction a finite number of times, covering the compact unit interval as \([0, 1] = [0, t_0] \cup [t_0, t_1] \cup \cdots \cup [t_N, 1],\) will prove that \(\delta(P_0) = \delta(P_t).\)

In view of \((3.19),\) the Kato-Nagy unitary \([Ka, \text{Sec. I.6.8}]\)
\[
W(k) := (1 - (P_0(k) - P_{t_0}(k))^2)^{-1/2} (P_{t_0}(k)P_0(k) + (1 - P_{t_0}(k))(1 - P_0(k))) \in \mathcal{U}(\mathcal{H})
\]
is well-defined and provides an intertwiner between Ran \(P_0(k)\) and Ran \(P_{t_0}(k),\) namely
\[
P_{t_0}(k) = W(k)P_0(k)W(k)^{-1}.
\]
Moreover, one immediately realizes that the map \(k \mapsto W(k)\) inherits from the two families of projectors the following properties:

(W1) the map \(B_{\text{eff}} \ni k \mapsto W(k) \in \mathcal{U}(\mathcal{H})\) is \(C^\infty\)-smooth;
(W2) the map \(k \mapsto W(k)\) is \(\tau\)-covariant, in the sense that whenever \(k\) and \(k + \lambda\) are both in \(B_{\text{eff}}\) for \(\lambda \in \Lambda,\) then
\[
W(k + \lambda) = \tau(\lambda)W(k)\tau(\lambda)^{-1};
\]
(W3) the map \(k \mapsto W(k)\) is time-reversal symmetric, in the sense that whenever \(k\) and \(-k\) are both in \(B_{\text{eff}},\) then
\[
W(-k) = \Theta W(k)\Theta^{-1}.
\]

Let now \(\{\Psi_0(k)\}_{k \in B_{\text{eff}}}\) be a continuous Bloch frame for \(\{P_0(k)\}_{k \in \mathbb{R}^2}.\) Extending the action of the unitary \(W(k) \in \mathcal{U}(\mathcal{H})\) to \(m\)-frames component-wise, we can define \(\Psi_{t_0}(k) = W(k)\Psi_0(k)\) for \(k \in B_{\text{eff}},\) and obtain a continuous Bloch frame \(\{\Psi_{t_0}(k)\}_{k \in B_{\text{eff}}}\) for \(\{P_{t_0}(k)\}_{k \in \mathbb{R}^2}.\) Following the procedure illustrated in Sections 3.2 and 3.3 we can produce two symmetric Bloch frames for \(\{P_0(k)\}_{k \in \mathbb{R}^2}\) and \(\{P_{t_0}(k)\}_{k \in \mathbb{R}^2},\) namely
\[
\Phi_0(k) = \Psi_0(k) \triangleleft \hat{U}_0(k) \quad \text{and} \quad \Phi_{t_0}(k) = \Psi_{t_0}(k) \triangleleft \hat{U}_{t_0}(k), \quad k \in \partial B_{\text{eff}}.
\]
From the above equalities, we deduce that
\[
\Phi_{t_0}(k) = \Psi_{t_0}(k) \triangleleft \hat{U}_{t_0}(k) = (W(k)\Psi_0(k)) \triangleleft \hat{U}_{t_0}(k) = W(k) (\Phi_0(k) \triangleleft \hat{U}_{t_0}(k)) = (W(k)\Phi_0(k)) \triangleleft (\hat{U}_{t_0}(k)^{-1} \hat{U}_{t_0}(k)) = (W(k)\Phi_0(k)) \triangleleft \hat{U}_{t_0}(k)(\hat{U}_{t_0}(k))
\]
where we have used that the action of a linear operator in \(\mathcal{B}(\mathcal{H}),\) extended component-wise to \(m\)-frames, commutes with the right-action of \(\mathcal{U}(\mathbb{C}^m).\) It is easy to verify...
that, in view of properties (W1), (W2) and (W3), the frame \( \{W(k)\hat{\Phi}_0(k)\}_{k \in \partial B_{\text{eff}}} \) gives a continuous Bloch frame for \( \{P_t_0(k)\}_{k \in \mathbb{R}^2} \) which still satisfies the vertex conditions (V) and the edge symmetries (E), since \( \hat{\Phi}_0 \) does. Hence the matrix \( X(k) := \hat{U}_0(k)^{-1}\hat{U}_t_0(k) \) satisfies hypothesis (X2) and in view of Proposition 3 its determinant has even degree. We conclude that

\[
\delta(P_0) = \deg([\det \hat{U}_0]) \equiv \deg([\det \hat{U}_t_0]) = \delta(P_{t_0}) \mod 2,
\]

which is what we wanted to show. \( \square \)
4. Comparison with the Fu-Kane index

In this Section, we will compare our $\mathbb{Z}_2$ invariant $\delta$ with the $\mathbb{Z}_2$ invariant $\Delta$ proposed by Fu and Kane [FK], and show that they are equal. For the reader’s convenience, we recall the definition of $\Delta$, rephrasing it in our terminology.

Let $\Psi(k) = \{\psi_1(k), \ldots, \psi_m(k)\}$ be a global $\tau$-equivariant [7] Bloch frame. Define the unitary matrix $w(k) \in \mathcal{U}(\mathbb{C}^m)$ by

$$w(k)_{ab} := \langle \psi_a(-k), \Theta \psi_b(k) \rangle.$$ (4.1)

Comparing (4.1) with (Fk) changes when the inversion or translation sym-

One immediately checks how $w(k)$ changes when the inversion or translation sym-

or in matrix form $w(\theta(k)) = -w(k)^T$. Moreover, by using the $\tau$-equivariance of the frame $\Psi$ we obtain

$$w(t_\lambda(k))_{ab} = \langle \psi_a(t_\lambda(k)), \Theta \psi_b(t_\lambda(k)) \rangle = \langle \psi_a(t_\lambda k), \Theta \psi_b(k) \rangle =$$

$$= \langle \psi_a(-k), \Theta \psi_b(k) \rangle = \langle \psi_a(-k), \Theta \psi_b(k) \rangle = w(k)_{ab}$$

because $\tau(-\lambda)$ is unitary; in matrix form we can thus write $w(t_\lambda(k)) = w(k)$.

Combining both these facts, we see that at the vertices $k_\lambda$ of the effective unit cell we get

$$-w(k_\lambda)^T = w(\theta(k_\lambda)) = w(t_{-\lambda}(k_\lambda)) = w(k_\lambda)$$

(7) This assumption is crucial in the definition of the Fu-Kane index, whereas the definition of our $\mathbb{Z}_2$ invariant does not need $\Psi$ to be already $\tau$-equivariant. Nonetheless, the existence of a global $\tau$-equivariant Bloch frame is guaranteed by a straightforward modification of the proof in [Pa], as detailed in [MP].

(8) Indeed, spelling out (4.1) one obtains

$$\Theta \psi_b(k) = \sum_{c=1}^m \psi_c(-k)w(k)_{cb}$$

and taking the scalar product of both sides with $\psi_a(-k)$ yields

$$\langle \psi_a(-k), \Theta \psi_b(k) \rangle = \sum_{c=1}^m \langle \psi_a(-k), \psi_c(-k) \rangle w(k)_{cb} = \sum_{c=1}^m \delta_{ac}w(k)_{cb} = w(k)_{ab}$$

because $\{\psi_a(-k)\}_{a=1,\ldots,m}$ is an orthonormal frame in Ran $P(-k)$. 


because by definition \( t_{\lambda} \theta(k_{\lambda}) = k_{\lambda} \), or equivalently \( \theta(k_{\lambda}) = t_{-\lambda}(k_{\lambda}) \). In other words, the matrix \( w(k_{\lambda}) \) is skew-symmetric, and hence it has a well-defined Pfaffian, satisfying \( (\text{Pf} \, w(k_{\lambda}))^2 = \det w(k_{\lambda}) \). The Fu-Kane index \( \Delta \) is then defined as [FK Eqn.s (3.22) and (3.25)]

\[
(4.2) \quad \Delta := P_\theta(1/2) - P_\theta(0) \mod 2,
\]

where for \( k_\ast \in \{0, 1/2\} \)

\[
(4.3) \quad P_\theta(k_\ast) := \frac{1}{2\pi i} \left( \int_{0}^{1/2} \text{d}k_2 \, \text{tr} \left( w(k_\ast, k_2)^* \partial_{k_2} w(k_\ast, k_2) \right) - 2 \log \frac{\text{Pf} \, w(k_\ast, 1/2)}{\text{Pf} \, w(k_\ast, 0)} \right).
\]

We are now in position to prove the above-mentioned equality between our \( \mathbb{Z}_2 \) invariant \( \delta \) and the Fu-Kane index \( \Delta \).

**Theorem 5.** Let \( \{P(k)\}_{k \in \mathbb{R}^2} \) be a family of projectors satisfying Assumption [1] and let \( \delta = \delta(P) \in \mathbb{Z}_2 \) as in (3.16). Moreover, let \( \Delta \in \mathbb{Z}_2 \) be the Fu-Kane index defined in (4.2). Then

\[
\delta = \Delta \in \mathbb{Z}_2.
\]

**Proof.** First we will rewrite our \( \mathbb{Z}_2 \) invariant \( \delta \), in order to make the comparison with \( \Delta \) more accessible. Recall that \( \delta \) is defined as the degree of the determinant of the matrix \( \widehat{U}(k) \), for \( k \in \partial B_{\text{eff}} \), satisfying \( \widehat{\Phi}(k) = \Psi(k) \triangleleft \widehat{U}(k) \), where \( \Phi(k) \) is as in (3.6).

The unitary \( \widehat{U}(k) \) coincides with the unitary \( \widehat{\Phi}(k) \) for \( k \in E_1 \cup E_2 \cup E_3 \), where \( \widehat{U}(k) \) is a continuous path interpolating the unitary matrices \( U(v_i) \), \( i = 1, 2, 3, 4 \), i.e. the solutions to the vertex conditions (compare Sections 3.2 and 3.3). The definition of \( \widehat{U}(k) \) for \( k \in E_4 \cup E_5 \cup E_6 \) is then obtained by imposing the edge symmetries on the corresponding frame \( \Phi(k) \), as in Section 3.3.

We will first compute explicitly the extension of \( \widehat{U} \) to \( k \in E_4 \cup E_5 \cup E_6 \). For \( k \in E_4 \), say \( k = (1/2, k_2) \) with \( k_2 \geq 0 \), we obtain

\[
\begin{align*}
\Phi(k) &= \tau_{e_1} \Theta \Phi(t_{e_1} \theta(k)) \triangleleft \varepsilon = \\
&= \tau_{e_1} \Theta \left( \Psi(t_{e_1} \theta(k)) \triangleleft \widehat{U}(t_{e_1} \theta(k)) \right) \triangleleft \varepsilon = \\
&= \tau_{e_1} \left( \Theta \tau_{e_1} \Psi(-k) \triangleleft \overline{\widehat{U}(1/2, -k_2)} \right) \triangleleft \varepsilon = \\
&= (\tau_{e_1} \tau_{-e_1} \Theta \Psi(-k)) \triangleleft (\overline{\widehat{U}(1/2, -k_2)} \varepsilon) = \\
&= (\Psi(k) \triangleleft w(-k)) \triangleleft (\overline{\widehat{U}(1/2, -k_2)} \varepsilon) = \\
&= \Psi(k) \triangleleft (w(-k) \overline{\widehat{U}(1/2, -k_2)} \varepsilon).
\end{align*}
\]

This means that

\[
(4.4) \quad \widehat{U}(k) = w(-k) \overline{\widehat{U}(1/2, -k_2)} \varepsilon, \quad k = (1/2, k_2) \in E_4.
\]
For $k \in E_5$, say $k = (k_1, 1/2)$, we obtain

$$
\hat{\Phi}(k) = \tau_{e_2} \hat{\Phi}(t_{-e_2}(k)) = \tau_{e_2} (\Psi(t_{-e_2}(k)) \triangleleft \tilde{U}(t_{-e_2}(k))) = \\
\tau_{e_2} \tau_{-e_2} \Psi(k) \triangleleft \tilde{U}(k_1, -1/2) = \Psi(k) \triangleleft \tilde{U}(k_1, -1/2),
$$
or equivalently

$$
(4.5) \quad \tilde{U}(k) = \tilde{U}(k_1, -1/2), \quad k = (k_1, 1/2) \in E_5.
$$

Finally, for $k \in E_6$, say $k = (0, k_2)$ with $k_2 \geq 0$, we obtain

$$
\hat{\Phi}(k) = \Theta \hat{\Phi}(\theta(k)) \triangleleft \varepsilon = \Theta (\Psi(\theta(k)) \triangleleft \tilde{U}(\theta(k))) \triangleleft \varepsilon = \\
(\Theta \Psi(-k)) \triangleleft (\tilde{U}(0, -k_2)\varepsilon) = (\Psi(k) \triangleleft w(-k)) \triangleleft (\tilde{U}(0, -k_2)\varepsilon) = \\
\Psi(k) \triangleleft (w(-k)\tilde{U}(0, -k_2)\varepsilon).
$$

This means that

$$
(4.6) \quad \tilde{U}(k) = w(-k)\tilde{U}(0, -k_2)\varepsilon, \quad k = (0, k_2) \in E_6.
$$

Notice that, as $w(-1/2, k_2) = w(t_{-e_1}(1/2, k_2)) = w(1/2, k_2)$, we can actually summarize (4.5) and (4.6) as

$$
\hat{U}(k_*, k_2) = w(k_*, -k_2)\tilde{U}(k_*, -k_2)\varepsilon, \quad k_* \in \{0, 1/2\}, \quad k_2 \in [0, 1/2].
$$

Since $\tilde{U}$ and $\tilde{U}$ coincide on $E_1$ and $E_3$, we can further rewrite this relation as

$$
(4.7) \quad w(k_*, k_2) = \tilde{U}(k_*, -k_2)\varepsilon^{-1}\tilde{U}(k_*, k_2)^T, \quad (k_*, k_2) \in S_*^1,
$$

where $S_*^1$ denotes the edge $E_1 \cup E_6$ for $k_* = 0$ (respectively $E_3 \cup E_4$ for $k_* = 1/2$), with the edge-points identified: the identification is allowed in view of (4.5) and the fact that $w(\lambda(k)) = w(k)$. 
We are now able to compute the degree of the determinant of $\hat{U}$. Firstly, an easy computation \(^{(9)}\) shows that

$$\deg([\det \hat{U}]) = \frac{1}{2\pi i} \oint_{\partial B_{\text{eff}}} dz \, \partial_z \log \det \hat{U}(z) = \frac{1}{2\pi i} \oint_{\partial B_{\text{eff}}} \left( \hat{U}(z)^* \partial_z \hat{U}(z) \right) = \sum_{i=1}^{6} \frac{1}{2\pi i} \int_{E_i} dz \, \tr(\hat{U}(z)^* \partial_z \hat{U}(z)).$$

Clearly we have

$$\int_{E_i} dz \, \tr(\hat{U}(z)^* \partial_z \hat{U}(z)) = \int_{E_i} dz \, \tr(\hat{U}(z)^* \partial_z \hat{U}(z)) \quad \text{for } i = 1, 2, 3,$$

\(^{(9)}\) If $\hat{U}(z) \in \mathbb{U}(\mathbb{C}^m)$ has spectrum $\{e^{i\lambda_j(z)}\}_{j=1, \ldots, m}$, then

$$\partial_z \log \det \hat{U}(z) = \sum_{j=1}^{m} e^{-i\lambda_j(z)} \partial_z e^{i\lambda_j(z)}.$$

On the other hand, writing the spectral decomposition of $\hat{U}(z)$ as

$$\hat{U}(z) = \sum_{j=1}^{m} e^{i\lambda_j(z)} P_j(z), \quad P_j(z)^* = P_j(z) = P_j(z)^2, \quad \tr(P_j(z)) = 1,$$

one immediately deduces that

$$\hat{U}(z)^* = \sum_{j=1}^{m} e^{-i\lambda_j(z)} P_j(z) \quad \text{and} \quad \partial_z \hat{U}(z) = \sum_{j=1}^{m} \left( \partial_z e^{i\lambda_j(z)} \right) P_j(z) + e^{i\lambda_j(z)} (\partial_z P_j(z)).$$

Notice now that, taking the derivative with respect to $z$ of the equality $P_j(z)^2 = P_j(z)$, one obtains

$$P_j(z) \partial_z P_j(z) = (\partial_z P_j(z)) (1 - P_j(z))$$

so that

$$\partial_z P_j(z) = P_j(z) (\partial_z P_j(z)) (1 - P_j(z)) + (1 - P_j(z)) (\partial_z P_j(z)) P_j(z).$$

From this, it follows by the ciclicity of the trace and the relation $P_j(z) P_\ell(z) = \delta_{j, \ell} P_j(z)$ that

$$\tr(P_\ell(z) (\partial_z P_j(z))) = \tr(P_j(z) P_\ell(z) (\partial_z P_j(z)) (1 - P_j(z))) + \tr((1 - P_j(z)) P_\ell(z) (\partial_z P_j(z)) P_j(z)) = 0.$$

We are now able to compute

$$\tr(\hat{U}(z)^* \partial_z \hat{U}(z)) = \sum_{j, \ell=1}^{m} \tr(e^{-i\lambda_j(z)} P_\ell(z) \left( \partial_z e^{i\lambda_j(z)} \right) P_j(z)) +$$

$$+ e^{-i(\lambda_j(z) - \lambda_j(z))} \tr(P_\ell(z) (\partial_j P_j(z))) =$$

$$= \sum_{j, \ell=1}^{m} e^{-i\lambda_j(z)} \left( \partial_z e^{i\lambda_j(z)} \right) \delta_{j, \ell} \tr(P_j(z)) = \sum_{j=1}^{m} e^{-i\lambda_j(z)} \partial_z e^{i\lambda_j(z)}.$$
because $\hat{U}$ and $\tilde{U}$ coincide on $E_1 \cup E_2 \cup E_3$. Using now Equation (4.5) we compute

$$
\int_{E_5} dz \, \text{tr} (\hat{U}(z) \partial_z \hat{U}(z)) = \int_{-1/2}^0 dk_1 \, \text{tr} (\hat{U}(k_1, 1/2) \partial_{k_1} \hat{U}(k_1, 1/2)) = -\int_0^{1/2} dk_1 \, \text{tr} (\hat{U}(k_1, -1/2) \partial_{k_1} \hat{U}(k_1, -1/2)) = -\int_{E_2} dz \, \text{tr} (\hat{U}(z) \partial_z \hat{U}(z))
$$

or equivalently, in view of (4.8) for $i = 2$,

$$
(4.9) \quad \left( \int_{E_2} + \int_{E_5} \right) dz \, \text{tr} (\hat{U}(z) \partial_z \hat{U}(z)) = 0.
$$

Making use of (4.7), we proceed now to evaluate the integrals on $E_1, E_3, E_4$ and $E_0$, which give the non-trivial contributions to $\text{deg}([\det \hat{U}])$. Indeed, Equation (4.7) implies

$$
\begin{align*}
{w}(k_*, k_2) &= \overline{\hat{U}(k_*, k_2)} \in \hat{U}(k_*, -k_2), \\
\partial_{k_2} w(k_*, k_2) &= -\partial_{k_2} \hat{U}(k_*, -k_2) \varepsilon^{-1} \hat{U}(k_*, k_2)^T + \hat{U}(k_*, -k_2) \varepsilon^{-1} \partial_{k_2} \hat{U}(k_*, k_2)^T,
\end{align*}
$$

from which we can compute

$$
\text{tr} (w(k_*, k_2) \partial_{k_2} w(k_*, k_2)) = -\text{tr} (\hat{U}(k_*, -k_2)^* \partial_{k_2} \hat{U}(k_*, -k_2) \varepsilon^{-1} \hat{U}(k_*, k_2)^T \overline{\hat{U}(k_*, k_2)} \varepsilon) + \\
+ \text{tr} (\overline{\hat{U}(k_*, k_2)} \varepsilon \hat{U}(k_*, -k_2)^* \hat{U}(k_*, -k_2) \varepsilon^{-1} \partial_{k_2} \hat{U}(k_*, k_2)^T)
\begin{align*}
= & -\text{tr} (\hat{U}(k_*, -k_2)^* \partial_{k_2} \hat{U}(k_*, -k_2)) + \text{tr} (\overline{\hat{U}(k_*, k_2)} \partial_{k_2} \hat{U}(k_*, k_2)^T) \\
= & -\text{tr} (\hat{U}(k_*, -k_2)^* \partial_{k_2} \hat{U}(k_*, -k_2)) + \text{tr} (\hat{U}(k_*, k_2)^* \partial_{k_2} \hat{U}(k_*, k_2)).
\end{align*}
$$

Integrating both sides of the above equality for $k_2 \in [0, 1/2]$ yields to (4.10)

$$
\int_{-1/2}^{1/2} dk_2 \, \text{tr} (w(k_*, k_2)^* \partial_{k_2} w(k_*, k_2)) = -\int_{-1/2}^0 dk_2 \, \text{tr} (\hat{U}(k_*, k_2)^* \partial_{k_2} \hat{U}(k_*, k_2)) + \\
+ \int_{0}^{1/2} dk_2 \, \text{tr} (\hat{U}(k_*, k_2)^* \partial_{k_2} \hat{U}(k_*, k_2)) = \\
= (-1)^{1+2k_*} \int_{S^1_*} dz \, \text{tr} (\hat{U}(z)^* \partial_z \hat{U}(z)) + \\
+ 2 \int_{0}^{1/2} dk_2 \, \text{tr} (\hat{U}(k_*, k_2)^* \partial_{k_2} \hat{U}(k_*, k_2)).
$$

The sign $s_* := (-1)^{1+2k_*}$ appearing in front of the integral along $S^1_* \text{ depends on the different orientations of the two circles, for } k_* = 0 \text{ and for } k_* = 1/2, \text{ parametrized by the coordinate } z = k_2.$
Now, notice that

\[ \int_{0}^{1/2} \frac{d k_2}{2} \text{tr} \left( \hat{U}(k_*, k_2)^* \partial_{k_2} \hat{U}(k_*, k_2) \right) = \int_{0}^{1/2} \frac{d k_2}{2} \partial_{k_2} \log \det \hat{U}(k_*, k_2) \]

(4.11)

\[ \equiv \log \frac{\det \hat{U}(k_*, 1/2)}{\det \hat{U}(k_*, 0)} \mod 2 \pi i. \]

Furthermore, evaluating Equation (4.7) at the six vertices \( k_\lambda \), we obtain

\[ w(k_\lambda) = \hat{U}(k_\lambda) \epsilon^{-1} \hat{U}(k_\lambda)^T \]

which implies that

(4.12)

\[ \text{Pf} w(k_\lambda) = \det \hat{U}(k_\lambda) \text{Pf} \epsilon^{-1} \]

by the well known property \( \text{Pf}(CAC^T) = \det(C) \text{Pf}(A) \), for a skew-symmetric matrix \( A \) and a matrix \( C \in M_n(\mathbb{C}) \).

Substituting the latter equality in the right-hand side of Equation (4.11) allows us to rewrite (4.10) as

\[ \frac{1}{2 \pi i} \left( \int_{0}^{1/2} \frac{d k_2}{2} \text{tr}(w(k_*, k_2)^* \partial_{k_2} w(k_*, k_2)) - 2 \log \frac{\text{Pf}(w(k_*, 1/2))}{\text{Pf}(w(k_*, 0))} \right) \equiv \]

\[ \equiv \frac{s_\epsilon}{2 \pi i} \int_{S_1^*} dz \text{tr} \left( \hat{U}(z)^* \partial_z \hat{U}(z) \right) \mod 2. \]

On the left-hand side of this equality, we recognize \( P_\theta(k_\epsilon) \), as defined in (4.3). Taking care of the orientation of \( S_1^* \), we conclude, also in view of (4.9), that

\[ \Delta \equiv P_{\theta}(1/2) - P_{\theta}(0) \mod 2 \]

\[ \equiv \frac{1}{2 \pi i} \left( \int_{E_1} + \int_{E_3} + \int_{E_4} + \int_{E_6} \right) dz \text{tr} \left( \hat{U}(z)^* \partial_z \hat{U}(z) \right) \mod 2 \]

\[ \equiv \deg([\det \hat{U}]) \equiv \delta \mod 2 \]

which is what we wanted to show. \( \square \)

**Remark 5 (On the role of Pfaffians).** Equation (4.7) is the crucial point in the above argument. Indeed, since \( \det \epsilon = 1 \) (compare Remark 2), from (4.7) it follows that

(4.13)

\[ \det w(k_\epsilon, k_2) = \det \hat{U}(k_\epsilon, -k_2) \det \hat{U}(k_\epsilon, k_2), \quad (k_\epsilon, k_2) \in S_1^1. \]

If we evaluate this equality at the six vertices \( k_\lambda \), we obtain

(4.14)

\[ \det w(k_\lambda) = (\det \hat{U}(k_\lambda))^2 = (\text{Pf}(w(k_\lambda)))^2. \]

Looking at Equation (4.13), we realize that the expression \( \det \hat{U}(k_\epsilon, k_2) \) serves as a “continuous prolongation” along the edges \( E_1, E_3, E_4, E_6 \) of the Pfaffian \( \text{Pf}(w(k_\lambda)) \), which is well-defined only at the six vertices \( k_\lambda \) (where the matrix \( w \) is skew-symmetric), in a way which is moreover compatible with time-reversal symmetry,
since in (4.13) both $\det \tilde{U}(k_*, k_2)$ and $\det \tilde{U}(k_*, -k_2)$ appear. This justifies the rather mysterious and apparently \textit{ad hoc} presence of Pfaffians in the Fu-Kane formula for the $\mathbb{Z}_2$ index $\Delta$.

In view of the equality $\Delta = \delta \in \mathbb{Z}_2$, we have a clear interpretation of the Fu-Kane index as the obstruction to the existence of a global continuous symmetric Bloch frame, as claimed in [FK] App. A.
5. A SIMPLER FORMULA FOR THE $\mathbb{Z}_2$ INVARIANT

The fact that the $\mathbb{Z}_2$ invariant $\delta$, as defined in (3.16), is well-defined and independent of the choice of an interpolation of the vertex unitaries $U(k_\lambda)$ (see Section 3.5.2) shows that its value depends only on the value of $\hat{U}$ at the vertices. This dependence can be made explicit. In this Section, we will provide a way to compute $\delta \in \mathbb{Z}_2$ using data coming just from the four time-reversal invariant momenta $v_1, \ldots, v_4$ which are inequivalent modulo translational and inversion symmetries of $\mathbb{R}^2$ (this terminology is borrowed from [FKM]). This should be compared with [FK, Equation (3.26)].

In the previous Section (compare Equation (4.10)), we have rewritten our invariant as

$$ \delta = \tilde{P}_\theta(1/2) - \tilde{P}_\theta(0) \mod 2, $$

with

$$ -\tilde{P}_\theta(k_\ast) := \frac{1}{2\pi i} \left( \int_{-1/2}^0 \text{d}k_2 \text{tr} \left( w(k_\ast, k_2)^* \partial_{k_2} w(k_\ast, k_2) \right) + 2 \int_{-1/2}^0 \text{d}k_2 \text{tr} \left( \hat{U}(k_\ast, k_2)^* \partial_{k_2} \hat{U}(k_\ast, k_2) \right) \right) = \frac{1}{2\pi i} \left( \log \frac{\det w(k_\ast, 0)}{\det w(k_\ast, -1/2)} - 2 \log \frac{\det \hat{U}(k_\ast, 0)}{\det \hat{U}(k_\ast, -1/2)} \right). $$

In view of (4.14), the above expression can be rewritten as

$$ \delta = \sum_{i=1}^4 \tilde{\eta}_{v_i} \mod 2, \quad \text{where} \quad \tilde{\eta}_{v_i} := \frac{1}{2\pi i} \left( \log \left( \det \hat{U}(v_i) \right)^2 - 2 \log \det \hat{U}(v_i) \right). $$

Notice that, since $\deg([\det \hat{U}])$ is an integer, the value $(-1)^{\deg([\det \hat{U}])}$ is independent of the choice of the determination of $\log(-1)$ and is determined by the parity of $\deg([\det \hat{U}])$, i.e. by $\delta = \deg([\det \hat{U}]) \mod 2$. Moreover, this implies also that

$$ (-1)^\delta = \prod_{i=1}^4 (-1)^\tilde{\eta}_{v_i} $$

and each $(-1)^{\tilde{\eta}_{v_i}}$ can be computed with any determination of $\log(-1)$ (as long as one chooses the same for all $i \in \{1, \ldots, 4\}$). Noticing that, using the principal value of the complex logarithm,

$$ (-1)^{(\log \alpha)/(2\pi i)} = (e^{i\pi}(\log \alpha)/(2\pi i)) = e^{(\log \alpha)/2} = \sqrt{\alpha}, $$

it follows that we can rewrite the above expression for $(-1)^\delta$ as

$$ (-1)^\delta = \prod_{i=1}^4 \sqrt{\left( \det \hat{U}(v_i) \right)^2 \det \hat{U}(v_i)} $$

where the branch of the square root is chosen in order to evolve continuously from $v_1$ to $v_2$ along $E_1$, and from $v_3$ to $v_4$ along $E_3$. This formula is to be compared with
Equation (3.26)] for the Fu-Kane index $\Delta$, namely

$$
(5.3) \quad (-1)^\Delta = \prod_{i=1}^{4} \sqrt{\frac{\det w(v_i)}{\text{Pf } w(v_i)}}.
$$

Recall now that the value of $\hat{U}$ at the vertices $k_\lambda$ is determined by solving the vertex conditions, as in Section 3.2. $\hat{U}(k_\lambda) = U(k_\lambda)$ is related to the obstruction unitary $U_{\text{obs}}(k_\lambda)$ by the relation (3.5). In particular, from (3.5) we deduce that

$$
\det U_{\text{obs}}(k_\lambda) = (\det U(k_\lambda))^2
$$

so that (5.2) may be rewritten as

$$
(5.4) \quad (-1)^\delta = \prod_{i=1}^{4} \sqrt{\frac{\det U_{\text{obs}}(v_i)}{\det U(v_i)}}.
$$

This reformulation shows that our $\mathbb{Z}_2$ invariant can be computed starting just from the “input” Bloch frame $\Psi$ (provided it is continuous on $\mathbb{B}_{\text{eff}}$), and more specifically from its values at the vertices $k_\lambda$. Indeed, the obstruction $U_{\text{obs}}(k_\lambda)$ at the vertices is defined by (3.3) solely in terms of $\Psi(k_\lambda)$; moreover, $U(k_\lambda)$ is determined by $U_{\text{obs}}(k_\lambda)$ as explained in the proof of Lemma 1.

We have thus the following algorithmic recipe to compute $\delta$:

- given a continuous Bloch frame $\Psi(k) = \{\psi_a(k)\}_{a=1,\ldots,m}, \ k \in \mathbb{B}_{\text{eff}}$, compute the unitary matrix

$$
U_{\text{obs}}(k_\lambda)_{a,b} = \sum_{c=1}^{m} \langle \psi_a(k_\lambda), \tau(\lambda)\Theta\psi_c(k_\lambda) \rangle \varepsilon_{cb},
$$

defined as in (3.3), at the four inequivalent time-reversal invariant momenta $k_\lambda = v_1, \ldots, v_4$;

- compute the spectrum $\{e^{i\lambda_1^{(i)}}, \ldots, e^{i\lambda_m^{(i)}}\} \subset U(1)$ of $U_{\text{obs}}(v_i)$, so that in particular

$$
\det U_{\text{obs}}(v_i) = \exp \left( i \left( \lambda_1^{(i)} + \cdots + \lambda_m^{(i)} \right) \right);
$$

normalize the arguments of such phases so that $\lambda^{(i)}_j \in [0, 2\pi)$ for all $j \in \{1, \ldots, m\}$;

- compute $U(v_i)$ as in the proof of Lemma 1 in particular we obtain that

$$
\det U(v_i) = \exp \left( i \left( \frac{\lambda_1^{(i)}}{2} + \cdots + \frac{\lambda_m^{(i)}}{2} \right) \right);
$$
• finally, compute $\delta$ from the formula (5.4), i.e.

$$(-1)^\delta = \prod_{i=1}^{4} \frac{\exp\left(i \left(\lambda_1^{(i)} + \cdots + \lambda_m^{(i)}\right)\right)}{\exp\left(i \left(\frac{\lambda_1^{(i)}}{2} + \cdots + \frac{\lambda_2^{(i)}}{2}\right)\right)}.$$ 

**Remark 6 (How can it be that $\delta = -1$?).** The ratio $\sqrt{\det U_{\text{obs}}(k\lambda)/\det U(k\lambda)}$ can very well be equal to $-1$. Indeed, to evaluate $\sqrt{\det U_{\text{obs}}(k\lambda)}$ one first computes the product of the phases constituting the spectrum of the matrix $U_{\text{obs}}(k\lambda)$, reducing its argument modulo $2\pi$, and then takes the (positive) square root; while to evaluate $\det U(k\lambda)$ one first takes the (positive) square roots of the element of the spectrum of $U_{\text{obs}}(k\lambda)$, and then computes their products, reducing the final argument modulo $2\pi$ if necessary. These procedures (product, square root and reduction modulo $2\pi$ of the argument) need not commute.
6. Construction of a symmetric Bloch frame in 3d

In this Section, we will show how to reproduce the constructive algorithm for a global continuous symmetric Bloch frame outlined in Section 3 also in the 3-dimensional setting \((k \in \mathbb{R}^3)\). In particular, we will recover the four \(\mathbb{Z}_2\) indices proposed by Fu, Kane and Mele \([\text{FKM}]\). We will first focus on the topological obstructions that arise, and then provide the construction of a symmetric Bloch frame in 3d when the procedure is unobstructed.

6.1. Vertex conditions and edge extension. The 3-dimensional unit cell is defined, in complete analogy with the 2-dimensional case, as

\[
\mathbb{B}^{(3)} := \left\{ k = \sum_{j=1}^{3} k_j e_j \in \mathbb{R}^3 : -\frac{1}{2} \leq k_i \leq \frac{1}{2}, \ i = 1, 2, 3 \right\}
\]

(the superscript \((3)\) stands for “3-dimensional”), where \(\{e_1, e_2, e_3\}\) is a basis in \(\mathbb{R}^3\) such that \(\Lambda = \text{Span}_\mathbb{Z} \{e_1, e_2, e_3\}\). If a continuous Bloch frame is given on \(\mathbb{B}^{(3)}\), then it can be extended to a \(\tau\)-equivariant Bloch frame on \(\mathbb{R}^3\) by considering its \(\tau\)-translates, provided it satisfies the obvious compatibility conditions of \(\tau\)-periodicity on the faces of the unit cell (i.e. on its boundary). Similarly, if one wants to study frames which are also time-reversal invariant, then one can restrict the attention to the effective unit cell

\[
\mathbb{B}_{\text{eff}}^{(3)} := \left\{ k = (k_1, k_2, k_3) \in \mathbb{B}^{(3)} : k_1 \geq 0 \right\}.
\]

The (effective) unit cell is pictured in Figure 2.

Vertices of the (effective) unit cell are defined again as those points \(k_\lambda\) which are invariant under the transformation \(t_\lambda \theta\): these are the points with half-integer coordinates with respect to the lattice generators \(\{e_1, e_2, e_3\}\). The vertex conditions for a symmetric Bloch frame read exactly as in (V), and can be solved analogously to the 2-dimensional case with the use of Lemma 1. This leads to the definition of a unitary matrix \(U(k_\lambda)\) at each vertex. The definition of \(U(\cdot)\) can be extended to the edges joining vertices of \(\mathbb{B}_{\text{eff}}^{(3)}\) by using the path-connectedness of the group \(\mathfrak{U}(\mathbb{C}^m)\), as in Section 3.3. Actually, we need to choose such an extension only on the edges which are plotted with a thick line in Figure 2; then we can obtain the definition of \(U(\cdot)\) to all edges by imposing edge symmetries, which are completely analogous to those in (E).

6.2. Extension to the faces: four \(\mathbb{Z}_2\) obstructions. We now want to extend the definition of the matrix \(U(k)\), mapping a reference Bloch frame \(\Psi(k)\) to a symmetric Bloch frame \(\Phi(k)\), to \(k \in \partial \mathbb{B}_{\text{eff}}^{(3)}\). The boundary of \(\mathbb{B}_{\text{eff}}^{(3)}\) consists now of six faces, which
we denote as follows:

\[
F_{1,0} := \left\{ (k_1, k_2, k_3) \in \partial \mathbb{B}_{\text{eff}}^{(3)} : k_1 = 0 \right\},
\]

\[
F_{1,+} := \left\{ (k_1, k_2, k_3) \in \partial \mathbb{B}_{\text{eff}}^{(3)} : k_1 = \frac{1}{2} \right\},
\]

\[
F_{i,\pm} := \left\{ (k_1, k_2, k_3) \in \partial \mathbb{B}_{\text{eff}}^{(3)} : k_i = \pm \frac{1}{2} \right\}, \quad i \in \{2, 3\}.
\]

Notice that \(F_{1,0}\) and \(F_{1,+}\) are both isomorphic to a full unit cell \(\mathbb{B}^{(2)}\) (the superscript \(^{(2)}\) stands for “2-dimensional”), while the faces \(F_{i,\pm}, i \in \{2, 3\}\), are all isomorphic to a 2d effective unit cell \(\mathbb{B}_{\text{eff}}^{(2)}\).

We start by considering the four faces \(F_{i,\pm}, i \in \{2, 3\}\). From the 2-dimensional algorithm, we know that to extend the definition of \(U(\cdot)\) from the edges to one of these faces we need for the associated \(\mathbb{Z}_2\) invariant \(\delta_{i,\pm}\) to vanish. Not all these four invariants are independent, though: indeed, we have that \(\delta_{i,+} = \delta_{i,-}\) for \(i = 2, 3\). In fact, suppose for example that \(\delta_{i,-}\) vanishes, so that we can extend the Bloch frame \(\Phi\) to the face \(F_{i,-}\). Then, by setting \(\Phi(t_{e_i}(k)) := \tau_{e_i} \Phi(k)\) for \(k \in F_{i,-}\), we get an extension of the frame \(\Phi\) to \(F_{i,+}\): it follows that also \(\delta_{i,+}\) must vanish. Viceversa, exchanging the roles of the subscripts + and – one can argue that if \(\delta_{i,+} = 0\) then
also \( \delta_{i,-} = 0 \); in conclusion, \( \delta_{i,+} = \delta_{i,-} \in \mathbb{Z}_2 \), as claimed. We remain for now with only two independent \( \mathbb{Z}_2 \) invariants, namely \( \delta_{2,+} \) and \( \delta_{3,+} \).

We now turn our attention to the faces \( F_{1,0} \) and \( F_{1,+} \). As we already noticed, these are \( 2d \) unit cells \( \mathbb{B}^{(2)} \). Each of them contains three thick-line edges (as in Figure 2), on which we have already defined the Bloch frame \( \Phi \); this allows us to test the possibility to extend it to the effective unit cell which they enclose. If we are indeed able to construct such an extension to this effective unit cell \( \mathbb{B}^{(2)} \), then we can extend it to the whole face by using the time reversal operator \( \Theta \) in the usual way: in fact, both \( F_{1,0} \) and \( F_{1,+} \) are such that if \( k \) lies on it then also \(-k\) lies on it (up to periodicity, or equivalently translational invariance). The obstruction to the extension of the Bloch frame to \( F_{1,0} \) and \( F_{1,+} \) is thus encoded again in two \( \mathbb{Z}_2 \) invariants \( \delta_{1,0} \) and \( \delta_{1,+} ; \) together with \( \delta_{2,+} \) and \( \delta_{3,+} \), they represent the obstruction of the extension of the symmetric Bloch frame from the edges of \( \mathbb{B}^{(3)} \) to the boundary \( \partial \mathbb{B}^{(3)} \).

Suppose now that we are indeed able to obtain such an extension to \( \partial \mathbb{B}^{(3)} \), i.e. that all four \( \mathbb{Z}_2 \) invariants vanish. Then we have a map \( \tilde{U} : \partial \mathbb{B}^{(3)} \rightarrow \mathcal{U}(\mathbb{C}_m) \), such that at each \( k \in \partial \mathbb{B}^{(3)} \) the unitary matrix \( \tilde{U}(k) \) maps the reference Bloch frame \( \Psi(k) \) to a symmetric Bloch frame \( \tilde{\Phi}(k) = \Psi(k) \circ \tilde{U}(k) \). In order to get a continuous symmetric Bloch frame defined on the whole \( \mathbb{B}^{(3)} \), it is thus sufficient to extend the map \( \tilde{U} : \partial \mathbb{B}^{(3)} \rightarrow \mathcal{U}(\mathbb{C}_m) \) to a continuous map \( U : \mathbb{B}^{(3)} \rightarrow \mathcal{U}(\mathbb{C}_m) \).

Topologically, the boundary of the effective unit cell in 3 dimensions is equivalent to a sphere: \( \partial \mathbb{B}^{(3)} \simeq S^2 \). Moreover, it is known that, if \( X \) is any topological space, then a continuous map \( f : S^2 \rightarrow X \) extends to a continuous map \( F : D^3 \rightarrow X \), defined on the 3-ball \( D^3 \) that the sphere encircles, if and only if its homotopy class \( [f] \in [S^2; X] = \pi_2(X) \) is trivial (compare the analogous discussion in Section 3.4). In our case, where \( X = \mathcal{U}(\mathbb{C}_m) \), it is a well-known fact that \( \pi_2(\mathcal{U}(\mathbb{C}_m)) = 0 \) [Hus, Ch.8, Sec. 12], so that actually any continuous map from the boundary of the effective unit cell to the unitary group extends continuously to a map defined on the whole \( \mathbb{B}^{(3)} \). In other words, there is no topological obstruction to the continuous extension of a symmetric frame from \( \partial \mathbb{B}^{(3)} \) to \( \mathbb{B}^{(3)} \), and hence to \( \mathbb{R}^3 \): indeed, one can argue, as in Proposition 1 that a symmetric Bloch frame on \( \mathbb{B}^{(3)} \) can always be extended to all of \( \mathbb{R}^3 \), by imposing \( \tau \)-equivariance and time-reversal symmetry.

In conclusion, we have that all the topological obstruction that can prevent the existence of a global continuous symmetric Bloch frame is encoded in the four \( \mathbb{Z}_2 \) invariants \( \delta_{1,0} \) and \( \delta_{i,+} \), for \( i \in \{1, 2, 3\} \), given by

\[
(6.1) \quad \delta_i(P) := \delta \left( P_{|F_i} \right), \quad F_i \in \{ F_{1,0}, F_{1,+}, F_{2,+}, F_{3,+} \}.
\]
6.3. Proof of Theorem \[3\] We have now understood how topological obstruction may arise in the construction of a global continuous symmetric Bloch frame, by sketching the 3-dimensional analogue of the method developed in Section \[3\] for the 2d case. This Subsection is devoted to detailing a more precise constructive algorithm for such a Bloch frame in 3d, whenever there is no topological obstruction to its existence. As in the 2d case, we will start from a “naïve” choice of a continuous Bloch frame \(\Psi(k)\), and symmetrize it to obtain the required symmetric Bloch frame \(\Phi(k) = \Psi(k) + U(k)\) on the effective unit cell \(B_{\text{eff}}^{(3)}\) (compare \(3\,2\)). We will apply this scheme first on vertices, then on edges, then (whenever there is no topological obstruction) to faces, and then to the interior of \(B_{\text{eff}}^{(3)}\).

The two main “tools” in this algorithm are provided by the following Lemmas, which are “distilled” from the procedure elaborated in Section \[3\].

Lemma 2 (From 0d to 1d). Let \(\{P(k)\}_{k \in \mathbb{R}}\) be a family of projectors satisfying Assumption\[7\]. Denote \(B_{\text{eff}}^{(1)} = \{k = k_1 e_1 : -1/2 \leq k_1 \leq 0\} \simeq [-1/2, 0]\). Let \(\Phi(-1/2)\) be a frame in \(\text{Ran} P(-1/2)\) such that

\[\Phi(-1/2) = \tau_{-e_1} \Theta \Phi(-1/2) \triangleleft \varepsilon,\]

i.e. \(\Phi\) satisfies the vertex condition \((\triangledown)\) at \(k_{-e_1} = -(1/2)e_1 \in B_{\text{eff}}^{(1)}\). Then one constructs a continuous Bloch frame \(\{\Phi_{\text{eff}}(k)\}_{k \in B_{\text{eff}}^{(1)}}\) such that

\[\Phi_{\text{eff}}(-1/2) = \Phi(-1/2) \quad \text{and} \quad \Phi_{\text{eff}}(0) = \Theta \Phi_{\text{eff}}(0) \triangleleft \varepsilon.\]

Proof. Solve the vertex condition at \(k_\lambda = 0 \in B_{\text{eff}}^{(1)}\) using Lemma\[1\] and then extend the frame to \(B_{\text{eff}}^{(1)}\) as in Section \[5.3\].

Lemma 3 (From 1d to 2d). Let \(\{P(k)\}_{k \in \mathbb{R}^2}\) be a family of projectors satisfying Assumption\[7\]. Let \(v_i\) and \(E_i\) denote the edges of the effective unit cell \(B_{\text{eff}}^{(2)}\), as defined in Section \[3.4\]. Let \(\{\Phi(k)\}_{k \in E_1 \cup E_2 \cup E_3}\) be a continuous Bloch frame for \(\{P(k)\}_{k \in \mathbb{R}^2}\), satisfying the vertex conditions \((\triangledown)\) at \(v_1, v_2, v_3\) and \(v_4\). Assume that

\[\delta(P) = 0 \in \mathbb{Z}_2.\]

Then one constructs a continuous Bloch frame \(\{\Phi_{\text{eff}}(k)\}_{k \in B_{\text{eff}}^{(2)}}\), satisfying the vertex conditions \((\triangledown)\) and the edge symmetries \((\bigtriangleup)\), and moreover such that

\[\Phi_{\text{eff}}(k) = \Phi(k) \quad \text{for} \ k \in E_1 \cup E_2.\]
extends to the whole $\mathbb{B}_{\text{eff}}^{(2)}$. The fact that $X(k)$ can be chosen to be constantly equal to the identity matrix on $E_1 \cup E_2 \cup E_5 \cup E_6$ shows that (6.2) holds. \hfill \Box

We are now ready to prove Theorem 3.

Proof of Theorem 3. Consider the region $Q = \mathbb{B}_{\text{eff}}^{(3)} \cap \{k_2 \leq 0, k_3 \geq 0\}$. We label its vertices as $v_1 = (0, -1/2, 0), v_2, v_3, v_4 \in Q \cap \{k_2 = -1/2\}$ (counted counterclockwise) and $v_5 = (0, 0, 0), v_6, v_7, v_8 \in Q \cap \{k_2 = 0\}$ (again counted counterclockwise). We also let $E_{ij}$ denote the edge joining $v_i$ and $v_j$. The labels are depicted in Figure 3.

Step 1. Choose a continuous Bloch frame $\{\Psi(k)\}_{k \in \mathbb{B}_{\text{eff}}^{(3)}}$ for $\{P(k)\}_{k \in \mathbb{R}^3}$. Solve the vertex conditions at all $v_i$’s, using Lemma 1 to obtain frames $\Phi_{\text{ver}}(v_i), i = 1, \ldots, 8$.

Step 2. Using repeatedly Lemma 2 extend the definition of $\Phi_{\text{ver}}$ to the edges $E_{12}, E_{15}, E_{23}, E_{26}, E_{34}, E_{37}$ and $E_{48}$, to obtain frames $\Phi_{\text{edg}}(k)$.

Step 3. Use Lemma 3 to extend further the definition of $\Phi_{\text{edg}}$ as follows.

3a. Extend the definition of $\Phi_{\text{edg}}$ on $F_{3,+}$: this can be done since $\delta_{3,+}$ vanishes. This will change the original definition of $\Phi_{\text{edg}}$ only on $E_{37}$.

3b. Extend the definition of $\Phi_{\text{edg}}$ on $F_{2,-}$: this can be done since $\delta_{2,-} = \delta_{2,+}$ vanishes. This will change the original definition of $\Phi_{\text{edg}}$ only on $E_{34}$.

3c. Extend the definition of $\Phi_{\text{edg}}$ on $F_{1,0} \cap \{k_3 \geq 0\}$: this can be done since $\delta_{1,0}$ vanishes. This will change the original definition of $\Phi_{\text{edg}}$ only on $E_{15}$. (Here we give $F_{1,0}$ the opposite orientation to the one inherited from $\partial \mathbb{B}_{\text{eff}}^{(3)}$, but this is inessential.)

3d. Extend the definition of $\Phi_{\text{edg}}$ on $F_{1,+} \cap \{k_3 \geq 0\}$. Although we have already changed the definition of $\Phi_{\text{edg}}$ on $E_{37} \cup E_{34}$, this extension can still be performed since we have proved in Section 3.5.2 that $\delta_{1,+}$ is independent of the choice of the extension of the frame along edges, and hence vanishes by hypothesis. The extension will further modify the definition of $\Phi_{\text{edg}}$ only on $E_{48}$.

We end up with a Bloch frame $\Phi_S$ defined on

$$S := F_{2,-} \cup F_{3,+} \cup (F_{1,0} \cap \{k_3 \geq 0\}) \cup (F_{1,+} \cap \{k_3 \geq 0\}).$$

Step 4. Extend the definition of $\Phi_S$ to $F_{1,0} \cap \{k_3 \leq 0\}$ and $F_{1,+} \cap \{k_3 \leq 0\}$ by setting

$$\Phi_{S'}(k) := \Phi_S(k) \quad \text{for } k \in S,$$
$$\Phi_{S'}(\theta(k)) := \Theta \Phi_S(k) \triangleq \varepsilon \quad \text{for } k \in F_{1,0} \cap \{k_3 \geq 0\}, \quad \text{and}$$
$$\Phi_{S'}(e_i \theta(k)) := \tau_{e_i} \Theta \Phi_S(k) \triangleq \varepsilon \quad \text{for } k \in F_{1,+} \cap \{k_3 \geq 0\}.$$

This extension is continuous. Indeed, continuity along $E_{15} \cup \theta(E_{15}) = F_{1,0} \cap \{k_3 = 0\}$ (respectively $E_{48} \cup e_i \theta(E_{48}) = F_{1,+} \cap \{k_3 = 0\}$) is a consequence of the edge symmetries that we have imposed on $\Phi_S$ in Step 3c (respectively in Step 3d). What we have to verify is that the definition of $\Phi_{S'}$ that we have just given on
Figure 3. Steps in the proof of Theorem 3

t_{e_2} \theta(E_{12}) = (F_{1,0} \cap \{k_3 \leq 0\}) \cap F_{2,-} \quad \text{and} \quad t_{e_1-e_2} \theta(E_{34}) = (F_{1,+} \cap \{k_3 \leq 0\}) \cap F_{2,-}

agrees with the definition of $\Phi_S$ on the same edges that was achieved in Step 3b.

We look at $t_{e_2} \theta(E_{12})$, since the case of $t_{e_1-e_2} \theta(E_{34})$ is analogous. If $k \in E_{12}$, then $\Phi_S(t_{e_2} \theta(k)) = \tau_{-e_2} \Theta \Phi_S(k) \triangleleft \varepsilon$, since in Step 3b we imposed the edge symmetries on $F_{3,-}$. On the other hand, $\Phi_{S'}(k) = \Phi_S(k)$ on $E_{12} \subset S$ by definition of $\Phi_{S'}$: we
get then also
\[ \Phi_S(t_{-e_2}\theta(k)) = \tau_{-e_2}\Theta\Phi_S(k) \prec \varepsilon = \tau_{-e_2}\Theta\Phi_{S'}(k) \prec \varepsilon = \tau_{-e_2}\Theta\tau_{-e_2}\Phi_{S'}(t_{e_2}(k)) \prec \varepsilon \]

because of the edge symmetries satisfied by \( \Phi_{S'} \) on the shorter edges of \( F_{1,0} \cap \{ k_3 \geq 0 \} \). In view of \( (P_3) \) and of the definition of \( \Phi_{S'} \) on \( F_{1,0} \cap \{ k_3 \leq 0 \} \), we conclude that
\[ \Phi_S(t_{-e_2}\theta(k)) = \Theta\Phi_{S'}(t_{e_2}(k)) \prec \varepsilon = \Phi_{S'}(\theta t_{e_2}(k)) = \Phi_{S'}(t_{-e_2}\theta(k)) \]
as wanted. This shows that \( \Phi_{S'} \) is continuous on
\[ S' := S \cup (F_{1,0} \cap \{ k_3 \leq 0 \}) \cup (F_{1,+} \cap \{ k_3 \leq 0 \}) \).

Step 5. Extend the definition of \( \Phi_{S'} \) to \( F_{3,-} \) by setting
\[ \Phi_{S'}(k) := \Phi_{S'}(k) \quad \text{for } k \in S', \quad \text{and} \]
\[ \Phi_{S'}(t_{-e_3}(k)) := \tau_{-e_3}\Phi_{S'}(k) \quad \text{for } k \in F_{3,+}. \]

This extension is continuous on \( t_{-e_3}(E_{23}) = F_{2,-} \cap F_{3,-} \) because in Step 3b we have imposed on \( \Phi_S \) the edge symmetries on the shorter edges of \( F_{2,-}. \) Similarly, \( \Phi_{S'} \) and \( \Phi_{S''} \) agree on \( \theta(E_{26}) \cup t_{-e_3}(E_{26}) = F_{1,0} \cap F_{3,-} \) and on \( t_{-e_3}(E_{37}) \cup \theta t_{e_1}(E_{37}) = F_{1,+} \cap F_{3,-}, \) because by construction \( \Phi_{S'} \) is \( \tau \)-equivariant. We have constructed so far a continuous Bloch frame \( \Phi_{S''} \) on \( S'' := S' \cup F_{3,-}. \)

Step 6. Extend the definition of \( \Phi_{S''} \) to \( F_{2,+} \) by setting
\[ \hat{\Phi}(k) := \Phi_{S''}(k) \quad \text{for } k \in S'', \quad \text{and} \]
\[ \hat{\Phi}(t_{e_2}(k)) := \tau_{e_2}\Phi_{S''}(k) \quad \text{for } k \in F_{2,-}. \]

Similarly to what was argued in Step 5, the edge symmetries (i.e. \( \tau \)-equivariance) on \( \partial F_{2,-} \) and \( \partial F_{2,+} \) imply that this extension is continuous. The Bloch frame \( \hat{\Phi} \) is now defined and continuous on \( \partial B^{(3)}_{\text{eff}}. \)

Step 7. Finally, extend the definition of \( \hat{\Phi} \) on the interior of \( B^{(3)}_{\text{eff}} \). As was argued before at the end of Section \( \text{[072]} \) this step is topologically unobstructed. Thus, we end up with a continuous symmetric Bloch frame \( \Phi_{\text{eff}} \) on \( B^{(3)}_{\text{eff}}. \) Set now
\[ \Phi_{\text{uc}}(k) := \begin{cases} \Phi_{\text{eff}}(k) & \text{if } k \in B^{(3)}_{\text{eff}}, \\ \Theta\Phi_{\text{eff}}(\theta(k)) \prec \varepsilon & \text{if } k \in B^{(3)} \setminus B^{(3)}_{\text{eff}}. \end{cases} \]

The symmetries satisfied by \( \Phi_{\text{eff}} \) on \( F_{1,0} \) (imposed in Step 4) imply that the Bloch frame \( \Phi_{\text{uc}} \) is still continuous. We extend now the definition of \( \Phi_{\text{uc}} \) to the whole \( \mathbb{R}^3 \) by setting
\[ \Phi(k) := \tau_{k'}\Phi_{\text{uc}}(k'), \quad \text{if } k = k' + \lambda \text{ with } k' \in B^{(3)} \setminus B^{(3)}_{\text{eff}}, \lambda \in \Lambda. \]

Again, the symmetries imposed on \( \Phi_{\text{uc}} \) in the previous Steps of the proof ensure that \( \Phi \) is continuous, and by construction it is also symmetric. This concludes the proof of Theorem 3. \( \square \)
6.4. Comparison with the Fu-Kane-Mele indices. In their work [FKM], Fu, Kane and Mele generalized the definition of $\mathbb{Z}_2$ indices for 2d topological insulators, appearing in [FK], to 3d topological insulators. There the authors mainly use the formulation of $\mathbb{Z}_2$ indices given by evaluation of certain quantities at the inequivalent time-reversal invariant momenta $k_\lambda$, as in (5.3). We briefly recall the definition of the four Fu-Kane-Mele $\mathbb{Z}_2$ indices for the reader’s convenience.

In the 3-dimensional unit cell $\mathbb{B}(3)$, there are only eight vertices which are inequivalent up to periodicity: these are the points $k_\lambda$ corresponding to $\lambda = (n_1/2, n_2/2, n_3/2)$, where each $n_j$ can be either 0 or 1. These are the vertices in Figure 2 that are connected by thick lines. Define the matrix $w$ as in (4.1), where $\Psi$ is a continuous and $\tau$-equivariant Bloch frame (whose existence is guaranteed again by the generalization of the results of [Pa] given in [MP]). Set

$$
\eta_{n_1,n_2,n_3} := \frac{\det w(k_\lambda)}{\text{Pf} w(k_\lambda)} \bigg|_{\lambda=(n_1/2,n_2/2,n_3/2)}.
$$

Then the four Fu-Kane-Mele $\mathbb{Z}_2$ indices $\nu_0, \nu_1, \nu_2, \nu_3 \in \mathbb{Z}_2$ are defined as [FKM, Eqn.s (2) and (3)]

$$
(-1)^{\nu_0} := \prod_{n_1,n_2,n_3 \in \{0,1\}} \eta_{n_1,n_2,n_3},
$$

$$
(-1)^{\nu_i} := \prod_{n_i=1, n_j \neq i \in \{0,1\}} \eta_{n_1,n_2,n_3}, \quad i \in \{1, 2, 3\}.
$$

In other words, the Fu-Kane-Mele 3d index $(-1)^{\nu_0}$ equals the Fu-Kane 2d index $(-1)^\Delta$ for the face where the $i$-th coordinate is set equal to 1/2, while the index $(-1)^{\nu_0}$ involves the product over all the inequivalent time-reversal invariant momenta $k_\lambda$.

Since our invariants $\delta_{i,0}$ and $\delta_{i,+}$, $i = 1, 2, 3$, are defined as the 2-dimensional $\mathbb{Z}_2$ invariants relative to certain (effective) faces on the boundary of the 3-dimensional unit cell, they also satisfy identities which express them as product of quantities to be evaluated at vertices of the effective unit cell, as in Section 5 (compare (5.2) and (5.4)). Explicitly, these expressions read as

$$
(-1)^{\delta_{i,0}} := \prod_{n_1=0,n_2,n_3 \in \{0,1\}} \hat{\eta}_{n_1,n_2,n_3},
$$

$$
(-1)^{\delta_{i,+}} := \prod_{n_i=1, n_j \neq i \in \{0,1\}} \hat{\eta}_{n_1,n_2,n_3}, \quad i \in \{1, 2, 3\},
$$

where (compare (5.2))

$$
\hat{\eta}_{n_1,n_2,n_3} := \frac{\sqrt{\det U(k_\lambda)^2}}{\det U(k_\lambda)} \bigg|_{\lambda=(n_1/2,n_2/2,n_3/2)}.
$$
As we have also shown in Section 4 that our 2-dimensional invariant $\delta$ agrees with the Fu-Kane index $\Delta$, from the previous considerations it follows at once that

$$\nu_i = \delta_{i,+} \in \mathbb{Z}_2, \ i \in \{1, 2, 3\}, \ \text{and} \ \nu_0 = \delta_{1,0} + \delta_{1,+} \in \mathbb{Z}_2.$$  

This shows that the four $\mathbb{Z}_2$ indices proposed by Fu, Kane and Mele are compatible with ours, and in turn our reformulation proves that indeed these $\mathbb{Z}_2$ indices represent the obstruction to the existence of a continuous symmetric Bloch frame in $3d$. The geometric rôle of the Fu-Kane-Mele indices is thus made transparent.

We also observe that, under this identification, the indices $\nu_i, i \in \{1, 2, 3\}$, depend manifestly on the choice of a basis $\{e_1, e_2, e_3\} \subset \mathbb{R}^d$ for the lattice $\Lambda$, while the index $\nu_0$ is independent of such a choice. This substantiates the terminology of [FKM], where $\nu_0$ is called “strong” invariant, while $\nu_1, \nu_2$ and $\nu_3$ are referred to as “weak” invariants.
Appendix A. Smoothing procedure

Throughout the main body of the paper, we have mainly considered the issue of the existence of a continuous global symmetric Bloch frame for a family of projectors \( \{ P(k) \}_{k \in \mathbb{R}^d} \) satisfying Assumption 1. This Appendix is devoted to showing that, if such a continuous Bloch frame exists, then also a smooth one can be found, arbitrarily close to it. The topology in which we measure “closeness” of frames is given by the distance

\[
\text{dist}(\Phi, \Psi) := \sup_{k \in \mathbb{R}^d} \left( \sum_{a=1}^{m} \| \phi_a(k) - \psi_a(k) \|_2^2 \right)^{1/2}
\]

for two global Bloch frames \( \Phi = \{ \phi_a(k) \}_{a=1, \ldots, m, k \in \mathbb{R}^d} \) and \( \Psi = \{ \psi_a(k) \}_{a=1, \ldots, m, k \in \mathbb{R}^d} \).

The following result holds in any dimension \( d \geq 0 \).

**Proposition 5.** Let \( \{ P(k) \}_{k \in \mathbb{R}^d} \) be a family of orthogonal projectors satisfying Assumption 1. Assume that a continuous global symmetric Bloch frame \( \Phi \) exists for \( \{ P(k) \}_{k \in \mathbb{R}^d} \). Then for any \( \mu > 0 \) there exists a smooth global symmetric Bloch frame \( \Phi_{\text{sm}} \) such that

\[
\text{dist}(\Phi, \Phi_{\text{sm}}) < \mu.
\]

**Proof.** We use the same strategy used to prove Proposition 5.1 in [FMP], to which we refer for most details.

As was already noticed (see Remark 3), a global Bloch frame gives a section of the principal \( \mathcal{U}(\mathbb{C}^m) \)-bundle \( \text{Fr}(P) \to T^d \), the frame bundle associated with the Bloch bundle \( P \to T^d \), whose fibre \( \text{Fr}(P)_k =: F_k \) over the point \( k \in T^d \) consists of all orthonormal bases in \( \text{Ran} \, P(k) \). The existence of a continuous global Bloch frame \( \Phi \) is thus equivalent to the existence of a continuous section of the frame bundle \( \text{Fr}(P) \).

By Steenrod’s ironing principle [St, Wo], there exists a smooth section of the frame bundle arbitrarily close to the latter continuous one; going back to the language of Bloch frames, this implies for any \( \mu > 0 \) the existence of a smooth global Bloch frame \( \Phi_{\text{sm}} \) such that

\[
\text{dist}(\Phi, \Phi_{\text{sm}}) < \frac{\mu}{2}.
\]

The Bloch frame \( \Phi_{\text{sm}} \) will not in general be also symmetric, so we apply a symmetrization procedure to \( \Phi_{\text{sm}} \) to obtain the desired smooth symmetric Bloch frame \( \Phi_{\text{sm}} \). In order to do so, we define the midpoint between two sufficiently close frames \( \Phi \) and \( \Psi \) in \( F_k \) as follows. Write \( \Psi = \Phi \circ U_{\Phi, \Psi} \), with \( U_{\Phi, \Psi} \) a unitary matrix. If \( \Psi \) is sufficiently close to \( \Phi \), then \( U_{\Phi, \Psi} \) is sufficiently close to the identity matrix \( I_m \) in the standard Riemannian metric of \( \mathcal{U}(\mathbb{C}^m) \) (see [FMP, Section 5] for details). As such, we have that \( U_{\Phi, \Psi} = \exp(A_{\Phi, \Psi}) \), for \( A_{\Phi, \Psi} \in \mathfrak{u}(\mathbb{C}^m) \) a skew-Hermitian matrix, and \( \exp: \mathfrak{u}(\mathbb{C}^m) \to \mathcal{U}(\mathbb{C}^m) \) the exponential map. We define then the midpoint

\[(10)\]
between $\Phi$ and $\Psi$ to be the frame

$$\tilde{M}(\Phi, \Psi) := \Phi \triangleleft \exp\left(\frac{1}{2} A_{\Phi, \Psi}\right).$$

Set

(A.1) \[\Phi_{\text{sm}}(k) := \tilde{M}(\tilde{\Phi}_{\text{sm}}(k), \Theta \tilde{\Phi}_{\text{sm}}(-k) \triangleleft \varepsilon).\]

The proof that $\Phi_{\text{sm}}$ defines a smooth global Bloch frame, which satisfies the $\tau$-equivariance property (F$\prime$\text{3}), and that moreover its distance from the frame $\Phi$ is less than $\mu$ goes exactly as the proof of [FMP, Prop. 5.1]. A slightly different argument is needed, instead, to prove that $\Phi_{\text{sm}}$ is also time-reversal symmetric, i.e. that it satisfies also (F$\prime$\text{4}). To show this, we need a preliminary result.

**Lemma 4.** Let $\Phi, \Psi \in F_k$ be two frames, and assume that $\Phi$ and $\Psi \triangleleft \varepsilon$ are sufficiently close. Then

(A.2) \[\tilde{M}(\Phi, \Psi \triangleleft \varepsilon) = \tilde{M}(\Phi \triangleleft \varepsilon^{-1}, \Psi) \triangleleft \varepsilon.\]

**Proof.** Notice first that

$$\Psi = \Phi \triangleleft U_{\Phi, \Psi} \implies \Psi \triangleleft \varepsilon = \Phi \triangleleft (U_{\Phi, \Psi} \varepsilon) \text{ and } \Psi = (\Phi \triangleleft \varepsilon^{-1}) \triangleleft (\varepsilon U_{\Phi, \Psi}),$$

which means that

$$U_{\Phi, \Psi} = U_{\Phi, \Psi} \varepsilon \text{ and } U_{\Phi, \Psi} = \varepsilon U_{\Phi, \Psi}.$$ Written

$$\varepsilon U_{\Phi, \Psi} = \exp(A) \text{ and } U_{\Phi, \Psi} \varepsilon = \exp(B)$$

for $A, B \in B_\delta(0) \subset \mathfrak{u}(\mathbb{C}^m)$, where $\delta > 0$ is such that $\exp: B_\delta(0) \subset \mathfrak{u}(\mathbb{C}^m) \to B_\delta(1_m) \subset \mathcal{U}(\mathbb{C}^m)$ is a diffeomorphism. Then we have that

(A.3) \[\exp \left(\varepsilon^{-1} A \varepsilon\right) = \varepsilon^{-1} \exp(A) \varepsilon = \varepsilon^{-1} \varepsilon U \varepsilon = U \varepsilon = \exp(B)\]

and, since the Hilbert-Schmidt norm $\|A\|_{\text{HS}}^2 := \text{tr}(A^* A)$ is invariant under unitary conjugation, also $\varepsilon^{-1} A \varepsilon \in B_\delta(0)$. It then follows from (A.3) that $B = \varepsilon^{-1} A \varepsilon$, because the exponential map is a diffeomorphism. From this we can conclude that

$$\tilde{M}(\Phi \triangleleft \varepsilon^{-1}, \Psi) \triangleleft \varepsilon = (\Phi \triangleleft \varepsilon^{-1}) \triangleleft \left(\exp\left(\frac{1}{2} A\right)\varepsilon\right) =$$

$$= \Phi \triangleleft \exp\left(\frac{1}{2} \varepsilon^{-1} A \varepsilon\right) = \Phi \triangleleft \exp\left(\frac{1}{2} B\right) =$$

$$= \tilde{M}(\Phi, \Psi \triangleleft \varepsilon)$$

which is exactly (A.2). \qed

say that the two frames $\Phi$ and $\Psi$ should be “sufficiently close”, we mean (here and in the following) that the unitary matrix $U_{\Phi, \Psi}$ lies in the ball $B_\delta(1_m)$. 

We are now in position to prove that $\Phi_{sm}$, defined in (A.1), satisfies $[F']$. Indeed, we compute

$$
\Theta \Phi_{sm}(k) \triangleleft \varepsilon = \Theta \tilde{M}(\tilde{\Phi}_{sm}(k), \Theta \tilde{\Phi}_{sm}(-k) \triangleleft \varepsilon) \triangleleft \varepsilon =
$$

$$
= \tilde{M}(\Theta \tilde{\Phi}_{sm}(k), \Theta^2 \tilde{\Phi}_{sm}(-k) \triangleleft \varepsilon) \triangleleft \varepsilon = \quad \text{(by [FMP], Eqn. (5.11))}
$$

$$
= \tilde{M}(\Theta \tilde{\Phi}_{sm}(k), \tilde{\Phi}_{sm}(-k) \triangleleft \varepsilon^{-1}) \triangleleft \varepsilon = \quad \text{(because $-\varepsilon = \varepsilon^{-1}$ by Remark 2)}
$$

$$
= \tilde{M}(\tilde{\Phi}_{sm}(-k) \triangleleft \varepsilon^{-1}, \Theta \tilde{\Phi}_{sm}(k)) \triangleleft \varepsilon = \quad \text{(because $\tilde{M}(\Phi, \Psi) = \tilde{M}(\Psi, \Phi)$)}
$$

$$
= \tilde{M}(\tilde{\Phi}_{sm}(-k), \Theta \tilde{\Phi}_{sm}(k) \triangleleft \varepsilon) = \Phi_{sm}(-k) = \Phi_{sm}(k) \quad \text{(by (A.2)).}
$$

This concludes the proof of the Proposition. □
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