Scuola Internazionale Superiore di Studi Avanzati - Trieste

Area of Mathematics
Ph.D. in Mathematical Physics

Thesis

Geometric phases in graphene and topological insulators

Candidate
Domenico Monaco

Supervisor
prof. Gianluca Panati
("La Sapienza" Università di Roma)

Internal co-Supervisor
prof. Ludwik Dąbrowski

Thesis submitted in partial fulfillment of the requirements for the degree of Philosophiæ Doctor

academic year 2014-15

SISSA - Via Bonomea 265 - 34136 TRIESTE - ITALY

Thesis defended in front of a Board of Examiners composed by

prof. Ludwik Dąbrowski, dr. Alessandro Michelangeli, and prof. Cesare Reina as internal members, and

prof. Gianluca Panati ("La Sapienza" Università di Roma), prof. Stefan Teufel (Eberhard Karls Universität Tübingen) as external members

on September 15th, 2015

Abstract

This thesis collects three of the publications that the candidate produced during his Ph.D. studies. They all focus on geometric phases in solid state physics.

We first study topological phases of 2-dimensional periodic quantum systems, in absence of a spectral gap, like *e. g.* (multilayer) graphene. A topological invariant $n_v \in \mathbb{Z}$, baptized eigenspace vorticity, is attached to any intersection of the energy bands, and characterizes the local topology of the eigenprojectors around that intersection. With the help of explicit models, each associated to a value of $n_v \in \mathbb{Z}$, we are able to extract the decay at infinity of the single-band Wannier function w in mono- and bilayer graphene, obtaining $|w(x)| \le \text{const} \cdot |x|^{-2}$ as $|x| \to \infty$.

Next, we investigate gapped periodic quantum systems, in presence of time-reversal symmetry. When the time-reversal operator Θ is of bosonic type, *i. e.* it satisfies $\Theta^2 = \mathbb{1}$, we provide an explicit algorithm to construct a frame of smooth, periodic and time-reversal symmetric (quasi-)Bloch functions, or equivalently a frame of almost-exponentially localized, real-valued (composite) Wannier functions, in dimension $d \le 3$. In the case instead of a fermionic time-reversal operator, satisfying $\Theta^2 = -\mathbb{1}$, we show that the existence of such a Bloch frame is in general topologically obstructed in dimension $d = 2$ and $d = 3$. This obstruction is encoded in $\mathbb{Z}_2$-valued topological invariants, which agree with the ones proposed in the solid state literature by Fu, Kane and Mele.

Acknowledgements

First and foremost, I want to thank my supervisor, Gianluca Panati, who lured me into Quantum Mechanics and Solid State Physics when I was already hooked on Topology and Differential Geometry, and then showed me that there isn't really that much of a difference if you know where to look.

During the years of my Ph.D. studies, I have had the occasion to discuss with several experts in Mathematics and Physics, who guided my train of thoughts into new and fascinating directions, and to whom I am definitely obliged. Big thanks to Jean Bellissard, Raffaello Bianco, Horia Cornean, Ludwik Dąbrowski, Giuseppe De Nittis, Gianfausto dell'Antonio, Domenico Fiorenza, Gian Michele Graf, Peter Kuchment, Alessandro Michelangeli, Adriano Pisante, Marcello Porta, Emil Prodan, Raffaele Resta, Shinsei Ryu, Hermann Schulz-Baldes, Clément Tauber, Stefan Teufel, and Andrea Trombettoni.

I am also extremely grateful to Riccardo Adami, Claudio Cacciapuoti, Raffaele Carlone, Michele Correggi, Pavel Exner, Luca Fanelli, Rodolfo Figari, Alessandro Giuliani, Ennio Gozzi, Gianni Landi, Mathieu Lewin, Gherardo Piacitelli, Alexander Sobolev, Jan Philip Solovej, Alessandro Teta, and Martin Zirnbauer, for inviting me to the events they organized and granting me the opportunity to meet many amusing and impressive people.

Contents

Introduction

1 Geometric phases of quantum matter

In the last 30 years, the origin of many interesting phenomena which were discovered in quantum mechanical systems was established to lie in *geometric phases* [45]. The archetype of such phases is named after sir Michael V. Berry [8], and was early related by Barry Simon [46] to the holonomy of a certain $U(1)$-bundle over the *Brillouin torus* (see Section 2.1). *Berry's phase* is a dynamical phase factor that is acquired by a quantum state on top of the standard energy phase, when the evolution is driven through a loop in some parameter space. In applications to condensed matter systems, this parameter space is usually the Brillouin zone. As an example, one of the most prominent incarnations of Berry's phase effects in solid state physics can be found in the *modern theory of polarization* [47], in which changes of the electronic terms in the polarization vector, $\Delta\mathbf{P}_{\mathrm{el}}$, through an adiabatic cycle are indeed expressed as differences of geometric phases. This result, first obtained by R.D. King-Smith and David Vanderbilt [26], was later elaborated by Raffaele Resta [42]. In more recent years, the Altland-Zirnbauer classification of random Hamiltonians in presence of discrete simmetries [1] sparked the interest in geometric labels attached to quantum phases of matter, and paved the way for the advent of *topological insulators* (see Section 1.2).

After being confined to the realm of high-energy physics and gauge theories, topology and geometry made their entrance, through Berry's phase, in the low-energy world of condensed matter systems. This Section is devoted to giving an informal overview on two instances of such geometric effects in solid state physics, namely the *quantum Hall effect* and the *quantum spin Hall effect*, which are of relevance also for the candidate's works presented in this thesis in Parts I and II.

1.1 Quantum Hall effect

One of the first and most striking occurrences of a topological index attached to a quantum phase of matter is that of the *quantum Hall effect* [50, 17].

The experimental setup for the Hall effect consists in putting a very thin slab of a crystal (making it effectively 2-dimensional) into a constant magnetic field, whose direction $\hat{z}$ is orthogonal to the plane Oxy in which the sample lies. If an electric current is induced, say, in direction $\hat{x}$, the charge carriers will experience a Lorentz force, which will make them accumulate along the edges in the transverse direction. If these edges are short-circuited, this will result in a transverse current flow j, called *Hall current* (see Figure 1).

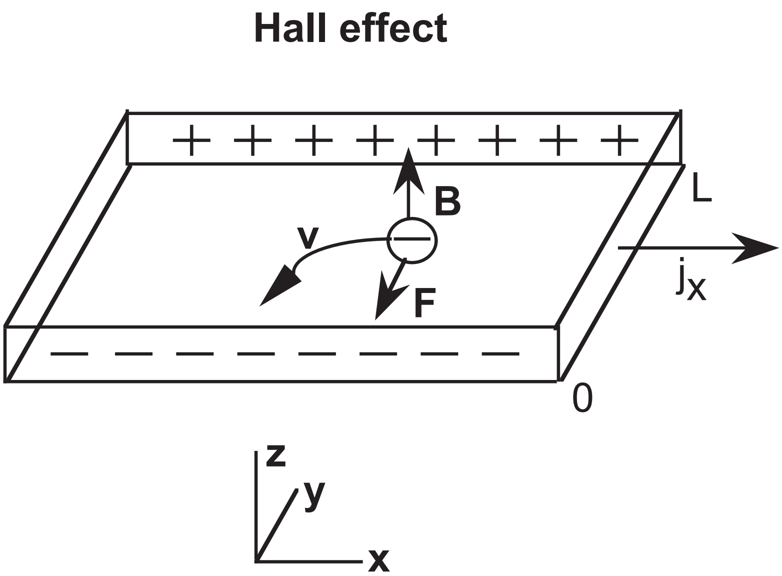


Fig. 1 The experimental setup for the (quantum) Hall effect.

The relation between this induced current and the applied electric field E is expressed by means of a 2×2 skew-symmetric tensor σ:

$$j = \sigma E, \quad \sigma = \begin{pmatrix} 0 & \sigma_{xy} \\ -\sigma_{xy} & 0 \end{pmatrix}.$$

The quantity σ_{xy} is called the *Hall conductivity*; since the setting is 2-dimensional[1], its inverse $\rho_{xy} = 1/\sigma_{xy}$ coincides with the *Hall resistivity*. The expected behaviour of this quantity as a function of the applied magnetic field B is linear, *i. e.* $\rho_{xy} \propto B$. In 1980, Klaus von Klitzing and his collaborators [49] performed the same experiment but at very low temperatures, so that quantum effects became relevant. What they observed was striking: the Hall resistivity displays *plateaus*, in which it stays *constant* as a function of the magnetic field, with sudden jumps between different plateaus (see Figure 2); moreover, the value of these plateaus comes exactly at inverses of integer numbers, in units of a fundamental quantum h/e^2 (where h is Planck's constant and e the charge of a carrier):

$$\sigma_{xy} = n\frac{e^2}{h}, \quad n \in \mathbb{Z}. \tag{1.1}$$

[1] Also the resistivity ρ is a skew-symmetric tensor, defined as the inverse of the conductivity tensor σ. In 2-dimensions, however, the resistivity tensor is characterized just by one non-zero entry ρ_{xy}.

This quantization phenomenon came to be known as the *quantum Hall effect*. The experimental precision of these measurements was incredible (in recent experiments this quantization rule can be measured up to an absolute error of $10^{-10} \sim 10^{-11}$), which lead also to applications in metrology, setting a new precision standard in the measurement of electric resistivity.

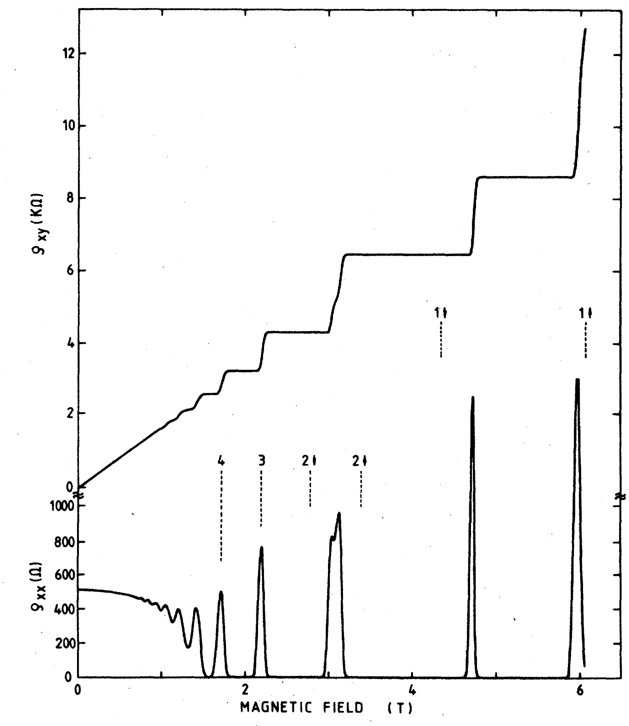


FIG. 14. Experimental curves for the Hall resistance $R_H = \rho_{xy}$ and the resistivity $\rho_{xx} \sim R_x$ of a heterostructure as a function of the magnetic field at a fixed carrier density corresponding to a gate voltage $V_g = 0$ V. The temperature is about 8 mK.

Fig. 2 The Hall resistivity ρ_{xy} as a function of the magnetic field B. The figure is taken from [50].

This peculiar quantization phenomenon rapidly attracted the attention of theoretical and mathematical physicists, seeking for its explanation: we refer to the review of Gian Michele Graf [17] where the author presents the three main intepretations that where proposed in the 1980's and 1990's in the mathematical physics community. The quantum Hall effect was put on mathematically rigorous grounds mainly by the group of Yosi Avron, Rudi Seiler, and Barry Simon [4, 5], as well as the one of Jean Bellissard and Hermann Schulz-Baldes [6, 23], with mutual exchanges of ideas. Elaborating on the pioneering work of Thouless, Kohmoto, Nightingale and den Nijs [48], both groups were able to interpret the integer appearing in the expression (1.1) for the Hall conductivity as a *Chern number* (see Section 2.2), explaining its topological origin and its quantization at the same time. The methods used by the two groups, however, are extremely different: Avron and his collaborators exploited techniques from differential geometry and gauge theory to formalize the so-called Laughlin argument, while Bellissard and his collaborators made use of results from noncommutative geometry and K-theory, establishing also a *bulk-edge corre-*

spondence, which makes their theory applicable also to *disordered* media. Having a framework that allows to include disorder is also convenient to qualify the quantization phenomenon as "topological": it should be robust against (small) perturbations of the system, among which one can include also randomly distributed impurities.

1.2 Quantum spin Hall effect and topological insulators

Almost 25 years after the discovery of the quantum Hall effect, topological phenomena made a new appeareance in the world of solid state physics, in what is now the flourishing field of *topological insulators* [19, 40, 14, 2]. These materials, first theorized and soon experimentally realized around 2005-2006, exhibit the peculiar feature of being insulating in the bulk but conducting on the boundary, thus becoming particularly appealing for applications *e. g.* in low-resistence current transport.

The founding pillar of this still very active research field is the work by Alexander Altland and Martin R. Zirnbauer [1]. Inspired by the classification of random matrix models by Dyson in terms of unitary (GUE), orthogonal (GOE) and symplectic (GSE) matrices (the so-called "threefold way"), Altland and Zirnbauer extended this classification to include also other *discrete* symmetries which are of interest for quantum systems, namely *charge conjugation* (or *particle-hole symmetry*), *time-reversal symmetry* and *chiral symmetry*. It was then realized that this classification could be used to produce models of *topological phases of quantum matter* in solid state physics, regarding quantum Hamiltonians as matrix-valued maps from the Brillouin zone which are subject to some of these symmetries. Around 2010, then, a number of *periodic tables of topological insulators* appeared [27, 43, 24, 25], discussing the topological labels that could be attached to these phases. From these tables it immediately becomes apparent that the number of possible symmetry classes is 10: this motivated the terminology "tenfold way" (see Table 1).

It should be stressed that the terminology "geometric" or "topological phase" is used, in this context, with a different acceptation than the one which applies, for example, to Berry's phase (a complex number of modulus 1, stemming from the holonomy of a $U(1)$ gauge theory). In the present framework, the term "phase" carries a meaning more similar to the one used in statistical mechanics and thermodynamics, to describe a particular class of physical states qualitatively characterized by the values of some macroscopic observable. As an example, one can use macroscopic magnetization to distinguish between the magnetic and non-magnetic phases of a thermodynamical system. In the quantum Hall effect, as we saw in the previous Section, it is instead the Hall conductivity that distinguishes the various (geometric) phases of the system; quantum Hall systems are indeed included in the Altland-Zirnbauer table, in the A class[2]. The explanation for the quantization of the Hall conductivity by means of Chern numbers can be also reformulated in terms of a Berry phase (see Section 2.2), motivating the slightly ambiguous use of the term "geometric phase"; another example is provided by the Berry phase interpretation of the Aharonov-Bohm effect [8]. The main difference that arises between geometric phases and thermodynamical phases is that in the former case they are characterized by a *topological* or *geometric index*, associated to the Hamiltonian of the system

[2] Other macroscopical observables related to different Altland-Zirnbauer symmetry classes are presented in [27].

Symmetry				Dimension							
AZ	T	C	S	1	2	3	4	5	6	7	8
A	0	0	0	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$
AIII	0	0	1	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0
AI	1	0	0	0	0	0	$\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$
BDI	1	1	1	$\mathbb{Z}$	0	0	0	$\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$
D	0	1	0	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$\mathbb{Z}$	0	$\mathbb{Z}_2$
DIII	-1	1	1	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$\mathbb{Z}$	0
AII	-1	0	0	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$\mathbb{Z}$
CII	-1	-1	1	$\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0
C	0	-1	0	0	$\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0
CI	1	-1	1	0	0	$\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0

Table 1 The periodic table of topological insulators. In the first column, "AZ" stands for the Altland-Zirnbauer (sometimes called Cartan) label [1]. The labels for the symmetries are: T (time-reversal), C (charge-conjugation), S (chirality). Time-reversal symmetry and charge conjugation are $\mathbb{Z}_2$-symmetries implemented antiunitarily, and hence can square to plus or minus the identity: this is the sign appearing in the respective columns (0 stands for a broken symmetry). Chirality is instead implemented unitarily: 0 and 1 stand for absent or present chiral symmetry, respectively. Notice that the composition of a time-reversal and a charge conjugation symmetry is of chiral type. The table repeats periodically after dimension 8 (*i. e.* for example the column corresponding to $d = 9$ would be equal to the one corresponding to $d = 1$, and so on).

or to its ground state manifold, and persist moreover in being distinct also at zero temperature.

Another strong motivation for the creation of these periodic tables came from the advent of *spintronics* [39], namely the observation that in certain materials spin-orbit interactions and time-reversal symmetry combine to generate a separation of robust *spin* (rather than charge) currents, located on the edge of the sample (see Figure 3), that could also be exploited in principle for applications to quantum computing. This framework resembles very much, as long as current generation is concerned, the situation described in the previous Section: indeed, this phenomenon was dubbed *quantum spin Hall effect*. The main difference between the latter and the quantum Hall effect is the fact that the quantity that stays quantized in the "quantum" regime is the *parity* of the number of (spin-filtered) stable edge modes[30]. From a theoretical viewpoint, the seminal works in the field of the quantum spin Hall effect and of quantum spin pumping are the ones by Eugene Mele, Charles Kane and Liang Fu [20, 21, 15, 16]; the first experimental confirmation of quantum spin Hall phenomena (in HgTe quantum wells) where obtained by the group of Shou-Cheng Zhang [7], see also [2] for a comprehensive list of experimentally realized topological insulators. The works by Fu, Kane and Mele were also the first to propose a $\mathbb{Z}_2$ *classification* for quantum spin Hall states, namely the presence of just two distinct classes (the usual insulator and the "topological" one).

As was already remarked, quantum spin Hall systems fall in the row that displays *time-reversal symmetry* (labelled by "AII" in Table 1) in periodic tables for topological insulators. The latter is a $\mathbb{Z}_2$-symmetry of some quantum systems, implemented by an antiunitary operator T acting on the Hilbert space $\mathcal{H}$ of the system. The time-

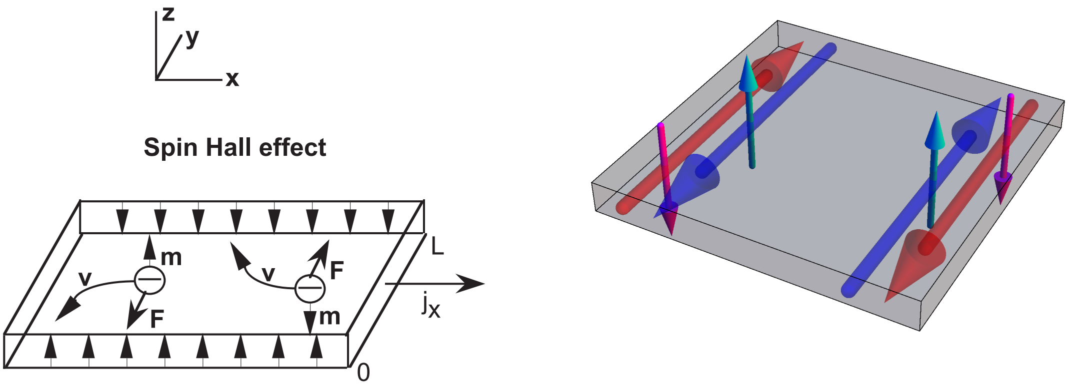


Fig. 3 The experimental setup for the (quantum) spin Hall effect, leading to the formation of spin edge currents.

reversal symmetry operator T is called *bosonic* or *fermionic* depending on whether $T^2 = +\mathbb{1}_{\mathcal{H}}$ or $T^2 = -\mathbb{1}_{\mathcal{H}}$, respectively[3]. This terminology is motivated by the fact that there are "canonical" time-reversal operators when $\mathcal{H} = L^2(\mathbb{R}^d) \otimes \mathbb{C}^{2s+1}$, with $s = 0$ and $s = 1/2$, is the Hilbert space of a spin-s particle: in the former case, T is just complex conjugation C on $L^2(\mathbb{R}^d)$ (and hence squares to the identity), while in the latter T is implemented as $C \otimes \mathrm{e}^{\mathrm{i}\pi S_y}$ on $\mathcal{H} = L^2(\mathbb{R}^d) \otimes \mathbb{C}^2$ (squaring to $-\mathbb{1}_{\mathcal{H}}$), where $S_y = \frac{1}{2}\sigma_2$ and $\sigma_2 = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}$ is the second Pauli matrix. Quantum spin Hall systems fall in the "fermionic" framework, because spin-orbit interactions are needed to play a rôle analogous to that of the external magnetic field in the quantum Hall effect.

Given the stringent analogy between quantum Hall and quantum spin Hall systems, and given also the geometric interpretation, in terms of Chern numbers, that was provided by the mathematical physics community for the labels attached to different quantum phases in the former, it is very tempting to conjecture a topological origin also for the $\mathbb{Z}_2$-valued labels that distinguish different quantum spin Hall phases. Although a heuristic argument for the interpretation of these quantum numbers in terms of topological data was already provided in the original Fu-Kane works [15], from a mathematically rigorous viewpoint the problem remained pretty much open, with the exclusion of pioneering works by Emil Prodan [38], Gian Michele Graf and Marcello Porta [18], Hermann Schulz-Baldes [44], and Giuseppe De Nittis and Kiyonori Gomi [10]. Among the aims of this dissertation is indeed the one to answer the above conjecture, and achieve a purely topological and obstruction-theoretic classification of quantum spin Hall systems in 2 and 3 dimensions (see Part II).

---

[3] Since time-reversal symmetry flips the arrow of time, it must not change the physical description of the system if it is applied twice. Hence T gives a projective unitary representation of the group $\mathbb{Z}_2$ on the Hilbert space $\mathcal{H}$, and as such $T^2 = \mathrm{e}^{\mathrm{i}\theta}\,\mathbb{1}_{\mathcal{H}}$. By antiunitarity, it follows that

$$\mathrm{e}^{\mathrm{i}\theta}\,T = T^2 T = T^3 = T T^2 = T\mathrm{e}^{\mathrm{i}\theta}\,\mathbb{1}_{\mathcal{H}} = \mathrm{e}^{-\mathrm{i}\theta}\,T$$

and consequently $\mathrm{e}^{\mathrm{i}\theta} = \pm 1$.

Before moving to the outline of the dissertation, in the next Section we recall the mathematical tools needed for the modeling of periodic gapped quantum systems, and the geometric classification of their quantum phases.

2 Analysis, geometry and physics of periodic Schrödinger operators

The aim of this Section is to present the main tools coming from analysis and geometry to describe crystalline systems from a mathematical point of view.

2.1 Analysis: Bloch-Floquet-Zak transform

Most of the solids which appear to be homogeneous at the macroscopic scale are modeled by a Hamiltonian operator which is invariant with respect to translations by vectors in a Bravais lattice $\Gamma = \mathrm{Span}_{\mathbb{Z}}\{a_1, \dots, a_d\} \simeq \mathbb{Z}^d \subset \mathbb{R}^d$ (see Figure 4). More precisely, the one-particle Hamiltonian H_Γ of the system is required to commute with these translation operators T_γ:

$$[H_\Gamma, T_\gamma] = 0 \quad \text{for all} \quad \gamma \in \Gamma. \tag{2.1}$$

This feature can be exploited to simplify the spectral analysis of H_Γ, and leads to the so-called *Bloch-Floquet-Zak transform*, that we review in this Section.

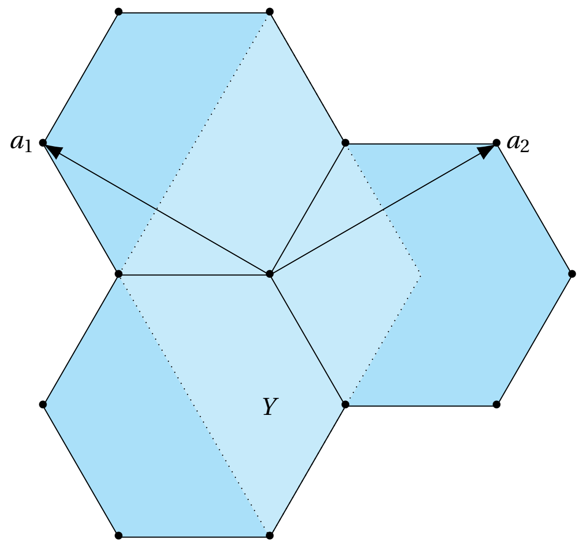


Fig. 4 The Bravais lattice Γ, encoding the periodicity of the crystal, should not be confused with the lattice of ionic cores of the medium. Indeed, also materials like *graphene* (see Part I of this dissertation), whose atoms are arranged to form a honeycomb (hexagonal) structure, are described by a Bravais lattice $\Gamma = \mathrm{Span}_{\mathbb{Z}}\{a_1, a_2\} \simeq \mathbb{Z}^2$. The lightly shaded part of the picture is a unit cell Y for Γ.

As an analogy, consider the free Hamiltonian $H_0 = -\frac{1}{2}\Delta$ on $L^2(\mathbb{R}^d)$, which commutes with all translation operators $(T_a\psi)(x) := \psi(x-a)$, $a \in \mathbb{R}^d$. Then, harmonic analysis provides a unitary operator $\mathcal{F}\colon L^2(\mathbb{R}^d) \to L^2(\mathbb{R}^d)$, namely the Fourier transform, which decomposes functions along the characters $\mathrm{e}^{\mathrm{i}k\cdot x}$ of the representation $T\colon \mathbb{R}^d \to \mathcal{U}(L^2(\mathbb{R}^d))$ and hence reduces H_0 to a multiplication operator in the momentum representation:

$$(\mathcal{F}\psi)(k) = (2\pi)^{-d}\int_{\mathbb{R}^d} \mathrm{d}x\, \mathrm{e}^{\mathrm{i}k\cdot x}\psi(x) \quad\Longrightarrow\quad \mathcal{F}H_0\mathcal{F}^{-1} = |k|^2.$$

We interpret this transformation to a multiplication operator as a "full diagonalization" of H_0. As we will now detail, the Bloch-Floquet-Zak transform operates in a similar way, but exploiting just the translations along vectors in the lattice Γ. It follows that only a "partial diagonalization" can be achieved, and in the Bloch-Floquet-Zak representation there will still remain a part of H_Γ which is in the form of a differential operator and accounts for the portion of the Hilbert space containing the degrees of freedom of a unit cell for Γ.

For the sake of concreteness we will mainly refer to the paradigmatic case of a periodic *real* Schrödinger operator, acting in appropriate (Hartree) units as

$$(H_\Gamma\psi)(x) := -\frac{1}{2}\Delta\psi(x) + V_\Gamma(x)\psi(x), \quad \psi \in L^2(\mathbb{R}^d), \tag{2.2}$$

where V_Γ is a real-valued Γ-periodic function. The latter condition implies immediately that H_Γ satisfies the commutation relation (2.1), where the translation operators are implemented on $L^2(\mathbb{R}^d)$ according to the natural definition

$$(T_\gamma\psi)(x) := \psi(x-\gamma), \quad \gamma \in \Gamma, \quad \psi \in L^2(\mathbb{R}^d).$$

Notice that $T\colon \Gamma \to \mathcal{U}(L^2(\mathbb{R}^d))$, $\gamma \mapsto T_\gamma$, provides a unitary representation of the lattice translation group Γ on the Hilbert space $L^2(\mathbb{R}^d)$. More general Hamiltonians can be treated by the same methods, like for example the *magnetic Bloch Hamiltonian*

$$(H_{\mathrm{MB}}\psi)(x) = \frac{1}{2}\left(-\mathrm{i}\nabla_x + A_\Gamma(x)\right)^2\psi(x) + V_\Gamma(x)\psi(x), \quad \psi \in L^2(\mathbb{R}^d)$$

and the *periodic Pauli Hamiltonian*

$$(H_{\mathrm{Pauli}}\psi)(x) = \frac{1}{2}\big((-\mathrm{i}\nabla_x + A_\Gamma(x))\cdot\sigma\big)^2\psi(x) + V_\Gamma(x)\psi(x), \quad \psi \in L^2(\mathbb{R}^3)\otimes\mathbb{C}^2,$$

where $A_\Gamma\colon \mathbb{R}^d \to \mathbb{R}^d$ is Γ-periodic and $\sigma = (\sigma_1, \sigma_2, \sigma_3)$ is the vector consisting of the three Pauli matrices. Another relevant case is that of Hamiltonians including a linear magnetic potential (thus inducing a constant magnetic field), whose magnetic flux per unit cell is a rational multiple of 2π (in appropriate units); in this case, the commutation relation (2.1) is satisfied, if one considers *magnetic translation operators* T_γ [51].

In view of the commutation relation (2.1), one may look for simultaneous eigenfunctions of H_Γ and the translations $\{T_\gamma\}_{\gamma\in\Gamma}$, *i. e.* for a solution to the problem

$$\begin{cases} (H_\Gamma \psi)(x) = E\psi(x) & E \in \mathbb{R}, \\ \left(T_\gamma \psi\right)(x) = \omega_\gamma \psi(x) & \omega_\gamma \in U(1). \end{cases} \tag{2.3}$$

The eigenvalues of the unitary operators T_γ provide an irreducible representation $\omega\colon \Gamma \to U(1)$, $\gamma \mapsto \omega_\gamma$, of the abelian group $\Gamma \simeq \mathbb{Z}^d$: it follows that ω_γ is a character, *i. e.*

$$\omega_\gamma = \omega_\gamma(k) = \mathrm{e}^{\mathrm{i}k\cdot\gamma}, \quad \text{for some } k \in \mathbb{T}^d_* := \mathbb{R}^d/\Gamma^*.$$

Here Γ^* denotes the dual lattice of Γ, given by those $\lambda \in \mathbb{R}^d$ such that $\lambda\cdot\gamma \in 2\pi\mathbb{Z}$ for all $\gamma \in \Gamma$. The quantum number $k \in \mathbb{T}^d_*$ is called *crystal* (or *Bloch*) *momentum*, and the quotient $\mathbb{T}^d_* = \mathbb{R}^d/\Gamma^*$ is often called *Brillouin torus*.

Thus, the eigenvalue problem (2.3) reads

$$\begin{cases} \left(-\tfrac{1}{2}\Delta + V_\Gamma\right)\psi(k,x) = E\psi(k,x) & E \in \mathbb{R}, \\ \psi(k, x-\gamma) = \mathrm{e}^{\mathrm{i}k\cdot\gamma}\,\psi(k,x) & k \in \mathbb{T}^d_*. \end{cases} \tag{2.4}$$

The above should be regarded as a PDE with k-dependent boundary conditions. The pseudo-periodicity dictated by the second equation prohibits the existence of non-zero solutions in $L^2(\mathbb{R}^d)$. One then looks for *generalized eigenfunctions* $\psi(k,\cdot)$, normalized by imposing

$$\int_Y \mathrm{d}y\,|\psi(k,y)|^2 = 1,$$

where Y is a fundamental unit cell for the lattice Γ.

Existence of solutions to (2.4) as above is guaranteed by *Bloch's theorem* [3], and are hence called *Bloch functions*. Bloch's theorem also gives that each solution ψ to (2.4) decomposes as

$$\psi(k,x) = \mathrm{e}^{\mathrm{i}k\cdot x}u(k,x) \tag{2.5}$$

where $u(k,\cdot)$ is, for any fixed k, a Γ-periodic function of x, thus living in the Hilbert space $\mathcal{H}_\mathrm{f} := L^2(\mathbb{T}^d)$, with $\mathbb{T}^d = \mathbb{R}^d/\Gamma$.

A more elegant and useful approach to obtain such Bloch functions (or rather their Γ-periodic part) is provided by adapting ideas from harmonic analysis, as was mentioned above. One introduces the so-called *Bloch-Floquet-Zak transform*,[4] acting on functions $w \in C_0(\mathbb{R}^d) \subset L^2(\mathbb{R}^d)$ by

$$(\mathcal{U}_{\mathrm{BFZ}}\, w)(k,x) := \frac{1}{|\mathbb{B}|^{1/2}} \sum_{\gamma\in\Gamma} \mathrm{e}^{-\mathrm{i}k\cdot(x-\gamma)}\, w(x-\gamma), \qquad x \in \mathbb{R}^d,\ k \in \mathbb{R}^d. \tag{2.6}$$

Here $\mathbb{B}$ denotes the fundamental unit cell for Γ^*, namely

$$\mathbb{B} := \left\{ k = \sum_{j=1}^d k_j b_j \in \mathbb{R}^d : -\frac{1}{2} \le k_j \le \frac{1}{2} \right\}$$

[4] A comparison with the *classical* Bloch-Floquet transform, appearing in physics textbooks, is provided in Remark 2.1.

where the dual basis $\{b_1, \ldots, b_d\} \subset \mathbb{R}^d$, spanning Γ^*, is defined by $b_i \cdot a_j = 2\pi\delta_{i,j}$.

Notice that from the definition (2.6) it follows at once that the function $\varphi(k,x) = (\mathcal{U}_{\mathrm{BFZ}}\, w)(k,x)$ is Γ-periodic in y and Γ^*-pseudoperiodic in k, *i. e.*

$$\varphi(k+\lambda, x) = \big(\tau(\lambda)\varphi\big)(k,x) := \mathrm{e}^{-\mathrm{i}\lambda\cdot x}\varphi(k,x), \quad \lambda \in \Gamma^*.$$

The operators $\tau(\lambda) \in \mathcal{U}(\mathcal{H}_{\mathrm{f}})$ defined above provide a unitary representation on $\mathcal{H}_{\mathrm{f}}$ of the group of translations by vectors in the dual lattice Γ^*.

The properties of the Bloch-Floquet-Zak transform are summarized in the following theorem, whose proof can be found in [29] or verified by direct inspection (see also [37]).

Theorem 2.1 (Properties of $\mathcal{U}_{\mathrm{BFZ}}$). *1. The definition* (2.6) *extends to give a unitary operator*

$$\mathcal{U}_{\mathrm{BFZ}} \colon L^2(\mathbb{R}^d) \to \mathcal{H}_\tau,$$

also called the Bloch-Floquet-Zak transform, where the Hilbert space of τ-equivariant L^2_{loc}-functions $\mathcal{H}_\tau$ is defined as

$$\mathcal{H}_\tau := \left\{\varphi \in L^2_{\mathrm{loc}}(\mathbb{R}^d; \mathcal{H}_{\mathrm{f}}) : \varphi(k+\lambda) = \tau(\lambda)\,\varphi(k) \textit{ for all } \lambda \in \Gamma^*, \textit{ for a.e. } k \in \mathbb{R}^d\right\}.$$

Its inverse is then given by

$$\big(\mathcal{U}_{\mathrm{BFZ}}^{-1}\varphi\big)(x) = \frac{1}{|\mathbb{B}|^{1/2}} \int_{\mathbb{B}} \mathrm{d}k\, \mathrm{e}^{\mathrm{i}k\cdot x}\varphi(k,x).$$

2. One can identify $\mathcal{H}_\tau$ with the constant fiber direct integral [41, Sec. XIII.16]

$$\mathcal{H}_\tau \simeq L^2(\mathbb{B}; \mathcal{H}_{\mathrm{f}}) \simeq \int_{\mathbb{B}}^{\oplus} \mathrm{d}k\, \mathcal{H}_{\mathrm{f}}, \quad \mathcal{H}_{\mathrm{f}} = L^2(\mathbb{T}^d).$$

Upon this identification, the following hold:

$$\begin{aligned}
\mathcal{U}_{\mathrm{BFZ}}\, T_\gamma\, \mathcal{U}_{\mathrm{BFZ}}^{-1} &= \int_{\mathbb{B}}^{\oplus} \mathrm{d}k \left(\mathrm{e}^{\mathrm{i}k\cdot\gamma}\, \mathbb{1}_{\mathcal{H}_{\mathrm{f}}}\right), \\
\mathcal{U}_{\mathrm{BFZ}} \left(-\mathrm{i}\frac{\partial}{\partial x_j}\right) \mathcal{U}_{\mathrm{BFZ}}^{-1} &= \int_{\mathbb{B}}^{\oplus} \mathrm{d}k \left(-\mathrm{i}\frac{\partial}{\partial y_j} + k_j\right), \qquad j \in \{1, \ldots, d\}, \\
\mathcal{U}_{\mathrm{BFZ}} f_\Gamma(x) \mathcal{U}_{\mathrm{BFZ}}^{-1} &= \int_{\mathbb{B}}^{\oplus} \mathrm{d}k\, f_\Gamma(y), \qquad \textit{if } f_\Gamma \textit{ is } \Gamma\textit{-periodic.}
\end{aligned}$$

In particular, if $H_\Gamma = -\frac{1}{2}\Delta + V_\Gamma$ is as in (2.2) *then*

$$\mathcal{U}_{\mathrm{BFZ}}\, H_\Gamma\, \mathcal{U}_{\mathrm{BFZ}}^{-1} = \int_{\mathbb{B}}^{\oplus} \mathrm{d}k\, H(k), \quad \textit{where} \quad H(k) = \frac{1}{2}\big(-\mathrm{i}\nabla_y + k\big)^2 + V_\Gamma(y). \tag{2.7}$$

3. Let $\varphi = \mathcal{U}_{\mathrm{BFZ}}\, w$ and $r \in \mathbb{N}$. Then the following are equivalent:

(i) $\varphi \in H^r_{\mathrm{loc}}(\mathbb{R}^d; \mathcal{H}_{\mathrm{f}}) \cap \mathcal{H}_\tau$;

(ii) $\langle x\rangle^r\, w \in L^2(\mathbb{R}^d)$, where $\langle x\rangle := (1+|x|^2)^{1/2}$.

In particular, $\varphi \in C^\infty(\mathbb{R}^d;\mathcal{H}_\mathrm{f}) \cap \mathcal{H}_\tau$ *if and only if* $\langle x\rangle^r w \in L^2(\mathbb{R}^d)$ *for all* $r \in \mathbb{N}$.

4. *Let* $\varphi = \mathcal{U}_\mathrm{BFZ} w$ *and* $\alpha > 0$. *Then the following are equivalent:*
   (i) φ *admits an analytic extension* Φ *in the strip*

$$\Omega_\alpha := \left\{ \kappa = (\kappa_1,\dots,\kappa_d) \in \mathbb{C}^d : |\Im \kappa_j| < \frac{\alpha}{2\pi\sqrt{d}} \text{ for all } j \in \{1,\dots,d\} \right\}, \tag{2.8}$$

   such that, if $\kappa = k + \mathrm{i}h \in \Omega_\alpha$ *with* $k,h \in \mathbb{R}^d$, *then* $k \mapsto \phi_h(k) := \Phi(k+\mathrm{i}h)$ *is an element of* $\mathcal{H}_\tau$ *with* $\mathcal{H}_\tau$*-norm uniformly bounded in* h;
   (ii) $\mathrm{e}^{\beta|x|} w \in L^2(\mathbb{R}^d)$ *for all* $0 \le \beta < \alpha$.

Whenever the operator V_Γ is Kato-small with respect to the Laplacian (*i. e.* infinitesimally Δ-bounded), *e. g.* if

$$V_\Gamma \in L^2_\mathrm{loc}(\mathbb{R}^d) \text{ for } d \le 3, \qquad \text{or} \qquad V_\Gamma \in L^p_\mathrm{loc}(\mathbb{R}^d) \text{ with } p > d/2 \text{ for } d \ge 4,$$

then the operator $H(k)$ appearing in (2.7), called the *fiber Hamiltonian*, is self-adjoint on the k-independent domain $\mathcal{D} = H^2(\mathbb{T}^d) \subset \mathcal{H}_\mathrm{f}$. The k-independence of the domain of self-adjointness, which considerably simplifies the mathematical analysis, is the main motivation to use the Bloch-Floquet-Zak transform (2.6) instead of the classical Bloch-Floquet transform (compare the following Remark). Notice in addition that the fiber Hamiltonians enjoy the τ-covariance relation

$$H(k+\lambda) = \tau(\lambda) H(k) \tau(\lambda)^{-1}, \quad k \in \mathbb{R}^d,\ \lambda \in \Gamma^*,$$

and that moreover, since V_Γ is real-valued,

$$H(-k) = C H(k) C^{-1}, \quad k \in \mathbb{R}^d$$

where $C\colon \mathcal{H}_\mathrm{f} \to \mathcal{H}_\mathrm{f}$ acts as complex conjugation. A similar relation holds also in the case of the periodic Pauli Hamiltonian $H_\mathrm{Pauli} = \frac{1}{2}((-\mathrm{i}\nabla_x + A_\Gamma)\cdot\sigma)^2 + V_\Gamma$, whose fiber Hamiltonian $H_\mathrm{Pauli}(k)$ satisfies

$$H_\mathrm{Pauli}(-k) = C_s H_\mathrm{Pauli}(k) C_s^{-1}$$

with $C_s = (\mathbb{1} \otimes \mathrm{e}^{-\mathrm{i}\pi S_y})C$ on $L^2(\mathbb{R}^3)\otimes\mathbb{C}^2$, and S_y the y-component of the spin operator. Since both C and C_s are antiunitary operators, these are instances of a *time-reversal symmetry* (in Bloch momentum space), as mentioned in the previous Section; in the first case it is of bosonic type, since $C^2 = \mathbb{1}$, while the second one is of fermionic type, since $C_s^2 = -\mathbb{1}$.

Remark 2.1 (Comparison with classical Bloch-Floquet theory). In most solid state physics textbooks [3], the *classical* Bloch-Floquet transform is defined as

$$(\mathcal{U}_\mathrm{BF}\, w)(k,x) := \frac{1}{|\mathbb{B}|^{1/2}} \sum_{\gamma\in\Gamma} \mathrm{e}^{\mathrm{i}k\cdot\gamma}\, w(x-\gamma), \qquad x \in \mathbb{R}^d,\ k \in \mathbb{R}^d, \tag{2.9}$$

for $w \in C_0(\mathbb{R}^d) \subset L^2(\mathbb{R}^d)$. The close relation with a discrete Fourier transform is thus more explicit in this formulation, and indeed the function $\psi(k,x) := (\mathcal{U}_\mathrm{BF}\, w)(k,x)$ will be Γ^*-periodic in k and Γ-pseudoperiodic in y:

$$\psi(k+\lambda, x) = \psi(k,x), \quad \lambda \in \Gamma^*,$$
$$\psi(k, x+\gamma) = \mathrm{e}^{\mathrm{i}k\cdot\gamma}\psi(k,x), \quad \gamma \in \Gamma.$$

As is the case for the modified Bloch-Floquet transform (2.6), the definition (2.9) extends to a unitary operator

$$\mathcal{U}_{\mathrm{BF}} \colon L^2(\mathbb{R}^d) \to \int_{\mathbb{B}}^{\oplus} \mathcal{H}_k \, \mathrm{d}k$$

where

$$\mathcal{H}_k := \left\{ \psi \in L^2_{\mathrm{loc}}(\mathbb{R}^d) : \psi(x+\gamma) = \mathrm{e}^{\mathrm{i}k\cdot\gamma}\psi(x) \ \forall \gamma \in \Gamma, \text{ for a.e. } x \in \mathbb{R}^d \right\}$$

(compare (2.4)). Moreover, a periodic Schrödinger operator of the form $H_\Gamma = -\frac{1}{2}\Delta + V_\Gamma$ becomes, in the classical Bloch-Floquet representation,

$$\mathcal{U}_{\mathrm{BF}}\, H_\Gamma\, \mathcal{U}_{\mathrm{BF}}^{-1} = \int_{\mathbb{B}}^{\oplus} H_{\mathrm{BF}}(k)\,\mathrm{d}k, \quad \text{where} \quad H_{\mathrm{BF}}(k) = -\frac{1}{2}\Delta_y + V_\Gamma(y).$$

Although the form of the operator $H_{\mathrm{BF}}(k)$, whose eigenfunctions $\psi(k,\cdot)$ appear in (2.7), looks simpler than the one of the fiber Hamiltonian $H(k)$ appearing in (2.11), one should observe that $H_{\mathrm{BF}}(k)$ acts on a *k-dependent* domain in the *k-dependent* Hilbert space $\mathcal{H}_k$. This constitutes the main disadvantage of working with the classical Bloch-Floquet transform (2.9), thus explaining why the modified definition (2.6) is preferred in the mathematical literature.

The two Bloch-Floquet representations (classical and modified) are nonetheless equivalent, since they are unitarily related by the operator

$$\mathcal{J} = \int_{\mathbb{B}}^{\oplus} \mathrm{d}k\, \mathcal{J}_k, \quad \text{where} \quad \mathcal{J}_k \colon \mathcal{H}_{\mathrm{f}} \to \mathcal{H}_k, \quad \left(\mathcal{J}_k \varphi\right)(y) = \mathrm{e}^{\mathrm{i}k\cdot y}\varphi(y), \quad k \in \mathbb{R}^d,$$

see (2.5), so that in particular $\mathcal{J}_k H(k) \mathcal{J}_k^{-1} = H_{\mathrm{BF}}(k)$. As a consequence, the spectrum of the fiber Hamiltonian is independent of the chosen definition. ◊

Under the assumption of Kato-smallness of V_Γ with respect to $-\Delta$, the fiber Hamiltonian $H(k)$, acting on $\mathcal{H}_{\mathrm{f}}$, has compact resolvent, by standard perturbation theory arguments [41, Thm.s XII.8 and XII.9]. We denote the eigenvalues of $H(k)$ as $E_n(k)$, $n \in \mathbb{N}$, labelled in increasing order according to multiplicity. The functions $k \mapsto E_n(k)$ are called *Bloch bands* in the physics literature (see Figure 5). Notice that the spectrum of the original Hamiltonian H_Γ can be reconstructed from that of the fiber Hamiltonians $H(k)$, leading to the well-known *band-gap* description:

$$\sigma(H_\Gamma) = \bigcup_{n\in\mathbb{N}} \bigcup_{k\in\mathbb{B}} E_n(k) = \{\lambda \in \mathbb{R} : \lambda = E_n(k) \text{ for some } n \in \mathbb{N},\ k \in \mathbb{B}.\} \tag{2.10}$$

The periodic part of the Bloch functions, appearing in (2.5), can be determined as a solution to the eigenvalue problem

$$H(k)u_n(k) = E_n(k)u_n(k), \quad u_n(k) \in \mathcal{D} \subset \mathcal{H}_{\mathrm{f}}, \quad \|u_n(k)\|_{\mathcal{H}_{\mathrm{f}}} = 1. \tag{2.11}$$

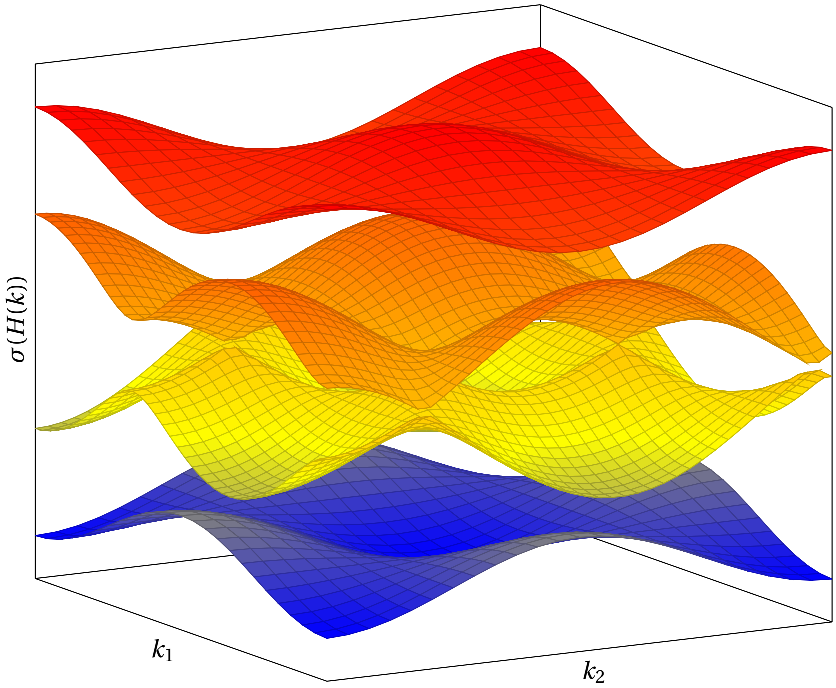


Fig. 5 The Bloch bands of a periodic Schrödinger operator.

Even if the eigenvalue $E_n(k)$ has multiplicity 1, the eigenfunction $u_n(k)$ is not unique, since another eigenfunction can be obtained by setting

$$\widetilde{u}_n(k,y) = \mathrm{e}^{\mathrm{i}\theta(k)} u_n(k,y)$$

where $\theta : \mathbb{T}^d \to \mathbb{R}$ is any measurable function. We refer to this fact as the *Bloch gauge freedom*.

2.2 Geometry: Bloch bundle

In real solids, Bloch bands intersect each other. However, in insulators and semiconductors the *Fermi energy* lies in a spectral gap, separating the occupied Bloch bands from the others. In this situation, it is convenient [9, 11] to regard all the bands below the gap as a whole, and to set up a multi-band theory.

More generally, we select a portion of the spectrum of $H(k)$ consisting of a set of $m \geq 1$ physically relevant Bloch bands:

$$\sigma_*(k) := \left\{ E_n(k) : n \in \mathcal{I}_* = \{n_0, \dots, n_0 + m - 1\} \right\}. \tag{2.12}$$

We assume that this set satisfies a *gap condition*, stating that it is separated from the rest of the spectrum of $H(k)$, namely

$$\inf_{k\in\mathbb{B}} \operatorname{dist}\big(\sigma_*(k), \sigma(H(k)) \setminus \sigma_*(k)\big) > 0 \tag{2.13}$$

(consider *e. g.* the collection of the yellow and orange bands in Figure 5). Under this assumption, one can define the spectral eigenprojector on $\sigma_*(k)$ as

$$P_*(k) := \chi_{\sigma_*(k)}(H(k)) = \sum_{n\in\mathcal{I}_*} |u_n(k,\cdot)\rangle\,\langle u_n(k,\cdot)|\,.$$

The family of spectral projectors $\{P_*(k)\}_{k\in\mathbb{R}^d}$ is the main character in the investigation of geometric effects in insulators, as will become clear in what follows. The equivalent expression for $P_*(k)$, given by the Riesz formula

$$P_*(k) = \frac{1}{2\pi\mathrm{i}} \oint_{\mathcal{C}} (H(k) - z\mathbb{1})^{-1}\, \mathrm{d}z, \tag{2.14}$$

where $\mathcal{C}$ is any contour in the complex plane winding once around the set $\sigma_*(k)$ and enclosing no other point in $\sigma(H(k))$, allows one to prove [36, Prop. 2.1] the following

Proposition 2.1. *Let $P_*(k) \in \mathcal{B}(\mathcal{H}_{\mathrm{f}})$ be the spectral projector of $H(k)$ corresponding to the set $\sigma_*(k) \subset \mathbb{R}$. Assume that σ_* satisfies the gap condition* (2.13)*. Then the family $\{P_*(k)\}_{k\in\mathbb{R}^d}$ has the following properties:*

(p_1) *the map $k \mapsto P_*(k)$ is analytic*[5] *from $\mathbb{R}^d$ to $\mathcal{B}(\mathcal{H}_{\mathrm{f}})$ (equipped with the operator norm);*
(p_2) *the map $k \mapsto P_*(k)$ is τ-covariant, i. e.*

$$P_*(k+\lambda) = \tau(\lambda)\, P_*(k)\, \tau(\lambda)^{-1}, \quad k \in \mathbb{R}^d,\ \lambda \in \Gamma^*.$$

(p_3) *the map $k \mapsto P_*(k)$ is time-reversal symmetric, i. e. there exists a antiunitary operator $T\colon \mathcal{H}_{\mathrm{f}} \to \mathcal{H}_{\mathrm{f}}$ such that*

$$T^2 = \pm\mathbb{1} \quad \textit{and} \quad P_*(-k) = T\, P_*(k)\, T^{-1}, \quad k \in \mathbb{R}^d.$$

Moreover, one has the following

(p_4) *compatibility property: $T\,\tau(\lambda) = \tau(-\lambda)\, T$ for all $\lambda \in \Lambda$.*

In this multi-band case, the notion of Bloch function is relaxed to that of a *quasi-Bloch function*, which is a normalized eigenstate of the spectral projector rather than of the fiber Hamiltonian:

$$P_*(k)\phi(k) = \phi(k), \quad \phi(k) \in \mathcal{H}_{\mathrm{f}}, \quad \|\phi(k)\|_{\mathcal{H}_{\mathrm{f}}} = 1. \tag{2.15}$$

Abstracting from the specific case of periodic, time-reversal symmetric Schrödinger operators, we consider a family of orthogonal projectors acting on a separable Hilbert space $\mathcal{H}$, satisfying the following

Assumption 2.1. The family of orthogonal projectors $\{P(k)\}_{k\in\mathbb{R}^d} \subset \mathcal{B}(\mathcal{H})$ enjoys the following properties:

[5] Here and in the following, "analyticity" is meant in the sense of admitting an analytic extension to a strip in the complex domain as in (2.8).

(P_1) *regularity*: the map $\mathbb{R}^d \ni k \mapsto P(k) \in \mathcal{B}(\mathcal{H})$ is analytic (respectively continuous, C^∞-smooth); in particular, the rank $m := \dim \operatorname{Ran} P(k)$ is constant in k;

(P_2) *τ-covariance*: the map $k \mapsto P(k)$ is covariant with respect to a unitary representation $\tau\colon \Lambda \to \mathcal{U}(\mathcal{H})$ of a maximal lattice $\Lambda \simeq \mathbb{Z}^d \subset \mathbb{R}^d$ on the Hilbert space $\mathcal{H}$, *i. e.*

$$P(k+\lambda) = \tau(\lambda)P(k)\tau(\lambda)^{-1}, \quad \text{for all } k \in \mathbb{R}^d, \lambda \in \Lambda;$$

(P_3) *time-reversal symmetry*: the map $k \mapsto P(k)$ is time-reversal symmetric, *i. e.* there exists an antiunitary operator $\Theta\colon \mathcal{H} \to \mathcal{H}$, called the *time-reversal operator*, such that

$$\Theta^2 = \pm \mathbb{1}_{\mathcal{H}} \quad \text{and} \quad P(-k) = \Theta P(k) \Theta^{-1}, \quad \text{for all } k \in \mathbb{R}^d.$$

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

(P_4) *compatibility condition*:

$$\Theta\tau(\lambda) = \tau(\lambda)^{-1}\Theta \quad \text{for all } \lambda \in \Lambda. \qquad \diamondsuit$$

The previous Assumptions retain only the fundamental $\mathbb{Z}^d$- and $\mathbb{Z}_2$-symmetries of the family of eigenprojectors of a time-reversal symmetric periodic gapped Hamiltonian, as in Proposition 2.1.

Following [35], one can construct a Hermitian vector bundle $\mathcal{E}_{\mathcal{P}} = \left(E_{\mathcal{P}} \xrightarrow{\pi} \mathbb{T}^d_*\right)$, with $\mathbb{T}^d_* := \mathbb{R}^d/\Lambda$, called the *Bloch bundle*, starting from a family of projectors $\mathcal{P} := \{P(k)\}_{k\in\mathbb{R}^d}$ satisfying properties (P_1) and (P_2) (see Figure 6). One proceeds as follows: Introduce the following equivalence relation on the set $\mathbb{R}^d \times \mathcal{H}$:

$$(k,\phi) \sim_\tau (k',\phi') \quad \text{if and only if} \quad \text{there exists } \lambda \in \Lambda \text{ such that } k' = k - \lambda \text{ and } \phi' = \tau(\lambda)\phi.$$

The total space of the Bloch bundle is then

$$E_{\mathcal{P}} := \left\{ [k,\phi]_\tau \in (\mathbb{R}^d \times \mathcal{H})/\sim_\tau : \phi \in \operatorname{Ran} P(k) \right\}$$

with projection $\pi([k,\phi]_\tau) = k \pmod{\Lambda} \in \mathbb{T}^d_*$. The condition $\phi \in \operatorname{Ran} P(k)$, or equivalently $P(k)\phi = \phi$, is independent of the representative $[k,\phi]_\tau$ in the $\sim_\tau$-equivalence class, in view of (P_2).

By using the Kato-Nagy formula [22, Sec. I.4.6], one shows that the previous definition yields an analytic vector bundle, which moreover inherits from $\mathcal{H}$ a natural Hermitian structure given by

$$\left\langle [k,\phi]_\tau, [k,\phi']_\tau \right\rangle := \left\langle \phi, \phi' \right\rangle_{\mathcal{H}}.$$

Indeed, pick $k_0 \in \mathbb{T}^d_*$, and let $U \subset \mathbb{T}^d_*$ be a neighbourhood of k_0 such that

$$\| P(k) - P(k_0) \|_{\mathcal{B}(\mathcal{H})} < 1 \quad \text{for all } k \in U.$$

The Kato-Nagy formula then provides a unitary operator $W(k;k_0) \in \mathcal{U}(\mathcal{H})$, depending analytically on k, such that

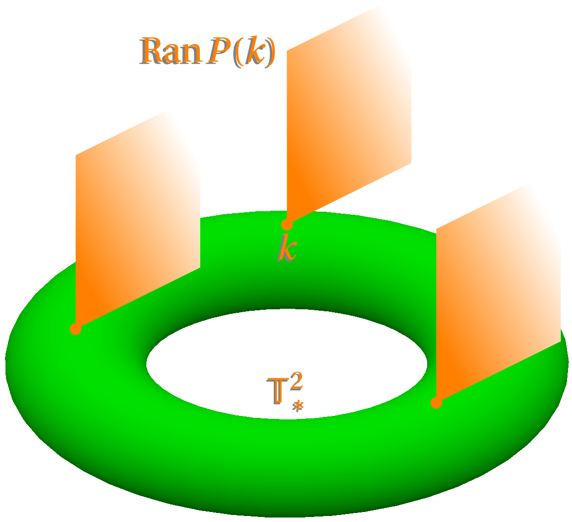


Fig. 6 The Bloch bundle over the 2-dimensional torus $\mathbb{T}^2_*$. The fiber over the point $k \in \mathbb{T}^2_*$ consists of the m-dimensional vector space $\operatorname{Ran} P(k)$.

$$P(k) = W(k; k_0) P(k_0) W(k; k_0)^{-1} \quad \text{for all } k \in U.$$

If $V \subset \mathbb{T}^d_*$ is a neighbourhood of a point $k_1 \in \mathbb{T}^d_*$ which intersects U, then the map $g_{UV}(k) := W(k; k_0)^{-1} W(k; k_1)$, viewed as a unitary $m \times m$ matrix between $\operatorname{Ran} P(k_1) \simeq \mathbb{C}^m$ and $\operatorname{Ran} P(k_0) \simeq \mathbb{C}^m$, provides an analytic transition function for the bundle $\mathcal{E}_{\mathcal{P}}$.

In this abstract framework, the rôle of quasi-Bloch functions is incorporated in the notion of a *Bloch frame*, as in the following

Definition 2.1 (Bloch frame). Let $\mathcal{P} = \{P(k)\}_{k \in \mathbb{R}^d}$ be a family of projectors satisfying Assumptions (P_1) and (P_2). A *local Bloch frame* for $\mathcal{P}$ on a region $\Omega \subset \mathbb{R}^d$ is a map

$$\Phi \colon \Omega \to \mathcal{H} \oplus \ldots \oplus \mathcal{H} = \mathcal{H}^m, \quad k \mapsto \Phi(k) := \{\phi_1(k), \ldots, \phi_m(k)\}$$

such that for a.e. $k \in \Omega$ the set $\{\phi_1(k), \ldots, \phi_m(k)\}$ is an orthonormal basis spanning $\operatorname{Ran} P(k)$. If $\Omega = \mathbb{R}^d$ we say that Φ is a *global Bloch frame*.

Moreover, we say that a (global) Bloch frame is

(F_1) *analytic* (respectively continuous, smooth) if the map $\phi_a : \mathbb{R}^d \to \mathcal{H}^m$ is analytic (respectively continuous, C^∞-smooth) for all $a \in \{1, \ldots, m\}$;
(F_2) τ*-equivariant* if

$$\phi_a(k + \lambda) = \tau(\lambda) \phi_a(k) \quad \text{for all } k \in \mathbb{R}^d,\ \lambda \in \Lambda,\ a \in \{1, \ldots, m\}. \qquad \Diamond$$

Remark 2.2. When the family of projectors $\mathcal{P}$ satisfies also (P_3), one can also ask a Bloch frame to be *time-reversal symmetric*, *i. e.* to satisfy a certain compatibility condition with the time-reversal operator Θ. We defer the treatement of time-reversal symmetric Bloch frames to Part II of this thesis. $\Diamond$

As was early noticed by several authors [28, 11, 34], there might be a competition between *regularity* (a local issue) and *periodicity* (a global issue) for a Bloch frame.

The existence of an analytic, τ-equivariant global Bloch frame for a family of projectors $\mathcal{P} = \{P(k)\}_{k\in\mathbb{R}^d}$ satisfying assumptions (P_1) and (P_2), which is equivalent to the existence of a basis of localized Wannier functions (see Section 2.3), is, in general, *topologically obstructed.* The main advantage of the geometric picture and the usefulness of the language of Bloch bundles is that it gives a way to measure and quantify this topological obstruction, and to look for sufficient conditions which guarantee its absence.

Indeed, the existence of a Bloch frame for $\mathcal{P}$ which satisfies (F_1) and (F_2) is equivalent to the *triviality*[6] of the associated Bloch bundle $\mathcal{E}_{\mathcal{P}}$. In fact, if the Bloch bundle $\mathcal{E}_{\mathcal{P}}$ is trivial, then an analytic Bloch frame $\{\phi_a\}_{a=1,\ldots,m}$ can be constructed by means of an analytic isomorphism $F : \mathbb{T}^d_* \times \mathbb{C}^m \xrightarrow{\sim} E_{\mathcal{P}}$ by setting $\phi_a(k) := F(k, e_a)$, where $\{e_a\}_{a=1,\ldots,m}$ is any orthonormal basis in $\mathbb{C}^m$. Viceversa, a global analytic Bloch frame $\{\phi_a\}_{a=1,\ldots,m}$ provides an analytic isomorphism $G : \mathbb{T}^d_* \times \mathbb{C}^m \xrightarrow{\sim} E_{\mathcal{P}}$ by setting

$$G(k, (v_1, \ldots, v_m)) = [k, v_1\phi_1(k) + \cdots + v_m\phi_m(k)]_\tau.$$

In general, the triviality of vector bundles on a low-dimensional torus $\mathbb{T}^d_*$ with $d \le 3$ is measured by the vanishing of its *first Chern class* [35, Prop. 4], defined in terms of the family of projectors $\{P(k)\}_{k\in\mathbb{R}^d}$ by the formula

$$\mathrm{Ch}_1(\mathcal{E}_{\mathcal{P}}) := \frac{1}{2\pi \mathrm{i}} \sum_{1\le\mu<\nu\le d} \Omega_{\mu\nu}(k)\, \mathrm{d}k_\mu \wedge \mathrm{d}k_\nu,$$

with

$$\Omega_{\mu\nu}(k) = \mathrm{Tr}_{\mathcal{H}} \left(P(k) \left[\partial_\mu P(k), \partial_\nu P(k) \right] \right).$$

In turn, due to the simple cohomological structure of the torus $\mathbb{T}^d_*$, the first Chern class vanishes if and only if the *Chern numbers*[7]

$$c_1(\mathcal{P})_{\mu\nu} := \frac{1}{2\pi \mathrm{i}} \int_{\mathbb{T}^2_{\mu\nu}} \mathrm{d}k_\mu \wedge \mathrm{d}k_\nu\, \Omega_{\mu\nu}(k) \in \mathbb{Z}, \quad 1 \le \mu < \nu \le d, \tag{2.16}$$

are all zero: here

$$\mathbb{T}^2_{\mu\nu} := \left\{ k = (k_1, \ldots, k_d) \in \mathbb{T}^d_* : k_\alpha = 0 \text{ if } \alpha \notin \{\mu, \nu\} \right\}.$$

---

[6] We recall that a vector bundle $\mathcal{E} = \left(E \xrightarrow{\pi} M\right)$ of rank m is called *trivial* if it is isomorphic to the product bundle $\mathcal{T} = \left(M \times \mathbb{C}^m \xrightarrow{\mathrm{pr}_1} M\right)$, where pr_1 is the projection on the first factor.

[7] In the framework of periodic Schrödinger operators, writing the spectral projector $P_*(k)$ in the ket-bra notation

$$P_*(k) = \sum_{a=1}^m |u_a(k)\rangle \langle u_a(k)|$$

then one can rewrite the formula for the Chern numbers as

$$c_1(\mathcal{P}_*)_{\mu,\nu} = \frac{1}{2\pi} \int_{\mathbb{T}^2_{\mu,\nu}} \mathrm{d}k_\mu \wedge \mathrm{d}k_\nu\, F_{\mu\nu}(k), \quad \text{with } F_{\mu\nu}(k) := 2 \sum_{a=1}^m \mathrm{Im} \left\langle \partial_\mu u_a(k), \partial_\nu u_a(k) \right\rangle_{\mathcal{H}_\mathrm{f}}.$$

The integrand $F_{\mu\nu}(k)$ can be recognized as the *Berry curvature, i. e.* the curvature of the Berry connection, appearing in the solid state literature [42].

The main result of [35], later generalized in [33] to the case of a fermionic time-reversal symmetry, is the following.

Theorem 2.2 ([35, Thm. 1], [33, Thm. 1]). *Let $d \le 3$, and let $\mathcal{P} = \{P(k)\}_{k\in\mathbb{R}^d}$ be a family of projectors satisfying Assumption 2.1 (in particular, it is time-reversal symmetric). Then the Bloch bundle $\mathcal{E}_{\mathcal{P}} = \left(E_{\mathcal{P}} \xrightarrow{\pi} \mathbb{T}^d_*\right)$ is trivial in the category of analytic Hermitian vector bundles.*

The above result then establishes the existence of analytic, τ-equivariant global Bloch frames in dimension $d \le 3$, whenever time-reversal symmetry is present.

2.3 Physics: Wannier functions and their localization

Coming back to periodic Schrödinger operators, we deduce some important physical consequences of the above geometric results. Recall that Bloch functions are defined as eigenfunctions of the fiber Hamiltonian $H(k)$ for a fixed crystal momentum $k \in \mathbb{R}^d$. One can use them to mimic eigenfunctions of the original periodic Schrödinger operator H_Γ, which strictly speaking do not exist since its spectrum (2.10) is in general purely absolutely continuous (unless there is a flat band $E_n(k) \equiv \text{const}$). In order to do so, one uses the Bloch-Floquet-Zak antitransform to bring Bloch functions back to the position-space representation.

More precisely, assume that σ_* in (2.12) consist of a single isolated Bloch band E_n (*i. e.* $m = 1$); the *Wannier function* w_n associated to a choice of the Bloch function $u_n(k,\cdot)$ for the band E_n, as in (2.11), is defined by setting

$$w_n(x) := \left(\mathcal{U}_{\mathrm{BFZ}}^{-1} u_n\right)(x) = \frac{1}{|\mathbb{B}|^{1/2}} \int_{\mathbb{B}} \mathrm{d}k\, \mathrm{e}^{\mathrm{i}k\cdot x} u_n(k,x). \tag{2.17}$$

In the multiband case ($m > 1$), the rôle of Bloch functions is played by quasi-Bloch functions, as in (2.15). The notion corresponding in position space to that of a Bloch frame $\{\phi_a\}_{a=1,\dots,m}$ is given by *composite Wannier functions* $\{w_1,\dots,w_m\} \subset L^2(\mathbb{R}^d)$, which are defined in analogy with (2.17) as

$$w_a(x) := \left(\mathcal{U}_{\mathrm{BFZ}}^{-1} \phi_a\right)(x) = \frac{1}{|\mathbb{B}|^{1/2}} \int_{\mathbb{B}} \mathrm{e}^{\mathrm{i}k\cdot x} \phi_a(k,x)\, \mathrm{d}k.$$

If we denote by

$$P_* := \mathcal{U}_{\mathrm{BFZ}}^{-1} \left(\int_{\mathbb{B}}^{\oplus} \mathrm{d}k\, P_*(k) \right) \mathcal{U}_{\mathrm{BFZ}}$$

the spectral projection of H_Γ corresponding to the relevant set of bands $\sigma_* = \bigcup_{k\in\mathbb{B}} \sigma_*(k)$, then it is not hard to prove [3] the following

Proposition 2.2. *Let $\Phi = \{\phi_a\}_{a=1,\dots,m}$ be a global Bloch frame for $\{P_*(k)\}_{k\in\mathbb{R}^d}$, and denote by $\{w_a\}_{a=1,\dots,m}$ the set of the corresponding composite Wannier functions. Then the set $\{T_\gamma w_a\}_{\gamma\in\Gamma; a=1,\dots,m}$ gives an* orthonormal basis *of* $\operatorname{Ran} P_*$.

Localization (that is, decay at infinity) of Wannier functions plays a fundamental rôle in the transport theory of electrons [3, 31]. One says that a set of composite

Wannier functions is *almost-exponentially localized* if it decays faster than any polynomial in the L^2-sense, *i. e.* if

$$\int_{\mathbb{R}^d} \left(1+|x|^2\right)^r |w_a(x)|^2 \,\mathrm{d}x < \infty \quad \text{for all } r \in \mathbb{N}, \quad a \in \{1,\dots,m\}.$$

One says instead that composite Wannier functions are *exponentially localized* if they decay exponentially in the L^2-sense, *i. e.* if

$$\int_{\mathbb{R}^d} \mathrm{e}^{2\beta|x|} |w_a(x)|^2 \,\mathrm{d}x < \infty \quad \text{for some } \beta > 0, \quad \text{for all } a \in \{1,\dots,m\}.$$

Due to the properties of the Bloch-Floquet-Zak transform listed in Theorem 2.1, one has that a set of almost-exponentially (respectively exponentially) localized composite Wannier functions exists if and only if there exists a smooth (respectively analytic), τ-equivariant Bloch frame for the family of spectral projectors $\{P_*(k)\}_{k\in\mathbb{R}^d}$. In view of the results of Proposition 2.1, we can rephrase the abstract result of Theorem 2.2 as

Corollary 2.1. *Let H_Γ be a periodic, time-reversal symmetric Schrödinger operator, acting on $L^2(\mathbb{R}^d)\otimes\mathbb{C}^N$ with $d \le 3$. Denote by σ_* a portion of the spectrum which satisfies the gap condition* (2.13)*, and denote by P_* the associated spectral projector. Then, there exists an orthonormal basis $\{T_\gamma w_a\}_{\gamma\in\Gamma; a=1,\dots,m}$ consisting of* exponentially localized *composite Wannier functions for* $\operatorname{Ran} P_*$.

Thus, we see that time-reversal symmetry is the crucial hypothesis to prove the existence of localized Wannier functions in insulators.

3 Structure of the thesis

After the above review on geometric phases and topological invariants of crystalline insulators, we are able to state the purpose of this dissertation. This thesis collects three of the publications that the candidate produced during his Ph.D. studies.

Part I contains the reproduction of [32]. The scope of this paper is to understand wheter geometric information can still be extracted from the datum of the spectral projector in the case when the gap condition (2.13) is *not* satisfied. We consider thus 2-dimensional crystals whose Fermi surface is first of all non-empty and degenerates to a discrete set of points, that is, semimetallic materials, whose prototypical model is (*multilayer*) *graphene*.

In these models, the associated family of eigenprojectors fails to be continuous at those points where eigenvalue bands touch. By adding a deformation parameter, which opens a gap between these bands (thus making the family of eigenprojectors smooth), one is able to recover a vector bundle, defined on a sphere (or a pointed cylinder) in the now 3-dimensional parameter space, surrounding a degenerate point. The first Chern number of this bundle, which characterizes completely its isomorphism class by the same arguments contained in [35], is then the integer-valued topological invariant, baptized *eigenspace vorticity*, which is associated to the eigenvalue intersection. It is proved that this definition provides a stronger notion than that of *pseudospin winding number* (at least in 2-band systems, where the latter is defined), which appeared in the literature of solid state physics and was also aimed at quantifying a geometric phase in presence of eigenvalue intersections.

With the help of explicit models for the local geometry around eigenvalue crossings, the authors of [32] were also able to establish the decay rate of Wannier functions in mono- and bilayer graphene. More precisely, if $w \in L^2(\mathbb{R}^2)$ is the Wannier function associated to, say, the valence band of such materials, then

$$\int_{\mathbb{R}^2} \mathrm{d}x\, |x|^{2\alpha} |w(x)|^2 < +\infty \quad \text{for all } 0 \le \alpha < 1.$$

Part II contains instead the reproduction of [12] and [13]. In both these papers, the starting datum is that of a family of projectors as in Assumption 2.1 with $d \le 3$; in [12] the time-reversal operator is assumed to be of bosonic type, while in [13] it is of fermionic type, squaring respectively to $+\mathbb{1}$ or $-\mathbb{1}$. The aim is to give an *explicit algorithmic construction* of smooth and τ-equivariant Bloch frames, whose existence was proved by abstract geometric methods in [35] and [33] (compare Theorem 2.2), investigating moreover if a certain compatibility condition with time-reversal symmetry can be enforced. The results depend crucially on the bosonic or fermionic nature of the time-reversal symmetry operator. Indeed, contrary to the bosonic case, in the fermionic framework there may be *topological obstructions* to the existence of smooth, τ-equivariant *and time-reversal symmetric* Bloch frames in dimensions $d = 2$ and $d = 3$. More explicitly, the results of [12] and [13] can be summarized as follows.

The thesis closes illustrating some perspectives and reporting some recent developments on the line of research initiated during the Ph.D. studies of the candidate.

Theorem ([12], [13]). *Let $\mathcal{P} = \{P(k)\}_{k\in\mathbb{R}^d}$ be a family of projectors satisfying Assumption 2.1. Assume that $1 \le d \le 3$. Then a global Bloch frame for $\mathcal{P}$ satisfying smoothness, τ-equivariance and time-reversal symmetry exists:*

If $\Theta^2 = +\mathbb{1}$ *always;*
If $\Theta^2 = -\mathbb{1}$ *according to the dimension:*

If $d = 1$ always;
If $d = 2$ if and only if

$$\delta(\mathcal{P}) = 0 \in \mathbb{Z}_2,$$

where $\delta(\mathcal{P})$ is a topological invariant of $\mathcal{P}$, defined in [13, Eqn. (3.16)];
If $d = 3$ if and only if

$$\delta_{1,0}(\mathcal{P}) = \delta_{1,+}(\mathcal{P}) = \delta_{2,+}(\mathcal{P}) = \delta_{3,+}(\mathcal{P}) = 0 \in \mathbb{Z}_2,$$

where $\delta_{1,0}(\mathcal{P})$, $\delta_{1,+}(\mathcal{P})$, $\delta_{2,+}(\mathcal{P})$ and $\delta_{3,+}(\mathcal{P})$ are topological invariants of $\mathcal{P}$, defined in [13, Eqn. (6.1)].

In particular, in the bosonic setting, the algorithm produces, via Bloch-Floquet-Zak antitransform, an orthonormal basis for the spectral subspace of a periodic, time-reversal symmetric Hamiltonian, consisting of composite Wannier functions which are almost-exponentially localized *and real-valued* (compare Corollary 2.1). For what concerns the fermionic setting, instead, it is interesting to notice that the obstructions are encoded into $\mathbb{Z}_2$*-valued* indices, rather than in integer-valued invariants like the Chern numbers (2.16). This is indeed in agreement with the periodic tables of topological insulators, and provides a geometric origin for these invariants in the periodic framework. In particular, in [13] the authors show that such invariants $\delta, \delta_{j,s} \in \mathbb{Z}_2$, which are the mod 2 reduction of the degree of the determinant of a unitary-valued map suitably defined on the boundary of half the Brillouin zone, coincide numerically with the ones proposed by L. Fu, C. Kane and E. Mele in the literature on time-reversal symmetric topological insulators [15, 16].

References

1. ALTLAND, A.; ZIRNBAUER, M. : Non-standard symmetry classes in mesoscopic normal-superconducting hybrid structures, *Phys. Rev. B* **55**, 1142–1161 (1997).
2. ANDO, Y. : Topological insulator materials, *J. Phys. Soc. Jpn.* **82**, 102001 (2013).
3. ASHCROFT, N.W.; MERMIN, N.D. : Solid State Physics. Harcourt (1976).
4. AVRON, J.E.; SEILER, R.; YAFFE, L.G. : Adiabatic theorems and applications to the quantum Hall effect, *Commun. Math. Phys.* **110**, 33–49 (1987).
5. AVRON, J.E.; SEILER, R.; SIMON, B. : Charge deficiency, charge transport and comparison of dimensions, *Commun. Math. Phys.* **159**, 399–422 (1994).
6. BELLISSARD, J.; VAN ELST, A.; SCHULZ-BALDES, H. : The noncommutative geometry of the quantum Hall effect, *J. Math. Phys* **35**, 5373–5451 (1994).
7. BERNEVIG, B.A.; HUGHES, T.L.; ZHANG, SH.-CH. : Quantum Spin Hall Effect and Topological Phase Transition in HgTe Quantum Wells, *Science* **15**, 1757–1761 (2006).
8. BERRY, M.V. : Quantal phase factors accompanying adiabatic changes, *Proc. R. Lond.* **A392**, 45–57 (1984).
9. BLOUNT, E.I. : Formalism of Band Theory, in: SEITZ, F.; TURNBULL, D. (eds.) : Solid State Physics, vol. 13, 305–373. Academic Press (1962).
10. DE NITTIS, G.; GOMI, K. : Classification of "Quaternionic" Bloch-bundles, *Commun. Math. Phys.* **339** (2015), 1–55.
11. DES CLOIZEAUX, J. : Analytical properties of n-dimensional energy bands and Wannier functions, *Phys. Rev.* **135**, A698–A707 (1964).
12. FIORENZA, D.; MONACO, D.; PANATI, G. : Construction of real-valued localized composite Wannier functions for insulators, *Ann. Henri Poincaré* (2015), DOI 10.1007/s00023-015-0400-6.
13. FIORENZA, D.; MONACO, D.; PANATI, G. : $\mathbb{Z}_2$ invariants of topological insulators as geometric obstructions, available at `arXiv:1408.1030`.
14. FRUCHART, M. ; CARPENTIER, D. : An introduction to topological insulators, *Comptes Rendus Phys.* **14**, 779–815 (2013).
15. FU, L.; KANE, C.L. : Time reversal polarization and a $\mathbb{Z}_2$ adiabatic spin pump, *Phys. Rev. B* **74**, 195312 (2006).
16. FU, L.; KANE, C.L.; MELE, E.J. : Topological insulators in three dimensions, *Phys. Rev. Lett.* **98**, 106803 (2007).
17. GRAF, G.M. : Aspects of the Integer Quantum Hall Effect, *P. Symp. Pure Math.* **76**, 429–442 (2007).
18. GRAF, G.M.; PORTA, M. : Bulk-edge correspondence for two-dimensional topological insulators, *Commun. Math. Phys.* **324**, 851–895 (2013).
19. HASAN, M.Z.; KANE, C.L. : Colloquium: Topological Insulators, *Rev. Mod. Phys.* **82**, 3045–3067 (2010).
20. KANE, C.L.; MELE, E.J. : $\mathbb{Z}_2$ Topological Order and the Quantum Spin Hall Effect, *Phys. Rev. Lett.* **95**, 146802 (2005).
21. KANE, C.L.; MELE, E.J. : Quantum Spin Hall Effect in graphene, *Phys. Rev. Lett.* **95**, 226801 (2005).
22. KATO, T. : Perturbation theory for linear operators. Springer, Berlin (1966).
23. KELLENDONK, J.; RICHTER, T.; SCHULZ-BALDES, H. : Edge current channels and Chern numbers in the integer quantum Hall effect, *Rev. Math. Phys.* **14**, 87–119 (2002).
24. KENNEDY, R.; GUGGENHEIM, C. : Homotopy theory of strong and weak topological insulators, available at `arXiv:1409.2529`.
25. KENNEDY, R.; ZIRNBAUER, M.R. : Bott periodicity for $\mathbb{Z}_2$ symmetric ground states of free fermion systems, available at `arXiv:1409.2537`.

26. KING-SMITH, R.D.; VANDERBILT, D. : Theory of polarization of crystalline solids, *Phys. Rev. B* **47**, 1651 (1993).
27. KITAEV, A. : Periodic table for topological insulators and superconductors, *AIP Conf. Proc.* **1134**, 22 (2009).
28. KOHN, W. : Analytic properties of Bloch waves and Wannier functions, *Phys. Rev.* **115**, 809 (1959).
29. KUCHMENT, P. : Floquet Theory for Partial Differential Equations. Vol. 60 of Operator Theory Advances and Applications. Birkhäuser Verlag (1993).
30. MACIEJKO, J.; HUGHES, T.L.; ZHANG, SH.-CH. : The quantum spin Hall effect, *Annu. Rev. Condens. Matter Phys.* **2**, 31–53 (2011).
31. MARZARI, N.; MOSTOFI, A.A.; YATES, J.R.; SOUZA I.; VANDERBILT, D. : Maximally localized Wannier functions: Theory and applications, *Rev. Mod. Phys.* **84**, 1419 (2012).
32. MONACO, D.; PANATI, G. : Topological invariants of eigenvalue intersections and decrease of Wannier functions in graphene, *J. Stat. Phys.* **155**, Issue 6, 1027–1071 (2014).
33. MONACO, D.; PANATI, G. : Symmetry and localization in periodic crystals: triviality of Bloch bundles with a fermionic time-reversal symmetry, *Acta Appl. Math.* **137**, Issue 1, 185–203 (2015).
34. NENCIU, G. : Dynamics of band electrons in electric and magnetic fields: Rigorous justification of the effective Hamiltonians, *Rev. Mod. Phys.* **63**, 91–127 (1991).
35. PANATI, G. : Triviality of Bloch and Bloch-Dirac bundles, *Ann. Henri Poincaré* **8**, 995–1011 (2007).
36. PANATI, G.; PISANTE, A. : Bloch bundles, Marzari-Vanderbilt functional and maximally localized Wannier functions, *Commun. Math. Phys.* **322**, 835–875 (2013).
37. PANATI, G.; SPARBER, C.; TEUFEL, S. : Effective dynamics for Bloch electrons: Peierls substitution and beyond, *Commun. Math. Phys.* **242**, 547–578 (2003).
38. PRODAN, E. : Robustness of the Spin-Chern number, *Phys. Rev. B* **80**, 125327 (2009).
39. QI, X.-L.; ZHANG, SH.-CH. : The quantum spin Hall effect and topological insulators, *Phys. Today* **63**, 33 (2010).
40. QI, X.-L.; ZHANG, SH.-CH. : Topological insulators and superconductors, *Rev. Mod. Phys.* **83**, 1057 (2011).
41. REED, M.; SIMON, B. : Methods of Modern Mathematical Physics, vol. IV: Analysis of Operators. Academic Press (1978).
42. RESTA, R. : Macroscopic polarization in crystalline dielectrics: the geometric phase approach, *Rev. Mod. Phys. 66*, Issue 3, 899–915 (1994).
43. RYU, S.; SCHNYDER, A.P.; FURUSAKI, A.; LUDWIG, A.W.W. : Topological insulators and superconductors: Tenfold way and dimensional hierarchy, *New J. Phys.* **12**, 065010 (2010).
44. SCHULZ-BALDES, H. : Persistence of spin edge currents in disordered Quantum Spin Hall systems, *Commun. Math. Phys.* **324**, 589–600 (2013).
45. SHAPERE, A.; WILCZEK, F. (eds.) : Geometric Phases in Physics. Vol. 5 of Advanced Series in Mathematical Physics. World Scientific, Singapore (1989).
46. SIMON, B. : Holonomy, the quantum adiabatic theorem, and Berry's phase, *Phys. Rev. Lett.* **51**, 2167–2170 (1983).
47. SPALDIN, N.A. : A beginner's guide to the modern theory of polarization, *J. Solid State Chem.* **195**, 2–10 (2012).
48. THOULESS, D.J.; KOHMOTO, M.; NIGHTINGALE, M.P.; DEN NIJS, M. : Quantized Hall conductance in a two-dimensional periodic potential, *Phys. Rev. Lett.* **49**, 405–408 (1982).
49. VON KLITZING, K.; DORDA, G.; PEPPER, M. : New method for high-accuracy determination of the fine-structure constant based on quantized Hall resistance, *Phys. Rev. Lett.* **45**, 494 (1980).
50. VON KLITZING, K. : The quantized Hall effect, *Rev. Mod. Phys.* **58**, Issue no. 3, 519–531 (1986).
51. ZAK, J. : Magnetic translation group, *Phys. Review* **134**, A1602 (1964).

Part I
Graphene

We reproduce here the content of the paper

MONACO, D.; PANATI, G. : Topological invariants of eigenvalue intersections and decrease of Wannier functions in graphene, *J. Stat. Phys.* **155**, Issue 6, 1027–1071 (2014).

Topological invariants of eigenvalue intersections and decrease of Wannier functions in graphene

Domenico Monaco and Gianluca Panati

Dedicated to Herbert Spohn, with admiration

Abstract We investigate the asymptotic decrease of the Wannier functions for the valence and conduction band of graphene, both in the monolayer and the multilayer case. Since the decrease of the Wannier functions is characterised by the structure of the Bloch eigenspaces around the Dirac points, we introduce a geometric invariant of the family of eigenspaces, baptised eigenspace vorticity. We compare it with the pseudospin winding number. For every value $n \in \mathbb{Z}$ of the eigenspace vorticity, we exhibit a canonical model for the local topology of the eigenspaces. With the help of these canonical models, we show that the single band Wannier function w satisfies $|w(x)| \le \text{const} \cdot |x|^{-2}$ as $|x| \to \infty$, both in monolayer and bilayer graphene.

Key words: Wannier functions, Bloch bundles, conical intersections, eigenspace vorticity, pseudospin winding number, graphene.

1 Introduction

The relation between topological invariants of the Hamiltonian and localization and transport properties of the electrons has become, after a profound paper by Thouless *et al.* [48], a paradigm of theoretical and mathematical physics. Besides the well-known example of the Quantum Hall effect [3, 13], the same paradigm applies to the macroscopic polarization of insulators under time-periodic deformations [21, 42, 36] and to many other examples [53]. While this relation has been deeply investigated in the case of gapped insulators, the case of semimetals remains, to our knowledge, widely unexplored. In this paper, we consider the prototypical example of graphene [6, 12, 4], both in the monolayer and in the multilayer realisations, and we investigate the relation between a *local* geometric invariant of the eigenvalue intersections and the electron localization.

Domenico Monaco
SISSA, Via Bonomea 265, 34136 Trieste, Italy
e-mail: dmonaco@sissa.it

Gianluca Panati
Dipartimento di Matematica “G. Castelnuovo”, “La Sapienza” Università di Roma, Piazzale A. Moro 2, 00185 Roma, Italy
e-mail: panati@mat.uniroma.it

A fundamental tool to study the localization of the electrons in periodic and almost-periodic systems is provided by Wannier functions [52, 28]. In the case of a single Bloch band isolated from the rest of the spectrum, the existence of an exponentially localized Wannier function was proved in dimension $d = 1$ by W. Kohn for centrosymmetric crystals [22]. The latter hypothesis has been later removed by J. de Cloizeaux [8]. A proof of existence for $d \leq 3$ has been obtained by J. de Cloizeaux for centrosymmetric crystals [7, 8], and by G. Nenciu [32] in the general case.

Whenever the Bloch bands intersect each other, there are two possible approaches. On the one hand, following de Cloizeaux [8], one considers a relevant family of Bloch bands which are separated by a gap from the rest of the spectrum (*e. g.* the bands below the Fermi energy in an insulator). Then the notion of Bloch function is relaxed to the weaker notion of *quasi-Bloch function*, and one investigates whether the corresponding *composite* Wannier functions are exponentially localized. An affirmative answer was provided by G. Nenciu for $d = 1$ [33], and only recently for $d \leq 3$ [5, 38]. On the other hand, one may focus on a *single* non-isolated band and estimate the asymptotic decrease of the corresponding single-band Wannier function, as $|x| \to \infty$. The rate of decrease depends, roughly speaking, on the regularity of the Bloch function at the intersection points.

In this paper we follow the second approach. We consider the case of graphene (both monolayer and bilayer) [6, 12] and we explicitly compute the rate of decrease of the Wannier functions corresponding to the conduction and valence band. Since the rate of decrease crucially depends on the behaviour of the Bloch functions at the Dirac points, we preliminarily study the topology of the Bloch eigenspaces around those points.

More precisely, we introduce a geometric invariant of the eigenvalue intersection, which encodes the behaviour of the Bloch eigenspaces at the singular point (Section 3.1). We show that our invariant, baptised *eigenspace vorticity*, equals the *pseudospin winding number* [39, 34, 27] whenever the latter is well-defined (Section 3.3). We prove, under suitable assumptions, that if the value of the eigenspace vorticity is $n_{\mathrm{v}} \in \mathbb{Z}$, then the local behaviour of the Bloch eigenspaces is described by the n_{v}-canonical model, explicitly described in Section 3.2. For example, monolayer and bilayer graphene correspond to the cases $n_{\mathrm{v}} = 1$ and $n_{\mathrm{v}} = 2$, respectively. The core of our topological analysis is Theorem 4.1, which shows that, in the relevant situations, the family of canonical models provides a complete classification of the local behaviour of the eigenspaces.

As a consequence of the previous geometric analysis, in Section 5 we are able to compute the rate of decrease of Wannier functions corresponding to the valence and conduction bands of monolayer and bilayer graphene. For both bands, we essentially obtain that

$$|w(x)| \leq \mathrm{const} \cdot |x|^{-2} \qquad \text{as } |x| \to \infty, \tag{1.1}$$

see Theorems 5.1 and 5.3 for precise statements.

The power-law decay in (1.1) suggests that electrons in the conduction or valence band are delocalized. The absence of localization and the finite metallic conductivity in monolayer graphene are usually explained as a consequence of the Dirac-like (conical) energy spectrum. Since bilayer graphene has the usual parabolic spectrum, "*the observation of the maximum resistivity* $\approx h/4e^2$ *[...] is most unexpected*" [34], thus challenging theoreticians to provide an explanation of the absence of localiza-

tion in bilayer graphene.
In this paper, we show that the absence of localization is not a direct consequence of the conical spectrum, but it is rather a consequence of the non-smoothness of the Bloch functions at the intersection points, which is in turn a consequence of a non-zero eigenspace vorticity, a condition which is verified by both mono- and multilayer graphene. While the existence of a local geometric invariant distinguishing monolayer graphene from bilayer graphene has been foreseen by several authors, as *e.g.* [34, 27, 39], our paper first demonstrates the relation between non-trivial local topology and absence of localization in position space.

While the Wannier functions in graphene are the motivating example, the importance of our topological analysis goes far beyond the specific case: we see a wide variety of possible applications, ranging from the topological phase transition in the Haldane model [17], to the analysis of the conical intersections arising in systems of ultracold atoms in optical lattices [54, 25, 47], to a deeper understanding of the invariants in 3-dimensional topological insulators [18, 19, 44]. As for the latter item, the applicability of our results is better understood in terms of edge states, following [18, Sec. IV]. Indeed, in a $3d$ crystal occupying the half-space, the edge states are decomposed with respect to a $2d$ crystal momentum; on the corresponding $2d$ Brillouin zone, there are four points invariant under time-reversal symmetry where surface Bloch bands may be doubly degenerate, yielding an intersection of eigenvalues. Although a detailed analysis is postponed to future work, we are confident that methods and techniques developed in this paper will contribute to a deeper understanding of the invariants of topological insulators.

Acknowledgments. We are indebted with D. Fiorenza and A. Pisante for many inspiring discussions, and with R. Bianco, R. Resta and A. Trombettoni for interesting comments and remarks. We are also grateful to the anonymous reviewers for their useful observations and suggestions. Financial support from the INdAM-GNFM project "Giovane Ricercatore 2011", and from the AST Project 2009 "Wannier functions" is gratefully acknowledged.

2 Basic concepts

In this Section, we briefly introduce the basic concepts and the notation, referring to [35, Section 2] for details.

2.1 Bloch Hamiltonians

To motivate our definition, we initially consider a periodic Hamiltonian $H_\Gamma = -\Delta + V_\Gamma$ where $V_\Gamma(x+\gamma) = V_\Gamma(x)$ for every γ in the periodicity lattice $\Gamma = \mathrm{Span}_{\mathbb{Z}}\{a_1, \dots, a_d\}$ (here $\{a_1, \dots, a_d\}$ is a linear basis of $\mathbb{R}^d$). We assume that the potential V_Γ defines an operator which is relatively bounded with respect to Δ with relative bound zero, in order to guarantee that H_Γ is self-adjoint on the domain $W^{2,2}(\mathbb{R}^d)$: when $d = 2$ (the relevant dimension for our subsequent analysis), for example, this holds whenever $V_\Gamma \in L^2_{\mathrm{loc}}(\mathbb{R}^2)$ [41, Thm. XIII.96]. To study such *Bloch Hamiltonians*, one introduces the (*modified*) *Bloch-Floquet transform* $\mathcal{U}_{\mathrm{BF}}$, acting on a function $w \in \mathcal{S}(\mathbb{R}^d)$ as

$$(\mathcal{U}_{\mathrm{BF}}\, w)\,(k,y) := \frac{1}{|\mathbb{B}|^{1/2}} \sum_{\gamma\in\Gamma} \mathrm{e}^{-\mathrm{i}k\cdot(y+\gamma)}\, w(y+\gamma), \quad k\in\mathbb{R}^d,\ y\in\mathbb{R}^d.$$

Here $\mathbb{B}$ is the fundamental unit cell for the dual lattice Γ^*, *i. e.* the lattice generated over the integers by the dual basis $\{a_1^*,\dots,a_d^*\}$ defined by the relations $a_i^*\cdot a_j = 2\pi\delta_{i,j}$. As can be readily verified, the function $\mathcal{U}_{\mathrm{BF}}\, w$ is Γ^*-pseudoperiodic and Γ-periodic, meaning that

$$\begin{aligned}
(\mathcal{U}_{\mathrm{BF}}\, w)\,(k+\lambda,y) &= \mathrm{e}^{-\mathrm{i}\lambda\cdot y}\,(\mathcal{U}_{\mathrm{BF}}\, w)\,(k,y) && \text{for } \lambda\in\Gamma^*,\\
(\mathcal{U}_{\mathrm{BF}}\, w)\,(k,y+\gamma) &= (\mathcal{U}_{\mathrm{BF}}\, w)\,(k,y) && \text{for } \gamma\in\Gamma.
\end{aligned}$$

Consequently, the function $(\mathcal{U}_{\mathrm{BF}}\, w)\,(k,\cdot)$, for fixed $k\in\mathbb{R}^d$, can be interpreted as an element of the k-independent Hilbert space $\mathcal{H}_{\mathrm{f}} = L^2(\mathbb{T}_Y^d)$, where $\mathbb{T}_Y^d = \mathbb{R}^d/\Gamma$ is a d-dimensional torus in position space.

The Bloch-Floquet transform $\mathcal{U}_{\mathrm{BF}}$, as defined above, extends to a unitary operator

$$\mathcal{U}_{\mathrm{BF}}\colon L^2(\mathbb{R}^d) \to \int_{\mathbb{B}}^{\oplus} \mathrm{d}k\, \mathcal{H}_{\mathrm{f}}$$

whose inverse is given by

$$\left(\mathcal{U}_{\mathrm{BF}}^{-1} u\right)(x) = \frac{1}{|\mathbb{B}|^{1/2}} \int_{\mathbb{B}} \mathrm{d}k\, \mathrm{e}^{\mathrm{i}k\cdot x}\, u(k,[x]), \quad x\in\mathbb{R}^d,$$

where $[x] := x \bmod \Gamma$. With the hypotheses on the potential V_Γ mentioned above, one verifies that H_Γ becomes a fibred operator in Bloch-Floquet representation, namely

$$\mathcal{U}_{\mathrm{BF}} H_\Gamma \mathcal{U}_{\mathrm{BF}}^{-1} = \int_{\mathbb{B}}^{\oplus} \mathrm{d}k\, H(k) \quad \text{where} \quad H(k) = (-\mathrm{i}\nabla_y + k)^2 + V_\Gamma. \tag{2.1}$$

Each $H(k)$ acts on the k-independent domain $\mathcal{D} := W^{2,2}(\mathbb{T}_Y^d) \subset \mathcal{H}_{\mathrm{f}}$, where it defines a self-adjoint operator. Since for any $\kappa_0\in\mathbb{C}^d$ one has

$$H(\kappa) = H(\kappa_0) + 2(\kappa-\kappa_0)\cdot(-\mathrm{i}\nabla_y) + (\kappa^2-\kappa_0^2)\mathbb{1}$$

and $(-\mathrm{i}\nabla_y)$ is relatively bounded with respect to $H(\kappa_0)$, the assignment $\kappa\mapsto H(\kappa)$ defines an entire family of type (A), and hence an entire analytic family in the sense of Kato [41, Thm. XII.9].

Moreover, all the operators $H(k)$, $k\in\mathbb{R}^d$, have compact resolvent, and consequently they only have pure point spectrum accumulating at infinity. We label the eigenvalues in increasing order, *i. e.* $E_0(k)\le\cdots\le E_n(k)\le E_{n+1}(k)\le\cdots$, repeated according to their multiplicity; the function $k\mapsto E_n(k)$ is usually called the *n-th Bloch band*. We denote by $u_n(k)$ the solution to the eigenvalue problem

$$H(k)u_n(k) = E_n(k)u_n(k), \quad u_n(k,\cdot)\in\mathcal{D}\subset\mathcal{H}_{\mathrm{f}}. \tag{2.2}$$

The function $k\mapsto\psi_n(k,y) = \mathrm{e}^{\mathrm{i}k\cdot y}u_n(k,y)$ is called the *n-th Bloch function* in the physics literature; $u_n(k,\cdot)$ is its Γ-periodic part.

2.2 From insulators to semimetals

In the case of an isolated Bloch band, or an isolated family of m Bloch bands $\{E_n, \dots, E_{n+m-1}\} = \{E_i\}_{i \in I}$, where "isolated" means that

$$\inf_k \{|E_i(k) - E_c(k)| : \; i \in I, c \notin I\} > 0, \tag{2.3}$$

one considers the orthogonal projector

$$P_I(k) = \sum_{n \in I} |u_n(k,\cdot)\rangle \langle u_n(k,\cdot)| \qquad \in \mathcal{B}(\mathcal{H}_{\mathrm{f}}). \tag{2.4}$$

It is known that, in view of condition (2.3), the map $k \mapsto P_I(k)$ is a $\mathcal{B}(\mathcal{H}_{\mathrm{f}})$-valued analytic and pseudoperiodic function (see, for example, [33] or [35, Proposition 2.1]). Thus, it defines a smooth vector bundle over the torus $\mathbb{T}_d^* = \mathbb{R}^d/\Gamma^*$ whose fibre at $k \in \mathbb{T}_d^*$ is $\operatorname{Ran} P_I(k)$. The triviality of such vector bundle, called *Bloch bundle* in [38], is equivalent to the existence of exponentially localized (composite) Wannier functions. By exploiting this geometric viewpoint, the existence of exponentially localized composite Wannier functions for a time-reversal-symmetric Hamiltonian has been proved, provided $d \leq 3$ [5, 38].

On the other hand, in metals and semimetals the relevant Bloch bands intersect each other. For example, in monolayer graphene the conduction and valence bands, here denoted by E_+ and E_- respectively, form a conical intersection at two inequivalent points K and K' (Dirac points), *i. e.* for $q = k - K$ one has

$$E_\pm(K+q) = \pm v_F |q| + o(|q|) \qquad \text{as } |q| \to 0, \tag{2.5}$$

where $v_F > 0$ is called the Fermi velocity and $E_\pm(K) = 0$ by definition of the zero of the energy. An analogous expansion holds when K is replaced by K'. The corresponding eigenprojectors

$$P_s(k) = |u_s(k,\cdot)\rangle \langle u_s(k,\cdot)|, \qquad s \in \{+,-\},$$

are not defined at $k = K$, nor does the limit $\lim_{k \to K} P_s(k)$ exist. This fact can be explicitly checked by using an effective tight-binding model Hamiltonian [51, 12, 4].

2.3 Tight-binding Hamiltonians in graphene

We provide some details about the latter claim. If the Bloch functions $\psi_s(k)$ for the Hamiltonian H_Γ were explicitly known, it would be natural to study the continuity of the eigenprojector by using the reduced 2-band Hamiltonian

$$\mathcal{H}_{\mathrm{red}}(k)_{r,s} = \left\langle \psi_r(k), H_\Gamma \, \psi_s(k) \right\rangle_{L^2(Y)} = \langle u_r(k), H(k) \, u_s(k) \rangle_{\mathcal{H}_{\mathrm{f}}} \tag{2.6}$$

where $r, s \in \{+,-\}$, Y is a fundamental cell for the lattice Γ and $H(k)$ is defined in (2.1). Focusing on $|q| \ll 1$, one notices that, since $H(K)u_\pm(K) = E_\pm(K)u_\pm(K) = 0$, a standard Hellman-Feynmann argument[1] yields

$$\mathcal{H}_{\text{red}}(K+q)_{r,s} = \big\langle u_r(K)\,,\, H(K+q)\, u_s(K)\big\rangle + \mathcal{O}(|q|^2). \tag{2.7}$$

Thus $q \mapsto \mathcal{H}_{\text{red}}(K+q)$ encodes, for $|q| \ll 1$, the local behaviour of the Hamiltonian and its eigenprojectors with respect to *fixed* Bloch functions, *i. e.* Bloch functions evaluated at the Dirac point.

Approximated Bloch functions can be explicitly computed in the tight-binding approximation. Within this approximation, the reduced Hamiltonian (2.6) is approximated by the effective Hamiltonian

$$\mathcal{H}_{\text{eff}}(k) = \begin{pmatrix} 0 & \gamma_k^* \\ \gamma_k & 0 \end{pmatrix} \quad \text{where} \quad \gamma_k = 1 + \mathrm{e}^{\mathrm{i}k\cdot a_2} + \mathrm{e}^{\mathrm{i}k\cdot(a_2-a_1)} \tag{2.8}$$

with $\{a_1, a_2\}$ the standard Bravais basis for graphene, as in [51, 12]. Thus, for $|q| \ll 1$ and denoting by θ_q the polar angle in the plane (q_1, q_2), *i. e.* $|q|\mathrm{e}^{\mathrm{i}\theta_q} = q_1 + \mathrm{i}q_2$, one obtains

$$\mathcal{H}_{\text{eff}}(K+q) = v_{\text{F}} \begin{pmatrix} 0 & q_1 - \mathrm{i}q_2 \\ q_1 + \mathrm{i}q_2 & 0 \end{pmatrix} + \mathcal{O}(|q|^2) = v_{\text{F}}|q| \begin{pmatrix} 0 & \mathrm{e}^{-\mathrm{i}\theta_q} \\ \mathrm{e}^{\mathrm{i}\theta_q} & 0 \end{pmatrix} + \mathcal{O}(|q|^2). \tag{2.9}$$

One easily checks (see Section) that the eigenprojectors of the leading-order Hamiltonian, which is proportional to

$$\mathcal{H}_{\text{mono}}(q) = |q| \begin{pmatrix} 0 & \mathrm{e}^{-\mathrm{i}\theta_q} \\ \mathrm{e}^{\mathrm{i}\theta_q} & 0 \end{pmatrix}, \tag{2.10}$$

are not continuous at $q = 0$, implying that – within the validity of the tight-binding approximation – also the eigenprojectors of $H(k)$ are not continuous at $k = K$, as claimed. In the case of bilayer graphene, the same approach yields a leading-order effective Hamiltonian proportional to

$$\mathcal{H}_{\text{bi}}(q) = |q|^2 \begin{pmatrix} 0 & \mathrm{e}^{-\mathrm{i}2\theta_q} \\ \mathrm{e}^{\mathrm{i}2\theta_q} & 0 \end{pmatrix} \tag{2.11}$$

---

[1] The Hellman-Feynmann-type argument goes as follows. Near a Dirac point, *i. e.* for $k = K + q$ and $|q| \ll 1$, one has

$$\begin{aligned}
\mathcal{H}_{\text{red}}(k)_{r,s} &= \langle u_r(k)\,,\, H(k)\, u_s(k)\rangle_{\mathcal{H}_{\text{f}}} \\
&= \langle u_r(K)\,,\, H(K)\, u_s(K)\rangle_{\mathcal{H}_{\text{f}}} + \\
&\quad + q\cdot\big(\langle \nabla_k u_r(K)\,,\, H(K)\, u_s(K)\rangle_{\mathcal{H}_{\text{f}}} + \langle H(K)\, u_r(K)\,,\, \nabla_k u_s(K)\rangle_{\mathcal{H}_{\text{f}}}\big) + \\
&\quad + q\cdot\langle u_r(K)\,,\, \nabla_k H(K)\, u_s(K)\rangle_{\mathcal{H}_{\text{f}}} + \mathcal{O}(|q|^2).
\end{aligned}$$

(Notice that the derivatives $\nabla_k H(k)$ exist in view of the above-mentioned analyticity of the family $k \mapsto H(k)$). Since $H(K)u_\pm(K) = 0$, all terms but the last vanish. Clearly,

$$\big\langle u_r(K)\,,\, H(K+q)\, u_s(K)\big\rangle = q\cdot\langle u_r(K)\,,\, \nabla_k H(K)\, u_s(K)\rangle + \mathcal{O}(|q|^2),$$

yielding the claim.

which also corresponds to a singular family of projectors. As pointed out by many authors [39, 27] the effective Hamiltonians (2.10) and (2.11) are related to different values of a "topological index". A rigorous definition of that index is the first task of our paper.

For the sake of completeness, we mention that according to [31] the low-energy effective Hamiltonian for multilayer graphene (with m layers and ABC stacking) is proportional to

$$\mathcal{H}_{\mathrm{multi}}(q) = |q|^m \begin{pmatrix} 0 & \mathrm{e}^{-\mathrm{i}m\theta_q} \\ \mathrm{e}^{\mathrm{i}m\theta_q} & 0 \end{pmatrix}, \qquad m \in \mathbb{N}^\times. \tag{2.12}$$

2.4 Singular families of projectors

Abstracting from the specific case of graphene, we study the topology of the Bloch eigenspaces around an eigenvalue intersection. We consider any periodic Hamiltonian and a selected Bloch band of interest E_s which intersects the other Bloch bands in finitely many points $K_1, \dots, K_M$. Focusing on one of them, named k_0, the crucial information is the behaviour of the function $k \mapsto P_s(k)$ in a neighbourhood $R \subset \mathbb{T}^*_d$ of the intersection point k_0. In view of the example of graphene, we set the following

Definition 2.1. Let $\mathcal{H}$ be a separable Hilbert space. A family of orthogonal projectors $\{P(k)\}_{k \in R \setminus \{k_0\}} \subset \mathcal{B}(\mathcal{H})$ such that $k \mapsto P(k)$ is C^∞-smooth in $\mathring{R} = R \setminus \{k_0\} \subset \mathbb{T}^*_d$ is called a **singular family** if it cannot be continuously extended to $k = k_0$, *i. e.* if $\lim_{k \to k_0} P(k)$ does not exist. In such a case, the point k_0 is called *singular point*. A family which is not singular is called *regular family*. ♢

In the case of insulators, the geometric structure corresponding to the regular family of projectors (2.4) is a smooth vector bundle, whose topological invariants can be investigated with the usual tools of differential geometry (curvature, Chern classes, ...). On the other hand, in the case of metals and semimetals one deals with a singular family of projectors, thus the usual geometric approach is not valid anymore. Indeed, in the case of conical intersections the interesting information is "hidden" in the singular point. In particular, if we assume for simplicity that the neighbourhood R is a small ball around the Dirac point k_0, then when $d = 2$ the set $R \setminus \{k_0\}$ can be continuously retracted to a circle S^1, and it is well known that every complex line bundle over S^1 is trivial, so it has no non-trivial topological invariants. In view of that, to define the topological invariants of a singular family of projectors we have to follow a different strategy, which is the content of Section 3. These invariants are also related to a distributional approach to the Berry curvature, as detailed in Appendix A.

3 Topology of a singular 2-dimensional family of projectors

Motivated by the example of graphene, in this paper we investigate the case of singular 2-dimensional families of projectors ($d = 2$, arbitrary rank). Since the relevant parameter is the codimension, this case corresponds to the generic case in the Born-

Oppenheimer theory of molecules [14, 15, 10]. The analysis of higher-codimensional cases will be addressed in a future paper.

For the moment being, we focus on just one singularity of the family of projectors, say at the point k_0. We will conduct a *local* analysis on the "topological behaviour" determined by such a singular point: hence we restrict our attention on a simply-connected region $R \subset \mathbb{T}_2^*$ containing k_0 such that for any other Bloch band E_n

$$E_s(k) \neq E_n(k) \quad \text{for all } k \in R \setminus \{k_0\}.$$

In other words, Bloch bands are allowed to intersect only at k_0 in the region R.

3.1 A geometric $\mathbb{Z}$-invariant: eigenspace vorticity

To define a local geometric invariant characterising the behaviour of a 2-dimensional family of projectors around the (possibly singular) point k_0, we start from the following

Datum 3.1. Let $\mathcal{H}$ be a separable Hilbert space, and let $R \subset \mathbb{T}_2^*$ be a simply connected region containing k_0. We consider a family of projectors $\{P_s(k)\}_{k \in R \setminus \{k_0\}} \subset \mathcal{B}(\mathcal{H})$ which is C^∞-smooth in $R \setminus \{k_0\}$. ♢

We restrict our attention to the local behaviour of the family $\{P_s(k)\}$ around k_0. Suppose $r > 0$ is so small that $U := \left\{k \in \mathbb{R}^2 : |k - k_0| < r\right\}$ is all contained in R. In order to define an integer-valued (local) geometric invariant n_{v}, baptised *eigenspace vorticity*,we provide the following computable recipe. First, introduce a smoothing parameter $\mu \in [-\mu_0, \mu_0]$, $\mu_0 > 0$, so that $\{P_s(k)\}_{R \setminus U}$ can be seen as the $\mu = 0$ case of a *deformed* family of projectors $\left\{P_s^\mu(k)\right\}$, which for $\mu \neq 0$ is defined and regular on the whole region R. We also assume that the dependence on μ of such a deformed family of projectors is at least of class C^2.

The deformed family $\left\{P_s^\mu(k)\right\}$ allows us to construct a vector bundle $\mathcal{L}_s$, which we call the *smoothed Bloch bundle*, over the set

$$B := \big(R \times [-\mu_0, \mu_0]\big) \setminus C,$$

where C denotes the "cylinder" $C := U \times (-\mu_0, \mu_0)$. The total space of this vector bundle is

$$\mathcal{L}_s := \left\{((k,\mu), v) \in B \times \mathcal{H} : v \in \operatorname{Ran} P_s^\mu(k)\right\}. \tag{3.1}$$

Explicitly, the fibre of $\mathcal{L}_s$ over a point $(k,\mu) \in B$ is the range of the projector $P_s^\mu(k)$. We may look at $\mathcal{L}_s$ as a collection of "deformations" of the bundle

$$\mathcal{L}_s^0 := \left\{(k, v) \in (R \setminus U) \times \mathcal{H} : v \in \operatorname{Ran} P_s(k)\right\}$$

over $R \setminus U$, which is defined solely in terms of the undeformed family $\{P_s(k)\}$.

We denote by ω_s the Berry curvature for the smoothed Bloch bundle $\mathcal{L}_s$. Posing for notational convenience $k_3 = \mu$ and $\partial_j = \partial/\partial k_j$, one has

(3.2)
$$\omega_s = \mathrm{i} \sum_{j,\ell=1}^{3} (\omega_s)_{j,\ell}(k)\, \mathrm{d}k_j \wedge \mathrm{d}k_\ell \quad \text{where } (\omega_s)_{j,\ell}(k) = \mathrm{Tr}\left(P_s^\mu(k)\left[\partial_j P_s^\mu(k), \partial_\ell P_s^\mu(k)\right]\right).$$

Set $\mathcal{C} := \partial C$ for the "cylindrical" internal boundary of the base space B, and

$$\mathring{C} := C \setminus \left\{(k = k_0, \mu = 0)\right\}$$

for the "pointed cylinder", which is the complement of B in

$$\widehat{B} := \left(R \times [-\mu_0, \mu_0]\right) \setminus \left\{(k = k_0, \mu = 0)\right\}.$$

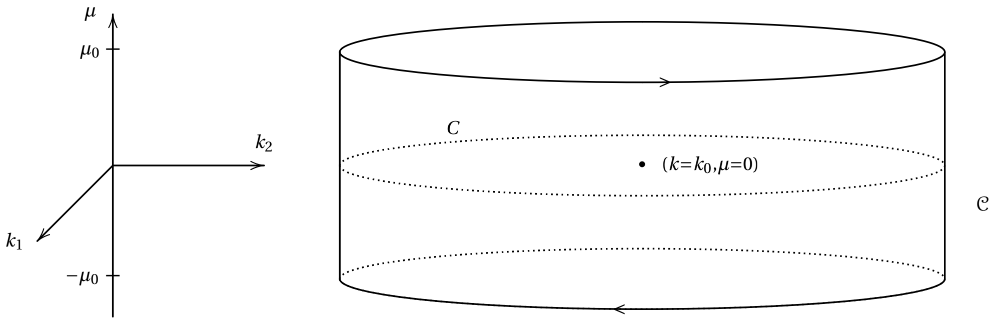


Fig. 1 The cylinder C and its surface $\mathcal{C}$. The boundary of this surface is oriented according to the outward normal direction.

Definition 3.1 (Eigenspace vorticity). Let $\{P_s(k)\}_{k \in R\setminus\{k_0\}}$ be a family of projectors as in Datum 3.1, and $\left\{P_s^\mu(k)\right\}_{(k,\mu)\in B}$ be a smoothed family of projectors, as described above. Let $\mathcal{L}_s$ be the vector bundle (3.1) over B, and denote by ω_s its Berry curvature, as in (3.2). The **eigenspace vorticity** of the smoothed family of projectors $\left\{P_s^\mu(k)\right\}_{k\in R\setminus\{k_0\}}$ (around the point $k_0 \in R$) is the integer

(3.3)
$$n_\mathrm{v} = n_\mathrm{v}(P_s) := -\frac{1}{2\pi}\int_{\mathcal{C}} \omega_s \in \mathbb{Z}.$$

◊

The number n_v is indeed an integer, because it equals (up to a conventional sign) the *first Chern number* of the vector bundle $\mathcal{L}_s \to \mathcal{C}$. This integer is the topological invariant that characterises the behaviour of $\left\{P_s^\mu(k)\right\}$ around k_0; in particular, when $\dim \mathrm{Ran}\, P(k) = 1$ for $k \neq k_0$, it selects one of the canonical models that will be introduced in the next Subsection. Notice that there is an ambiguity in the *sign* of the integer n_v defined in (3.3), related to the orientation of the cylindrical surface of integration $\mathcal{C}$. Indeed, if one exchanges μ with $-\mu$ one obtains the opposite value for n_v. This ambiguity is resolved once the orientation of the μ-axis is fixed.

Remark 3.1 (Deformations in computational physics). The above smoothing procedure corresponds to a common practice in computational solid-state physics[2].

[2] We are grateful to R. Bianco and R. Resta for pointing out this fact to us.

Indeed, the family $\{P_s(k)\}$ usually appears as the collection of the eigenprojectors corresponding to the eigenvalue $E_s(k)$ of a given Hamiltonian operator $H(k)$ (*e. g.* the Hamiltonian (2.6) or (2.10) for graphene). When dealing with an intersection of eigenvalues, to improve the numerical accuracy it is often convenient to consider a family of deformed Hamiltonians $H^\mu(k)$ and the corresponding eigenprojectors $P_s^\mu(k)$, in such a way that the eigenvalue intersection disappears when $\mu \neq 0$. For example, when dealing with monolayer graphene the deformed Hamiltonian is obtained by varying the electronegativity of the carbon atoms in the numerical code. ♢

Before we proceed, we have to comment on the well-posedness of our definition of eigenspace vorticity. First of all, the definition relies on the existence of a deformation $\left\{P_s^\mu(k)\right\}$ of the original family $\{P_s(k)\}$ as in Datum 3.1, which for $\mu \neq 0$ is regular also at $k = k_0$. Such a deformation indeed exists in all cases of practical interest, namely when $P_s(k)$ arises as the eigenprojector, relative to an eigenvalue $E_s(k)$, of a k-dependent Hamiltonian $H(k)$, such that at $k = k_0$ two of its eigenvalues coincide. Indeed, in view of the von Neumann-Wigner theorem [1, 50], the eigenvalue intersection for general Hermitian matrices is highly non-generic, *i. e.* it is a codimension-3 phenomenon. As the base B of the smoothed Bloch bunde is 3-dimensional, it may be assumed that the eigenvalue intersection – *i. e.* the singularity of the family of projectors – occurs only at the point $(k = k_0, \mu = 0)$; more precisely, the generic deformation $\left\{P_s^\mu(k)\right\}$ (which may be assumed to be the family of eigenprojectors of some deformed Hamiltonian $H^\mu(k)$) will satisfy this hypothesis.

In addition to this, we must investigate how the definition (3.3) of n_{v} depends on the specific choice of the deformation. Since n_{v} is a topological quantity, it is stable under small perturbations of the deformed family of projectors $\left\{P_s^\mu(k)\right\}$. This means that model Hamiltonians which are "close", in some suitable sense, will produce the same eigenspace vorticity. More formally, we argue as follows. Let $\widetilde{P}_s^\mu(k)$ be another smoothing deformation of the family of projectors $P_s(k)$, so that in particular

$$P_s^{\mu=0}(k) = P_s(k) = \widetilde{P}_s^{\mu=0}(k), \quad \text{for all } k \in R \setminus \{k_0\}.$$

Moreover, define the 2-form $\widetilde{\omega}_s$ and its components $(\widetilde{\omega}_s)_{j,\ell}(k)$, $j, \ell \in \{1, 2, 3\}$, as in (3.2), with $P_s^\mu(k)$ replaced by $\widetilde{P}_s^\mu(k)$.

Lemma 3.1 (Irrelevance of the choice among close deformations). *Suppose that the maps* $\widehat{B} \ni (k, \mu) \mapsto P_s^\mu(k) \in \mathcal{B}(\mathcal{H})$ *and* $\widehat{B} \ni (k, \mu) \mapsto \widetilde{P}_s^\mu(k) \in \mathcal{B}(\mathcal{H})$ *are of class* C^2*, and that*

$$\left\| P^\mu(k) - \widetilde{P}^\mu(k) \right\|_{\mathcal{B}(\mathcal{H})} < 1 \quad \textit{for all } (k, \mu) \in \mathcal{C}. \tag{3.4}$$

Then

$$\int_{\mathcal{C}} \omega_s = \int_{\mathcal{C}} \widetilde{\omega}_s. \tag{3.5}$$

Proof. By a result of Kato and Nagy [20, Sec. I.6.8], the hypothesis (3.4) implies that there exists a family of unitary operators $W^\mu(k)$ such that

$$\widetilde{P}_s^\mu(k) = W^\mu(k) P_s^\mu(k) W^\mu(k)^{-1}. \tag{3.6}$$

The explicit Kato-Nagy's formula

$$W^{\mu}(k) := \left(\mathbb{1} - (P^{\mu}_s(k) - \widetilde{P}^{\mu}_s(k))^2\right)^{-1/2} \left(\widetilde{P}^{\mu}_s(k) P^{\mu}_s(k) + (\mathbb{1} - \widetilde{P}^{\mu}_s(k))(\mathbb{1} - P^{\mu}_s(k))\right) \tag{3.7}$$

shows that the map $(k,\mu) \mapsto W^{\mu}(k)$ has the same regularity as $(k,\mu) \mapsto P^{\mu}_s(k) - \widetilde{P}^{\mu}_s(k)$[3].

Formula (3.6) implies that the vector bundles $\mathcal{L}_s$ and $\widetilde{\mathcal{L}}_s$, corresponding to the deformed families of projectors $\{P^{\mu}_s(k)\}$ and $\{\widetilde{P}^{\mu}_s(k)\}$ respectively, are isomorphic, the isomorphism being implemented fibre-wise by the unitary $W^{\mu}(k)$. Thus they have the same Chern number, *i. e.* equation (3.5) holds true.

Alternatively, for the sake of clarity, we provide an explicit proof of (3.5) by showing that the difference $\widetilde{\omega}_s - \omega_s$ is an exact form $\mathrm{d}\beta$ on $\mathcal{C}$; then by applying Stokes' theorem one gets

$$\int_{\mathcal{C}} (\widetilde{\omega}_s - \omega_s) = \int_{\mathcal{C}} \mathrm{d}\beta = 0$$

because $\mathcal{C}$ has no boundary. This will conclude the proof of the Lemma.

For the sake of readability, in the following we will use the abbreviations

$$P := P^{\mu}_s(k), \quad \widetilde{P} := \widetilde{P}^{\mu}_s(k), \quad W := W^{\mu}(k),$$
$$\omega_{j,\ell} := (\omega_s)_{j,\ell}(k), \quad \widetilde{\omega}_{j,\ell} := (\widetilde{\omega}_s)_{j,\ell}(k).$$

A lengthy but straightforward computation, that uses only the cyclicity of the trace, the relations $P^2 = P$ and $WW^{-1} = \mathbb{1} = W^{-1}W$ and their immediate consequences

$$P(\partial_j P) = \partial_j P - (\partial_j P)P \qquad \text{and} \qquad W^{-1}(\partial_j W) = -(\partial_j W^{-1})W,$$

yields to

$$\begin{aligned} \widetilde{\omega}_{j,\ell} - \omega_{j,\ell} = &\operatorname{Tr}\left\{P(\partial_j W^{-1})(\partial_\ell W) - P(\partial_\ell W^{-1})(\partial_j W)\right\} \\ &+ \operatorname{Tr}\left\{(\partial_j P)W^{-1}(\partial_\ell W) - (\partial_\ell P)W^{-1}(\partial_j W)\right\}. \end{aligned} \tag{3.9}$$

Summing term by term the two lines in (3.9), one gets

$$\begin{aligned} \widetilde{\omega}_{j,\ell} - \omega_{j,\ell} &= \operatorname{Tr}\left\{\left(P(\partial_j W^{-1}) + (\partial_j P)W^{-1}\right)(\partial_\ell W) - \left(P(\partial_\ell W^{-1}) + (\partial_\ell P)W^{-1}\right)(\partial_j W)\right\} = \\ &= \operatorname{Tr}\left\{\partial_j(PW^{-1})\partial_\ell W - \partial_\ell(PW^{-1})\partial_j W\right\} = \\ &= \operatorname{Tr}\left\{\partial_j\left(PW^{-1}(\partial_\ell W)\right) - PW^{-1}\partial_j\partial_\ell W - \partial_\ell\left(PW^{-1}(\partial_j W)\right) + PW^{-1}\partial_\ell\partial_j W\right\} = \\ &= \partial_j\left(\operatorname{Tr}\left\{PW^{-1}(\partial_\ell W)\right\}\right) - \partial_\ell\left(\operatorname{Tr}\left\{PW^{-1}(\partial_j W)\right\}\right), \end{aligned}$$

[3] The presence of the inverse square root does not spoil the regularity of $W^{\mu}(k)$. Indeed, setting $Q = Q^{\mu}(k) = (P^{\mu}_s(k) - \widetilde{P}^{\mu}_s(k))^2$, one can expand

$$(\mathbb{1} - Q)^{-1/2} = \sum_{n=0}^{\infty} \binom{-1/2}{n} (-Q)^n. \tag{3.8}$$

The above power series is absolutely convergent if $\|Q\| < 1$ (which follows from (3.4)), and in the same range it is term-by-term differentiable.

where we used the fact that $(k,\mu) \mapsto W^{\mu}(k)$ is at least of class C^2, so that the mixed second derivatives cancel. In summary, the explicit computation shows that

$$\widetilde{\omega}_{j,\ell} - \omega_{j,\ell} = \partial_j \operatorname{Tr}\left(P_s^{\mu}(k) W^{\mu}(k)^{-1} \partial_\ell W^{\mu}(k)\right) - \partial_\ell \operatorname{Tr}\left(P_s^{\mu}(k) W^{\mu}(k)^{-1} \partial_j W^{\mu}(k)\right)$$

which can be written in a more intrinsic form as

$$\widetilde{\omega}_s - \omega_s = \mathrm{d}\beta, \quad \text{with} \quad \beta = 2\,\mathrm{i}\operatorname{Tr}\left(P_s^{\mu}(k) W^{\mu}(k)^{-1} \mathrm{d}W^{\mu}(k)\right).$$

This concludes the proof. □

Remark 3.2 (Numerical evaluation of the eigenspace vorticity). The numerical evaluation of n_{v} can be performed by replacing the cylindrical surface $\mathcal{C}$ with any surface homotopically equivalent to it in $\widehat{B}$, *e.g.* with any polyhedron enclosing the point $(k_0, 0)$. Numerically, the eigenspace vorticity is evaluated by summing up contributions from all faces of the polyhedron. The integral of the curvature ω_s over each face is computed by a discretization scheme which approximates the integral of the Berry connection over the perimeter of the face (see *e.g.* [39] and references therein). The latter approach has been implemented by R. Bianco in the case of the Haldane model [17], and provided results in agreement with the analytical computation already in an 8-point discretization, by using a cube. ◊

Even with the above result, the value of n_{v} may still *a priori* depend on the choice of the specific deformation $\left\{P_s^{\mu}(k)\right\}$, and not only on the original family of projectors $\left\{P_s(k) = P_s^{\mu=0}(k)\right\}$. However, as we will explain in Section 3.3, when $\mathcal{H} = \mathbb{C}^2$ there exists a class of "distinguished deformations", called *hemispherical*, which provide a natural choice of deformation to compute the eigenspace vorticity. For such hemispherical deformations, the eigenspace vorticity indeed depends only on the undeformed family of projectors, *i. e.* on the Datum 3.1. In all the relevant examples, as the tight-biding model of graphene or the Haldane model, such hemispherical deformations appear naturally.

For the sake of clarity, in the next Subsection we introduce a family of *canonical models*, one for each value of $n_{\mathrm{v}} \in \mathbb{Z}$, having the property of being hemispherical. For the case of a general Hilbert space $\mathcal{H}$, the identification of a "distinguished" class of deformations is a challenging open problem.

3.2 The canonical models for an intersection of eigenvalues

In this Subsection, we introduce effective Hamiltonians whose eigenspaces model the topology of Bloch eigenspaces, locally around a point k_0 where Bloch bands intersect. These will be also employed as an example on how to perform the μ-deformation for a family of eigenprojectors.

Hereafter, we focus on the case of a system of two *non-degenerate* Bloch bands, *i. e.* $P_s(k)$ is a projector on $\mathcal{H} = \mathbb{C}^2$ and $\dim \operatorname{Ran} P_s(k) = 1$ for $k \neq k_0$.

The 1-canonical model

Assume from now on that $k \in U = \{k \in \mathbb{R}^2 : |k - k_0| < r\}$, where $r > 0$ is sufficiently small; as before, set $q = k - k_0$. We will mainly work in polar coordinates in momentum space, and hence denote by $(|q|, \theta_q)$ the coordinates of q, namely $q_1 + \mathrm{i} q_2 = |q|\, \mathrm{e}^{\mathrm{i}\theta_q}$.

Following [14], we consider the effective Hamiltonian[4]

$$H_{\text{eff}}(q) := \begin{pmatrix} q_1 & q_2 \\ q_2 & -q_1 \end{pmatrix} = |q| \begin{pmatrix} \cos\theta_q & \sin\theta_q \\ \sin\theta_q & -\cos\theta_q \end{pmatrix}. \tag{3.10}$$

The eigenvalues of this matrix are given by

$$E_\pm(q) = \pm |q|$$

and thus $H_{\text{eff}}(q)$ is a good candidate for modelling conical intersections locally (compare (2.5)). The eigenfunctions corresponding to $E_+(q)$ and $E_-(q)$ are respectively

$$\phi_{1,+}(q) = \mathrm{e}^{\mathrm{i}\theta_q/2} \begin{pmatrix} \cos(\theta_q/2) \\ \sin(\theta_q/2) \end{pmatrix}, \quad \phi_{1,-}(q) = \mathrm{e}^{\mathrm{i}\theta_q/2} \begin{pmatrix} -\sin(\theta_q/2) \\ \cos(\theta_q/2) \end{pmatrix}. \tag{3.11}$$

The phases are chosen so that these functions are single-valued when we identify $\theta_q = 0$ and $\theta_q = 2\pi$. We will call $\phi_{1,\pm}(q)$ the *canonical eigenvectors for the conical intersection* at the singular point k_0. These satisfy

$$\partial_{|q|} \phi_{1,\pm} = 0, \quad \partial_{\theta_q} \phi_{1,\pm} = \frac{1}{2} \left(\pm \phi_{1,\mp} + \mathrm{i} \phi_{1,\pm} \right). \tag{3.12}$$

The corresponding eigenprojectors are easily computed to be

$$P_{1,\pm}(q) = \pm \frac{1}{2|q|} \begin{pmatrix} q_1 \pm |q| & q_2 \\ q_2 & -q_1 \pm |q| \end{pmatrix} = \pm \frac{1}{2} \begin{pmatrix} \cos\theta_q \pm 1 & \sin\theta_q \\ \sin\theta_q & -\cos\theta_q \pm 1 \end{pmatrix}. \tag{3.13}$$

The above expressions show that the families $\{P_{1,\pm}(q)\}_{q \in \mathring{U}}$ are singular at $q = 0$, in the sense of Definition 2.1. As explained in Section 3.1, in order to compute their vorticities we have to introduce a smoothing parameter $\mu \in [-\mu_0, \mu_0]$ to remove the singularity: this is achieved by considering the so-called *avoided crossings* [15]. Explicitly, we deform the Hamiltonian (3.10) to get

$$H^\mu_{\text{eff}}(q) := \begin{pmatrix} q_1 & q_2 + \mathrm{i}\mu \\ q_2 - \mathrm{i}\mu & -q_1 \end{pmatrix} = |q| \begin{pmatrix} \cos\theta_q & \sin\theta_q + \mathrm{i}\eta \\ \sin\theta_q - \mathrm{i}\eta & -\cos\theta_q \end{pmatrix}, \tag{3.14}$$

where $\mu \in [-\mu_0, \mu_0]$ is a small real parameter and

$$\eta = \eta^\mu(q) := \frac{\mu}{|q|}.$$

[4] The Hamiltonian (3.10) is unitarily equivalent to the effective Hamiltonian for monolayer graphene (2.10), by conjugation with a *k-independent* unitary matrix. Thus, both (2.10) and (3.10) are reasonable choices for a canonical local model describing conical intersections of eigenvalues. We prefer the choice (3.10), since this Hamiltonian has real entries.

In this case, the eigenvalues are

$$E^{\mu}_{\pm}(q) := \pm\sqrt{|q|^2+\mu^2} = \pm|q|\sqrt{1+\eta^2}$$

and thus, if $\mu \neq 0$, the energy bands do not intersect.

As the matrix $H^{\mu}_{\mathrm{eff}}(q)$ is not real, we look for complex eigenfunctions of the form $v+\mathrm{i}u$. These can be found by solving the system

$$\begin{cases} \cos\theta_q\, v_1 + \sin\theta_q\, v_2 = \pm\sqrt{1+\eta^2}\, v_1 + \eta\, u_2, \\ -\sin\theta_q\, v_1 + \cos\theta_q\, v_2 = \mp\sqrt{1+\eta^2}\, v_2 + \eta\, u_1, \\ \cos\theta_q\, u_1 + \sin\theta_q\, u_2 = \pm\sqrt{1+\eta^2}\, u_1 - \eta\, v_2, \\ -\sin\theta_q\, u_1 + \cos\theta_q\, u_2 = \mp\sqrt{1+\eta^2}\, u_2 - \eta\, v_1, \end{cases} \tag{3.15}$$

with respect to the unknowns (v_1, v_2, u_1, u_2), and then imposing that they coincide, up to the phase $\mathrm{e}^{\mathrm{i}\theta_q/2}$, with (3.11) when $\mu = 0$ and $q \neq 0$ (a condition on (v_1, v_2)). After choosing the appropriate phase, one gets the *canonical eigenvectors for the avoided crossing*

$$\phi^{\mu}_{1,\pm}(q) := \frac{1}{\sqrt{1+\alpha^2}}\left[\phi_{1,\pm}(q) + \mathrm{i}\alpha\phi_{1,\mp}(q)\right] \tag{3.16}$$

where

$$\alpha = \alpha^{\mu}(q) := \frac{1-\sqrt{1+\eta^2}}{\eta} = \frac{|q|-\sqrt{|q|^2+\mu^2}}{\mu}. \tag{3.17}$$

One can easily check that the eigenprojectors associated to these eigenvectors are

$$\begin{aligned} P^{\mu}_{1,\pm}(q) &= \pm\frac{1}{2\sqrt{|q|^2+\mu^2}}\begin{pmatrix} q_1 \pm\sqrt{|q|^2+\mu^2} & q_2+\mathrm{i}\mu \\ q_2-\mathrm{i}\mu & -q_1\pm\sqrt{|q|^2+\mu^2}\end{pmatrix} = \\ &= \pm\frac{1}{2\sqrt{1+\eta^2}}\begin{pmatrix} \cos\theta_q \pm\sqrt{1+\eta^2} & \sin\theta_q+\mathrm{i}\eta \\ \sin\theta_q-\mathrm{i}\eta & -\cos\theta_q\pm\sqrt{1+\eta^2}\end{pmatrix}. \end{aligned}$$

It is convenient to describe the behavior of the eigenspaces in geometric terms. For a fixed choice of the index $s \in \{+,-\}$, we introduce a line bundle $\mathcal{P}_{1,s}$, called the *stratified bundle*, on the pointed cylinder $\mathring{C}$, whose fibre at the point $(q,\mu) \in \mathring{C}$ is just the range of the projector $P^{\mu}_{1,s}(q)$. As the stratified bundle $\mathcal{P}_{1,s}$ is (up to retraction of the basis) a line bundle over the 2-dimensional manifold $\mathcal{C}$, it is completely characterised by its first Chern number. The latter can be computed as the integral over $\mathcal{C}$ of the Berry curvature, which can be interpreted as an “inner” vorticity of the family $\{P_{1,s}(q)\}$ (compare Definition 3.1).

Explicitly, by using polar coordinates, the Berry curvature of the stratified bundle $\mathcal{P}_{1,\pm}$ reads

$$\begin{aligned}\omega_{1,\pm} = & -2\Big(\Im\left\langle \partial_{|q|}\phi^{\mu}_{1,\pm}(q), \partial_{\theta_q}\phi^{\mu}_{1,\pm}(q)\right\rangle_{\mathcal{H}_{\mathrm{f}}} \mathrm{d}|q|\wedge \mathrm{d}\theta_q + \\ & + \Im\left\langle \partial_{|q|}\phi^{\mu}_{1,\pm}(q), \partial_{\mu}\phi^{\mu}_{1,\pm}(q)\right\rangle_{\mathcal{H}_{\mathrm{f}}} \mathrm{d}|q|\wedge \mathrm{d}\mu + \\ & + \Im\left\langle \partial_{\theta_q}\phi^{\mu}_{1,\pm}(q), \partial_{\mu}\phi^{\mu}_{1,\pm}(q)\right\rangle_{\mathcal{H}_{\mathrm{f}}} \mathrm{d}\theta_q\wedge \mathrm{d}\mu\Big).\end{aligned} \tag{3.18}$$

By using (3.12), one computes the derivatives appearing in the above expression: this yields to

$$\begin{aligned}\partial_{|q|}\phi^{\mu}_{1,\pm} &= \frac{\mathrm{i}}{1+\alpha^2}\,\phi^{\mu}_{1,\mp}\partial_{|q|}\alpha, \\ \partial_{\mu}\phi^{\mu}_{1,\pm} &= \frac{\mathrm{i}}{1+\alpha^2}\,\phi^{\mu}_{1,\mp}\partial_{\mu}\alpha, \\ \partial_{\theta_q}\phi^{\mu}_{1,\pm} &= \frac{1}{2}\frac{1\mp\alpha}{\sqrt{1+\alpha^2}}\left(\pm\phi_{1,\mp} + \mathrm{i}\phi_{1,\pm}\right).\end{aligned} \tag{3.19}$$

As

$$\left\langle \phi^{\mu}_{1,\mp}(q), \pm\phi_{1,\mp}(q) + \mathrm{i}\phi_{1,\pm}(q)\right\rangle_{\mathcal{H}_{\mathrm{f}}} = \pm\frac{1\pm\alpha}{\sqrt{1+\alpha^2}}$$

one obtains

$$\omega_{1,\pm} = \pm\frac{1}{2}\left[\partial_{|q|}\left(\frac{\mu}{\sqrt{|q|^2+\mu^2}}\right)\mathrm{d}|q|\wedge\mathrm{d}\theta_q - \partial_{\mu}\left(\frac{\mu}{\sqrt{|q|^2+\mu^2}}\right)\mathrm{d}\theta_q\wedge\mathrm{d}\mu\right]. \tag{3.20}$$

Integrating the curvature of the Berry connection over the surface $\mathcal{C}$, one obtains the Chern number

$$\mathrm{ch}_1(\mathcal{P}_{1,\pm}) = \frac{1}{2\pi}\int_{\mathcal{C}}\omega_{1,\pm} = \mp 1$$

or equivalently

$$n_{\mathrm{v}}(P_{1,\pm}) = \pm 1.$$

The *n*-canonical model

We now exhibit model Hamiltonians $H_n(q)$, having Bloch bands $E_{\pm}(q) = \pm e(q)$ (with $e(0) = 0$ and $e(q) > 0$ for $q \neq 0$, in order to have eigenvalue intersections only at $q = 0$), such that the corresponding stratified bundles have a Chern number equal to an arbitrary $n \in \mathbb{Z}$, and that in particular $H_{\mathrm{eff}}(q) = H_{n=1}(q)$ when we choose $e(q) = |q|$ (*i. e.* when a conical intersection of bands is present). Notice that, if $P_{n,\pm}(q)$ are the eigenprojectors of the Hamiltonian $H_n(q)$, then

$$H_n(q) = E_+(q)P_{n,+}(q) + E_-(q)P_{n,-}(q). \tag{3.21}$$

Thus, it suffices to provide an *ansatz* for the eigenfunctions $\phi_{n,\pm}(q)$ of $H_n(q)$. Set

$$\phi_{n,+}(q) = \mathrm{e}^{\mathrm{i}n\theta_q/2}\begin{pmatrix}\cos(n\theta_q/2)\\ \sin(n\theta_q/2)\end{pmatrix}, \quad \phi_{n,-}(q) = \mathrm{e}^{\mathrm{i}n\theta_q/2}\begin{pmatrix}-\sin(n\theta_q/2)\\ \cos(n\theta_q/2)\end{pmatrix}. \tag{3.22}$$

Notice that, for even n, the functions $\cos(n\theta_q/2)$ and $\sin(n\theta_q/2)$ are already single-valued under the identification of $\theta_q = 0$ with $\theta_q = 2\pi$, but so is the phase $e^{in\theta_q/2}$, so there is no harm in inserting it. These functions will be called the *n-canonical eigenvectors*. As for their eigenprojectors, one easily computes

$$P_{n,\pm}(q) = \pm\frac{1}{2}\begin{pmatrix}\cos n\theta_q \pm 1 & \sin n\theta_q \\ \sin n\theta_q & -\cos n\theta_q \pm 1\end{pmatrix}. \tag{3.23}$$

By (3.21) above we get that the n-th Hamiltonian is

$$H_n(q) = e(q)\begin{pmatrix}\cos n\theta_q & \sin n\theta_q \\ \sin n\theta_q & -\cos n\theta_q\end{pmatrix} \tag{3.24}$$

provided that we show that the stratified bundles $\mathcal{P}_{n,\pm}$ have first Chern number equal to $\mp n$.

In order to evaluate $\mathrm{ch}_1(\mathcal{P}_{n,\pm})$, we perturb the Hamiltonian $H_n(q)$ in a way which is completely analogous to what we did for $H_{\mathrm{eff}}(q)$, and define

$$H_n^\mu(q) := e(q)\begin{pmatrix}\cos n\theta_q & \sin n\theta_q + i\eta \\ \sin n\theta_q - i\eta & -\cos n\theta_q\end{pmatrix}, \quad \eta = \frac{\mu}{e(q)}. \tag{3.25}$$

The eigenvalues of $H_n^\mu(q)$ are $E_\pm^\mu(q) = \pm e^\mu(q)$, where[5] $e^\mu(q) := e(q)\sqrt{1+\eta^2}$.

Its eigenfunctions can be found by solving a system similar to (3.15), obtained just by replacing θ_q with $n\theta_q$. After straightforward calculations, one eventually finds

$$\phi_{n,\pm}^\mu(q) := \frac{1}{\sqrt{1+\alpha^2}}\left[\phi_{n,\pm}(q) + i\alpha\phi_{n,\mp}(q)\right]$$

with the *same* α as in (3.17). One easily checks that the associated eigenprojectors are

$$P_{n,\pm}^\mu(q) = \pm\frac{1}{2\sqrt{1+\eta^2}}\begin{pmatrix}\cos n\theta_q \pm \sqrt{1+\eta^2} & \sin n\theta_q + i\eta \\ \sin n\theta_q - i\eta & -\cos n\theta_q \pm \sqrt{1+\eta^2}\end{pmatrix}. \tag{3.26}$$

Now notice that

$$\partial_{|q|}\phi_{n,\pm} = 0, \quad \partial_{\theta_q}\phi_{n,\pm} = \frac{n}{2}\left(\pm\phi_{n,\mp} + i\phi_{n,\pm}\right).$$

Hence, in order to compute the Berry curvature of the stratified bundle $\mathcal{P}_{n,\pm}$, one only has to modify the expression for all the derivatives (and related scalar products with other derivatives) computed above substituting $\phi_{1,\pm}^\mu(q)$ with $\phi_{n,\pm}^\mu(q)$, and multiplying by n the ones involving derivatives with respect to θ_q. Notice that the dependence of η, and consequently of $P_{n,\pm}^\mu(q)$, on $e(q)$ does not affect this computation, provided the hypothesis $e(0) = 0$ holds. Explicitly, this procedure yields to

[5] One could also choose to put a different eigenvalue $\tilde{e}(q,\mu)$ in front of the matrix in (3.25), because the topology of the stratified bundle depends only on the family of projectors $\{P_{n,\pm}^\mu(q)\}$ (which we will introduce in a moment). We will adhere to our definition of $e^\mu(q)$ in order to recover the model (3.14) when we set $n = 1$ and $e(q) = |q|$.

$$\omega_{n,\pm} = \pm\frac{n}{2}\left[\partial_{|q|}\left(\frac{\mu}{\sqrt{e(q)^2+\mu^2}}\right)\mathrm{d}|q|\wedge\mathrm{d}\theta_q - \partial_\mu\left(\frac{\mu}{\sqrt{e(q)^2+\mu^2}}\right)\mathrm{d}\theta_q\wedge\mathrm{d}\mu\right], \tag{3.27}$$

and correspondingly the "inner" vorticity of $\{P_{n,\pm}(q)\}$ equals

$$n_{\mathrm{v}}(P_{n,\pm}) = -\mathrm{ch}_1(\mathcal{P}_{n,\pm}) = -\frac{1}{2\pi}\int_{\mathcal{C}}\omega_{n,\pm} = \pm n,$$

as we wanted.

Remark 3.3 (The case $n = 0$). When $n = 0$, the functions $\phi_{0,\pm}(q)$ are constant, and hence are defined on the whole disc U. Correspondingly, the stratified bundles $\mathcal{P}_{0,\pm}$ are both isomorphic to the trivial line bundle $\big(U\times[-\mu_0,\mu_0]\big)\times\mathbb{C}$. Of course, the bundles $\mathcal{P}_{0,\pm}$ do not correspond to families of *singular* projectors; however, this notation will help us state our results in a neater way in the following. ◊

3.3 Comparison with the pseudospin winding number

In this Section we compare the *eigenspace vorticity* with the *pseudospin winding number* (PWN) which appears in the literature about graphene [39, 27]. While the former is defined in a wider context, it happens that these two indices agree whenever the latter is well-defined, including the relevant cases of monolayer and multilayer graphene. We also show that the pseudospin winding number is neither a Berry phase, as already noticed in [39], nor a topological invariant.

Definition of the pseudospin winding number.

We firstly rephrase the usual definition in a more convenient language. The starting point is the following

Datum 3.2. For $\mathcal{H} = \mathbb{C}^2$, let $\{P(k)\}\subset\mathcal{B}(\mathcal{H})$ be a family of orthogonal projectors defined on the circle $S^1 = \partial U$, where $U = \{k\in\mathbb{R}^2 : |k-k_0| < r\}$, for a suitable $r > 0$. We will also assume that the range of each projector $P(k)$ is 1-dimensional, because this is clearly the only interesting case. ◊

Let $\Psi : S^1 \to \mathbb{C}^2$ be a continuous map such that $\Psi(k)\in\operatorname{Ran}P(k)$ and $\Psi(k)\neq 0$ for every $k\in S^1$. Such a map does exist: Indeed, let $\mathcal{P}$ be the line bundle over S^1 corresponding to $\{P(k)\}$, whose total space is

$$\mathcal{P} = \left\{(k,v)\in S^1\times\mathbb{C}^2 :\ v\in\operatorname{Ran}P(k)\right\}.$$

The line bundle $\mathcal{P}$ is trivial, since every *complex* line bundle over S^1 is so. Therefore there exists a global non-zero continuous section of $\mathcal{P}$, here denoted by Ψ. Without loss of generality, we assume $\|\Psi(k)\|\equiv 1$.
With respect to a fixed orthonormal basis $\{e_1,e_2\}\subset\mathbb{C}^2$ one writes

$$\Psi(k) = \psi_1(k)e_1 + \psi_2(k)e_2. \tag{3.28}$$

Obviously, $\psi_1(k)$ and $\psi_2(k)$ can not be simultaneously zero. One makes moreover the following (sometimes implicit) assumption.

Assumption 3.1. Assume that for every $k \in S^1 = \{k \in \mathbb{R}^2 : |k - k_0| = r\}$ the numbers $\psi_1(k)$ and $\psi_2(k)$ are *both* non-zero. ◊

Under this assumption, which implies $\psi_j(k) = |\psi_j(k)| \mathrm{e}^{\mathrm{i}\theta_j(k)}$ with θ_j continuous, the map

$$g : S^1 \to U(1), \qquad g(k) = \operatorname{phase}\left(\frac{\psi_2(k)}{\psi_1(k)}\right) = \mathrm{e}^{\mathrm{i}(\theta_2(k) - \theta_1(k))}$$

is well-defined and continuous. Then the *pseudospin winding number* $n_{\mathrm{w}} = n_{\mathrm{w}}(P)$ is defined as the degree of the continuous map g. In terms of polar coordinates for $q = k - k_0$, namely $q = (|q|, \theta_q)$, one has

$$n_{\mathrm{w}} = n_{\mathrm{w}}(P) := \deg g = \frac{1}{2\pi\mathrm{i}} \oint_{S^1} \mathrm{d}k\, \overline{g(k)}\, \frac{\partial g}{\partial \theta_q}(k) \in \mathbb{Z}. \tag{3.29}$$

For example, when we take the eigenprojectors $P_\pm(k)$ of the effective tight-binding Hamiltonians (2.10) and (2.12) as our datum, the Assumption 3.1 is satisfied, with respect to the canonical basis of $\mathbb{C}^2$, by the global section (for the m-multilayer graphene Hamiltonian (2.12))

$$\Psi_{m,s}(q) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ s\,\mathrm{e}^{\mathrm{i}m\theta_q} \end{pmatrix}, \qquad m \in \mathbb{N}^\times, \tag{3.30}$$

where $s \in \{+, -\}$ refers to the choice of the upper (resp. lower) eigenvalue. It is then straightforward to check that

$$n_{\mathrm{w}} = \begin{cases} 1 & \text{for monolayer graphene,} \\ 2 & \text{for bilayer graphene,} \\ m & \text{for } m\text{-multilayer graphene.} \end{cases} \tag{3.31}$$

Remark 3.4 (Comparison with the Berry phase). We emphasise that, despite the formal similarity of the definitions, in general the pseudospin winding number is *not* a Berry phase, as clarified by Park and Marzari [39]. Indeed, g is not a wave function, but the ratio of the components of a single ($\mathbb{C}^2$-valued) wave function with respect to a chosen orthonormal basis.

On the other hand, if in some particular model it happens that

$$|\psi_2(k)/\psi_1(k)| = |g(k)| \equiv 1 \text{ for all } k \in S^1 \tag{3.32}$$

(as indeed happens in the case (3.30)), then the holonomy of the Berry connection $\mathcal{A}$ (*i. e.* the Berry phase) along the circle S^1 is

$$\operatorname{Hol}\mathcal{A} = \exp\left\{ -\oint_{S^1} \left\langle \Psi(k), \frac{\partial}{\partial\theta_q}\Psi(k) \right\rangle_{\mathbb{C}^2} \right\} = \mathrm{e}^{-\mathrm{i}\pi n_{\mathrm{w}}},$$

as can be checked by direct computation, assuming without loss of generality that the first component of $\Psi(k)$ is real, *i. e.* $\psi_1(k) = |\psi_1(k)|$. In such a case, n_{w} contains a more detailed information than the Berry phase, which is defined only modulo $2\pi\mathbb{Z}$. ♢

Remark 3.5 (Hartree-Fock corrections). It has been recently shown [16] that, when many-electron Coulomb interactions in monolayer graphene are taken into account, the leading order correction in the framework of the Hartree-Fock theory amounts to replace the effective Hamiltonian (2.10) with

$$\mathcal{H}^{(\mathrm{HF})}_{\mathrm{mono}}(q) = v_{\mathrm{eff}}(q)\,|q| \begin{pmatrix} 0 & \mathrm{e}^{-\mathrm{i}\theta_q} \\ \mathrm{e}^{\mathrm{i}\theta_q} & 0 \end{pmatrix},$$

where v_{eff} is an explicit function [16, Lemma 3.2]. The corresponding eigenprojectors coincide with those of the Hamiltonian (2.10). Therefore, the PWN equals the one computed in the tight-binding model. ♢

Geometrical reinterpretation.

We find convenient to reinterpret the definition of n_{w} in terms of projective geometry, in order to study the dependence of (3.29) on the choice of the basis appearing in (3.28).

We consider the complex projective space $\mathbb{C}P^1$ (the set of all complex lines in $\mathbb{C}^2$ passing through the origin), denoting by $[\psi_1, \psi_2]$ the line passing through the point $(\psi_1, \psi_2) \in \mathbb{C}^2 \setminus \{0\}$. In view of the identification $\mathbb{C}P^1 \simeq S^2$ via the stereographic projection from S^2 to the one-point compactification of the complex plane, the points $S = [0, 1]$ and $N = [1, 0]$ in $\mathbb{C}P^1$ are called South pole and North pole[6], respectively. Explicitly, stereographic projection is given by the map

$$\mathbb{C}P^1 \to \mathbb{C} \cup \{\infty\}, \quad [\psi_1, \psi_2] \mapsto \psi_1/\psi_2. \tag{3.33}$$

Since every rank-1 orthogonal projector is identified with a point in $\mathbb{C}P^1$ (its range), the Datum 3.2 yields a continuous map

$$\begin{array}{rccccl} G: & S^1 & \longrightarrow & \mathcal{B}(\mathbb{C}^2) & \longrightarrow & \mathbb{C}P^1 \\ & k & \longmapsto & P(k) & \longmapsto & \operatorname{Ran} P(k) = [\psi_1(k), \psi_2(k)] \end{array} \tag{3.34}$$

where, in the last equality, the choice of a basis in $\mathbb{C}^2$ is understood to write out the coordinates of $(\psi_1(k), \psi_2(k))$. With this identification, Assumption 3.1 is equivalent to the condition

(3.35) the range of the map G does not contain the points N and S in $\mathbb{C}P^1$.

Thus, in view of the previous Assumption, the range of G is contained in a tubular neighbourhood of the equator S^1_{eq} of $S^2 \simeq \mathbb{C}P^1$, and therefore the degree of G is well-defined. The latter is, up to a sign, the pseudospin winding number, *i. e.*

$$n_{\mathrm{w}} = -\deg G, \qquad G: S^1 \to \operatorname{Tub} S^1_{\mathrm{eq}} \subset S^2. \tag{3.36}$$

[6] Notice that, since the basis $\{e_1, e_2\}$ is orthonormal, the points $\{N, S\}$ are antipodal on S^2.

Indeed, clearly $G(k) = [\psi_1(k), \psi_2(k)] = [\psi_1(k)/\psi_2(k), 1]$; in view of our convention (3.33), we deduce that

$$\deg G = \deg g^{-1} = -\deg g = -n_{\mathrm{w}}$$

as claimed.

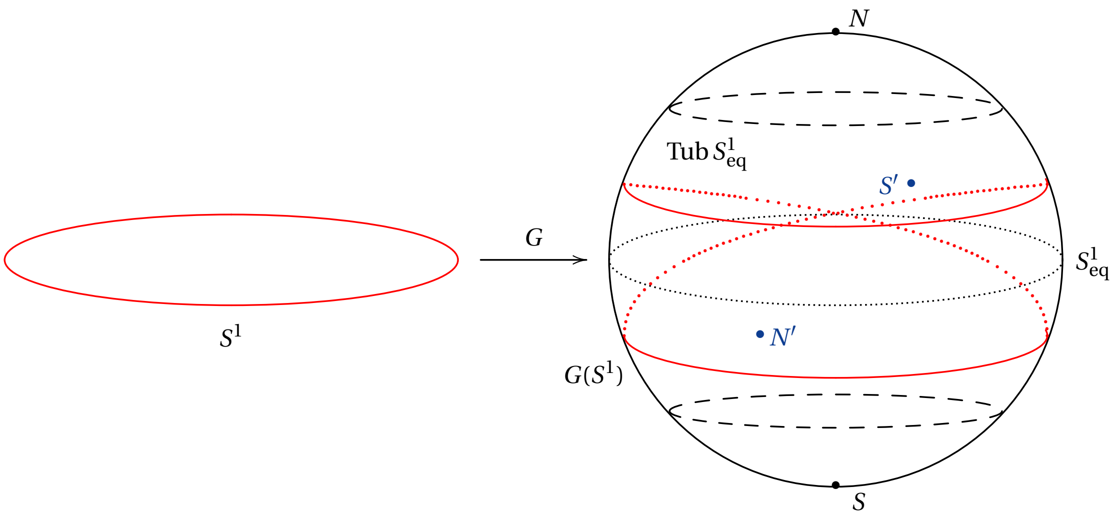


Fig. 2 An example of map $G\colon S^1 \to \mathrm{Tub}\, S^1_{\mathrm{eq}} \subset S^2$.

This reinterpretation shows that n_{w} is only a *conditional* topological invariant, in the sense that it is invariant only under continuous deformation of the Datum 3.2 *preserving Assumption* (3.35). The integer n_{w} cannot be invariant under arbitrary continuous deformations: Indeed, the map G in (3.34) can be continuosly deformed to a map G_{South} which is constantly equal to the South pole, and then to a map G_* which is constantly equal to an arbitrary point of the equator. Since $\deg(G_*) = 0$, we conclude that *the pseudospin winding number is not invariant under arbitrary continuous deformations of the family of projectors* appearing in Datum 3.2, or equivalently is not invariant under arbitrary continuous deformations of the corresponding Hamiltonian. In other words, n_{w} is a conditional topological invariant.

Finally, we point out that in general n_{w} is not independent of the choice of the basis appearing in (3.28), which corresponds to a choice of antipodal points $\{N, S\}$ in S^2. Indeed, in the example in Figure 2 one sees that $n_{\mathrm{w}} = 2$ with respect to the choice $\{N, S\}$, while the choice $\{N', S'\}$ yields $n'_{\mathrm{w}} = 0$.

There exists a single case in which n_{w} is independent of the basis (up to a sign), namely if

(3.37) the range of the map G is contained in a maximum circle E in S^2.

Indeed, in such a case one can identify E with the equator, thus inducing a canonical choice of the poles $\{N, S\}$, up to reordering (*i. e.* the only other possible choice is $N' = S$ and $S' = N$). This restrictive condition is indeed satisfied in the case of multilayer graphene, compare (3.30) and (3.37) recalling that the condition $|\psi_1(k)| - |\psi_2(k)| = 0$ corresponds to being on the equator.

In summary, the PWN is well-defined and independent of the basis only under the restrictive assumptions (3.35) and (3.37). These assumptions hold in the case of (multilayer) tight-binding graphene, but one cannot expect that they hold true in more general situations (*e. g.* deformed graphene, topological insulators, ...). Indeed, the Haldane Hamiltonian $H_{\mathrm{Hal}}(k)$ [17], which has been considered a paradigmatic model for many interesting effects in solid state physics, provides an example in which hypothesis (3.37) does not hold. The Hamiltonian $H_{\mathrm{Hal}}(k)$ is an effective 2×2 Hamiltonian, modelling a honeycomb crystal. It depends on several parameters: t_1 and t_2 which are hopping energies, ϕ which plays the role of an external magnetic flux, and M which is an on-site energy. If $|t_2/t_1| < 1/3$ and $M = \pm 3\sqrt{3}\,t_2 \sin(\phi)$, then the two bands of the Hamiltonian $H_{\mathrm{Hal}}(k)$ touch at (at least) one point k_0 in the Brillouin zone. We checked that, for the values of the parameters $t_1 = 1$, $t_2 = (1/4)\,t_1$, $\phi = \pi/8$ and $M = 3\sqrt{3}\,t_2 \sin(\phi)$ (in suitable units), the image of the map $G_{\mathrm{Hal}}(k) := \operatorname{Ran} P_{\mathrm{Hal}}(k)$, where $P_{\mathrm{Hal}}(k)$ is the spectral projection on the upper band of $H_{\mathrm{Hal}}(k)$ and k varies in a circle around k_0, does *not* lie on a maximum circle on the sphere $S^2 \simeq \mathbb{C}P^1$. Consequently, in the Haldane model, at least for these specific values of the parameters, the PWN is ill-defined.

Comparison of the two concepts.

In this Subsection, we are going to show that our eigenspace vorticity provides a more general and flexible definition of a topological invariant, which agrees with the PWN whenever the latter is well-defined, thus revealing its hidden geometric nature. In order to obtain, in the case $\mathcal{H} = \mathbb{C}^2$, a value of n_{v} which does not depend on the choice of the deformation, we will focus on a “distinguished” class of deformations, namely those corresponding to weakly hemispherical maps (Definition 3.2).

Advantages and disadvantages of the two indices are easily noticed. As for the pseudospin winding number, its definition depends only on the *undeformed* family of projectors, but it requires Assumption 3.1 to be satisfied, with respect to a suitable basis of $\mathbb{C}^2$. Moreover, (3.37) must also hold true for the definition of the PWN to be base-independent. Viceversa, the definition of the eigenspace vorticity requires the construction of a family of *deformed* projectors, but it does not require any special assumption on the unperturbed family of projectors.

As the reader might expect, we can prove that the eigenspace vorticity and the pseudospin winding number coincide whenever both are defined. This holds true, in particular, in the case of monolayer and multilayer graphene.

Firstly, we give an alternative interpretation of the eigenspace vorticity as the degree of a certain map. This will make the comparison between the two indices more natural.

Lemma 3.2. *Let $\{P(k)\}_{k\in R\setminus\{k_0\}}$ be a family of rank-1 projectors as in Datum 3.1, with $\mathcal{H} = \mathbb{C}^2$, and let $\{P^{\mu}(k)\}_{(k,\mu)\in B}$ be a deformation of it, as described in Section 3.1. Let $n_{\mathrm{v}} \in \mathbb{Z}$ be the eigenspace vorticity* (3.3) *of the deformed family $\{P^{\mu}(k)\}_{(k,\mu)\in B}$. Define the map $\widetilde{G}\colon \mathcal{C} \to \mathbb{C}P^1$ by $\widetilde{G}(k,\mu) := \operatorname{Ran} P^{\mu}(k)$, for $(k,\mu) \in \mathcal{C}$. Then*

$$n_{\mathrm{v}} = -\deg \widetilde{G}.$$

Proof. The integral formula for the degree of a smooth map $F\colon M \to N$ between manifolds of the same dimension [9, Theorem 14.1.1] states that, if ω is a top-degree form on N, then

$$\int_M F^* \omega = \deg F \int_N \omega. \tag{3.38}$$

Let ω_{FS} be the *Fubini-Study* 2-form on $\mathbb{C}P^1$, defined as

$$\omega_{\mathrm{FS}}(\zeta) = \mathrm{i}\overline{\partial}\partial \ln\left(1+|\zeta|^2\right) \mathrm{d}\zeta \wedge \mathrm{d}\overline{\zeta} = \frac{\mathrm{i}}{(1+|\zeta|^2)^2} \mathrm{d}\zeta \wedge \mathrm{d}\overline{\zeta}$$

on the open subset $\mathbb{C}P^1 \setminus \{S\} = \left\{[\psi_1, \psi_2] \in \mathbb{C}P^1 : \psi_1 \neq 0\right\} \simeq \mathbb{C}$ with complex coordinate $\zeta = \psi_2/\psi_1$ (here $\partial = \partial/\partial\zeta$ and $\overline{\partial} = \partial/\partial\overline{\zeta}$). One easily checks that

$$\frac{1}{2\pi} \int_{\mathbb{C}P^1} \omega_{\mathrm{FS}} = 1.$$

Moreover, it is also known [49, Section 3.3.2] that $(1/2\pi)\omega_{\mathrm{FS}}$ is the first Chern class $\mathrm{Ch}_1(\mathcal{S})$ of the *tautological bundle* $\mathcal{S}$ over $\mathbb{C}P^1$, whose fibre over the point representing the line $\ell \subset \mathbb{C}^2$ is the line ℓ itself. Instead, the bundle $\mathcal{L}$ associated with the family $\left\{P^\mu(k)\right\}$ has the range of the projector as its fibre over $(k,\mu) \in \mathcal{C}$; this means by definition that it is the pullback via $\widetilde{G}$ of the tautological bundle. By naturality of the Chern classes, we deduce that the Berry curvature 2-form ω, defined as in (3.2), is given by[7]

$$\omega = 2\pi\, \mathrm{Ch}_1(\mathcal{L}) = 2\pi\, \mathrm{Ch}_1(\widetilde{G}^* \mathcal{S}) = 2\pi\, \widetilde{G}^* \mathrm{Ch}_1(\mathcal{S}) = \widetilde{G}^* \omega_{\mathrm{FS}}.$$

This fact, together with the formula (3.38), yields to

$$n_{\mathrm{v}} = -\frac{1}{2\pi}\int_{\mathcal{C}} \omega = -\frac{1}{2\pi}\int_{\mathcal{C}} \widetilde{G}^* \omega_{\mathrm{FS}} = -\deg \widetilde{G} \left(\frac{1}{2\pi}\int_{\mathbb{C}P^1} \omega_{\mathrm{FS}}\right) = -\deg \widetilde{G}$$

as claimed. □

We now proceed to the proof of the equality between the pseudospin winding number and the eigenspace vorticity, provided (3.35) holds true. We consider also cases, *e. g.* perturbed graphene, in which a canonical orthonormal basis in $\mathbb{C}^2$ is provided by an unperturbed or reference Hamiltonian; so, condition (3.37) is not assumed. However, whenever the Hamiltonian is such that (3.37) holds true, then Step 1 in the following proof is redundant.

The class of deformations which we want to use to compute the eigenspace vorticity is defined as follows.

Definition 3.2 (Weakly hemispherical map). A map $F\colon \mathcal{C} \to S^2$ is called **hemispherical** (with respect to a choice of an equator $S^1_{\mathrm{eq}} \subset S^2$) if $F(S^1) \subset S^1_{\mathrm{eq}}$ and $F^{-1}(S^1_{\mathrm{eq}}) \subset S^1$, where $S^1 = \mathcal{C} \cap \left\{\mu = 0\right\}$. Equivalently, F is hemispherical if it maps the "upper half" of the cylinder (namely $\mathcal{C}_+ := \mathcal{C} \cap \left\{\mu > 0\right\}$) to the northern hemi-

[7] Notice that, without invoking the naturality of Chern classes, the equality $\omega = \widetilde{G}^* \omega_{\mathrm{FS}}$ can also be explicitly checked by a long but straightforward computation.

sphere S^2_+, the "equator" S^1 into S^1_{eq}, and the "lower half" of the cylinder (namely $\mathcal{C}_- := \mathcal{C} \cap \{\mu < 0\}$) to the southern hemisphere S^2_-.

A map $F \colon \mathcal{C} \to S^2$ is called **weakly hemisperical** if $F(S^1)$ is contained in a tubular neighbourhood $\mathrm{Tub}\, S^1_{\mathrm{eq}}$ of the equator, and it is homotopic to a hemispherical map via the *retraction along meridians.* ♢

The retraction along meridians is defined as follows. Choose two open neighbourhoods O_N and O_S of the North and South pole, respectively, which do not intersect the tubular neighbourhood $\mathrm{Tub}\, S^1_{\mathrm{eq}}$ containing $F(S^1)$. Let $\rho_t \colon S^2 \to S^2$ be the homotopy which as t goes from 0 to 1 expands O_N to the whole northern hemisphere and O_S to the whole southern hemisphere, while keeping the equator S^1_{eq} fixed (compare Figure 3). Then let $F' := \rho_1 \circ F$; the maps $\rho_t \circ F$ give an homotopy between F and F'. Then F is weakly hemispherical if F' is hemispherical.

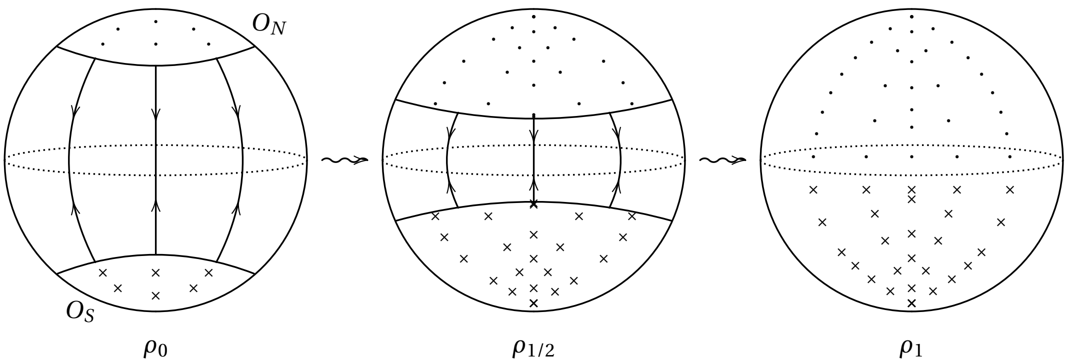


Fig. 3 The retraction ρ_t for $t = 0$, $t = 1/2$ and $t = 1$.

Proposition 3.1. *Let* $\{P(k)\}_{k \in \partial U}$ *be a family of projectors as in Datum 3.2 and let* $G \colon S^1 \to \mathbb{C}P^1$ *be the corresponding map, i. e.* $G(k) = \mathrm{Ran}\, P(k)$ *as in* (3.34)*. Suppose that Assumption 3.1 (or equivalently the condition* (3.35) *on G) holds. Let* $\{P^\mu(k)\}_{(k,\mu) \in \mathcal{C}}$ *be a deformed family of projectors, as in Section 3.1, and* $\widetilde{G} \colon \mathcal{C} \to \mathbb{C}P^1$ *be defined by* $\widetilde{G}(k,\mu) := \mathrm{Ran}\, P^\mu(k)$*. (Clearly* $\widetilde{G}(k,0) = G(k)$ *for* $k \in S^1$*.) Assume that* $\widetilde{G}$ *is weakly hemispherical. Then, up to a reordering of the basis involved in the definition of the pseudospin winding number, one has*

$$n_{\mathrm{w}}(P) = n_{\mathrm{v}}(P).$$

Proof. The proof will consist in modifying suitably the functions G and $\widetilde{G}$ (without leaving their respective homotopy classes), in order to compare their degrees. We divide the proof of this statement into a few steps.

Step 1: choice of suitable maps G *and* $\widetilde{G}$. Consider the composition $\widetilde{G}' := \rho_1 \circ \widetilde{G}$, which by hypothesis can be assumed to be a hemispherical map (up to a reordering of the poles, *i. e.* of the basis for the definition the PWN). As the degree of the map $\widetilde{G}$ depends only on the homotopy class of $\widetilde{G}$, we have that $\deg \widetilde{G} = \deg \widetilde{G}'$. The analogous statement holds also for G and $G' := \rho_1 \circ G$. In the following, we drop the "primes" and assume that G is such that $G(S^1) \subseteq S^1_{\mathrm{eq}}$ and that $\widetilde{G}$ is hemispherical.

Step 2: $\deg \widetilde{G} = \deg G$. The map $\widetilde{G}\big|_{\mathcal{C}_+} \colon \mathcal{C}_+ \to S^2_+$ is a map between manifolds with boundary, mapping $\partial \mathcal{C}_+ = S^1$ to $\partial S^2_+ = S^1_{\mathrm{eq}}$. By taking a regular value in S^2_+ to compute the degree of $\widetilde{G}$, we deduce from our hypotheses (Step 1) that the points in its preimage all lie in the upper half of the cylinder, so that $\deg \widetilde{G} = \deg\left(\widetilde{G}\big|_{\mathcal{C}_+}\right)$. On the other hand, the degree of a map between manifolds with boundary coincides with the degree of its restriction to the boundaries themselves [9, Theorem 13.2.1]. We conclude that

$$\deg \widetilde{G} = \deg\left(\widetilde{G}\big|_{\mathcal{C}_+}\right) = \deg\left(\widetilde{G}\big|_{\partial\mathcal{C}_+}\right) = \deg\left(\widetilde{G}\big|_{S^1}\right) = \deg G$$

as claimed.

Step 3: conclusion. To sum up, putting together Step 1 and Step 2, by (3.36) and Lemma 3.2 we conclude that

$$n_{\mathrm{v}} = -\deg \widetilde{G} = -\deg G = n_{\mathrm{w}}$$

and this ends the proof of the Proposition. □

Finally, we conclude that n_{v} is intrinsically defined when $\mathcal{H} = \mathbb{C}^2$. Indeed, the ambiguity in the choice of the deformation may be removed by choosing a deformation which corresponds to a weakly hemispherical map. Then the value of n_{v} is independent of the choice of a specific deformation among this class, in view of the following Corollary of the proof.

Corollary 3.1. *Let $\{P^\mu(k)\}_{(k,\mu)\in B}$ and $\{\widehat{P}^\mu(k)\}_{(k,\mu)\in B}$ be two deformations of the family $\{P(k)\}_{k\in R\setminus\{k_0\}}$, both corresponding to a weakly hemisperical map with respect to an equator $S^1_{\mathrm{eq}} \subset S^2$. Then*

$$n_{\mathrm{v}}(P) = n_{\mathrm{v}}(\widehat{P}).$$

An example of hemispherical deformation $\{P^\mu(k)\}$ for a family of projectors $\{P(k)\}$ is provided by the canonical models (3.23) and (3.26) of last Subsection, as the reader may easily check. Since the corresponding Hamiltonian $H_m(q)$, as in (3.24) with $n = m$ and $e(q) = |q|^m$, is unitarily conjugated to tight-binding the Hamiltonian (2.12) of m-multilayer graphene, we get that both the eigenspace vorticity and the PWN of graphene are equal to m, in accordance with (3.31) and the above Proposition.

As an example of a weakly hemispherical deformation, we can instead consider the eigenprojectors of the Haldane Hamiltonian, for example for the values of the parameters cited above. By Lemma 3.1, if the values of the parameters (M,ϕ) of $H_{\mathrm{Hal}}(k)$ are close to those corresponding to the tight-binding Hamiltonian of monolayer graphene, namely $(M,\phi) = (0,0)$, then its eigenprojectors will also have an eigenspace vorticity equal to 1 in absolute value, in accordance with the numerical evaluation of Remark 3.2.

4 Universality of the canonical models

In this Section, we prove that the local models provided by the projectors (3.23), together with their deformed version (3.26), are *universal*, meaning the following: if the "outer" eigenspace vorticity of the deformed family of projectors $\{P^\mu_s(k)\}$ is $N \in \mathbb{Z}$ and if we set $n_{\mathrm{v}} := sN$, with $s \in \{+,-\}$, then the n_{v}-canonical projections $\{P^\mu_{n_{\mathrm{v}},s}(k)\}$

will provide an extension of the family, initially defined in B, to the whole $\widehat{B}$ (the notation is the same of Section 3.1).

More precisely, we will prove the following statement.

Theorem 4.1. *Let $\mathcal{L}_s$ be the complex line bundle over B defined as in* (3.1)*. Let $N \in \mathbb{Z}$ be its vorticity around U, defined as in* (3.3)*, and set $n_{\mathrm{v}} := sN$ (recall that $s \in \{+,-\}$). Then there exists a complex line bundle $\widehat{\mathcal{L}}_s$ over $\widehat{B}$ such that*

$$\widehat{\mathcal{L}}_s\big|_B \simeq \mathcal{L}_s \quad \textit{and} \quad \widehat{\mathcal{L}}_s\big|_{\overset{\circ}{C}} \simeq \mathcal{P}_{n_{\mathrm{v}},s},$$

where $\mathcal{P}_{n_{\mathrm{v}},s}$ is the stratified bundle corresponding to the family of projectors (3.26) *for $n = n_{\mathrm{v}}$.*

The bundle $\widehat{\mathcal{L}}_s$, appearing in the above statement, allows one to interpolate the "external data" (the bundle $\mathcal{L}_s$) with the canonical model around the singular point (the stratified bundle $\mathcal{P}_{n_{\mathrm{v}},s}$).

The geometric core of the proof of Theorem 4.1 lies in the following result.

Lemma 4.1. *Under the hypotheses of Theorem 4.1, the restriction of the bundles $\mathcal{L}_s$ and $\mathcal{P}_{n_{\mathrm{v}},s}$ to the cylindrical surface $\mathcal{C}$ are isomorphic:*

$$\mathcal{L}_s\big|_{\mathcal{C}} \simeq \mathcal{P}_{n_{\mathrm{v}},s}\big|_{\mathcal{C}}.$$

Proof. The statement follows from the well-known facts that line bundles on any CW-complex X are completely classified by their first Chern *class*, living in $H^2(X;\mathbb{Z})$ (see [45]), and that when $X = \mathcal{C} \simeq S^2$ then $H^2(\mathcal{C};\mathbb{Z}) \simeq \mathbb{Z}$, the latter isomorphism being given by integration on $\mathcal{C}$ (or, more formally, by evaluation of singular 2-cocycles on the fundamental class $[\mathcal{C}]$ in homology). As a result, one deduces that line bundles on $\mathcal{C}$ are classified by their first Chern *number*. As $\mathcal{L}_s$ and $\mathcal{P}_{n_{\mathrm{v}},s}$ have the same Chern number, equal to $-N$, when restricted to the surface $\mathcal{C}$, they are isomorphic. □

Proof of Theorem 4.1. Vector bundles are given by "gluing" together (trivial) bundles defined on open sets covering the base space, so we can expect that we can glue $\mathcal{L}_s$ and $\mathcal{P}_{n_{\mathrm{v}},s}$ along $\mathcal{C}$, given that their restrictions on $\mathcal{C}$ are isomorphic (as was proved in Lemma 4.1). The only difficulty we have to overcome is that $\mathcal{C}$ is a *closed* subset of $\widehat{B}$.

We argue as follows. Let T be an open tubular neighbourhood of $\mathcal{C}$ in $\widehat{B}$, and let $\rho\colon T \to \mathcal{C}$ be a retraction of T on $\mathcal{C}$. As $T \cap \overset{\circ}{C}$ is a deformation retract of $\mathcal{C}$ via the map ρ, we may extend the definition of $\mathcal{L}_s$ to $T \cap \overset{\circ}{C}$ by letting

$$\mathcal{L}_s\big|_{T\cap\overset{\circ}{C}} := \rho^*\left(\mathcal{L}_s\big|_{\mathcal{C}}\right).$$

Similarly, we can extend $\mathcal{P}_{n_{\mathrm{v}},s}$ outside $\overset{\circ}{C}$ setting

$$\mathcal{P}_{n_{\mathrm{v}},s}\big|_{T\cap B} := \rho^*\left(\mathcal{P}_{n_{\mathrm{v}},s}\big|_{\mathcal{C}}\right).$$

With these definitions, one has

$$\mathcal{L}_s\big|_T \simeq \rho^*\left(\mathcal{L}_s\big|_{\mathcal{C}}\right) \tag{4.1a}$$

and similarly

$$\mathcal{P}_{n_v,s}\big|_T \simeq \rho^*\left(\mathcal{P}_{n_v,s}\big|_{\mathcal{C}}\right). \tag{4.1b}$$

In fact, let $\mathcal{V}$ denote either $\mathcal{L}_s$ or $\mathcal{P}_{n_v,s}$. It is known [30, Theorem 14.6] that all complex line bundles admit a morphism of bundles to $\mathcal{U}_{U(1)} = \left(EU(1) \xrightarrow{\pi} \mathbb{C}P^\infty\right)$, the tautological bundle[8] on $\mathbb{C}P^\infty$, and that their isomorphism classes are uniquely determined by the homotopy class of the map between the base spaces. Let

$$\begin{array}{ccc} E\left(\mathcal{V}|_T\right) & \longrightarrow & EU(1) \\ \downarrow & & \downarrow \\ T & \xrightarrow{f_T} & \mathbb{C}P^\infty \end{array} \qquad \text{and} \qquad \begin{array}{ccc} E\left(\rho^*\left(\mathcal{V}|_{\mathcal{C}}\right)\right) & \longrightarrow & EU(1) \\ \downarrow & & \downarrow \\ T & \xrightarrow{f_{\mathcal{C}}} & \mathbb{C}P^\infty \end{array}$$

be those two morphisms of bundles just described; then (4.1a) and (4.1b) will hold as long as we prove that f_T and $f_{\mathcal{C}}$ are homotopic. Now, the following diagram[9]

$$\begin{array}{ccc} T & \xrightarrow{f_{\mathcal{C}}} & \mathbb{C}P^\infty \\ {\scriptstyle\rho}\downarrow & \overset{\mathrm{Id}_T}{\searrow}\ \approx & \uparrow{\scriptstyle f_T} \\ \mathcal{C} & \xhookrightarrow[\iota]{} & T \end{array}$$

where $\iota\colon \mathcal{C} \hookrightarrow T$ denotes the inclusion map, is clearly commutative. By definition of deformation retract, the maps $\iota \circ \rho$ and Id_T are homotopic: hence

$$f_{\mathcal{C}} = f_T \circ \iota \circ \rho \approx f_T \circ \mathrm{Id} = f_T$$

as was to prove.

By Lemma 4.1 we have $\mathcal{L}_s\big|_{\mathcal{C}} \simeq \mathcal{P}_{n_v,s}\big|_{\mathcal{C}}$, and hence also

$$\rho^*\left(\mathcal{L}_s\big|_{\mathcal{C}}\right) \simeq \rho^*\left(\mathcal{P}_{n_v,s}\big|_{\mathcal{C}}\right).$$

Equations (4.1a) and (4.1b) thus give

$$\mathcal{L}_s\big|_T \simeq \mathcal{P}_{n_v,s}\big|_T.$$

Hence the two line bundles $\mathcal{L}_s$ and $\mathcal{P}_{n_v,s}$ are isomorphic on the *open* set T, and this allows us to glue them. □

Remark 4.1 (Families of projectors with many singular points). We conclude this Section with some observations regarding singular families of projectors with more than one singular point (but still a finite number of them). Denote by $S = \{K_1, \ldots, K_M\} \subset \mathbb{T}_2^*$ the set of singular points of the family of rank-1 projectors $\mathbb{T}_2^* \ni$

[8] The *infinite complex projective space* $\mathbb{C}P^\infty$ is defined as the inductive limit of the system of canonical inclusions $\mathbb{C}P^N \hookrightarrow \mathbb{C}P^{N+1}$; it can be thought of as the space of all lines sitting in some "infinite-dimensional ambient space" $\mathbb{C}^\infty$. It admits a *tautological line bundle* with total space

$$EU(1) := \left\{(\ell, v) \in \mathbb{C}P^\infty \times \mathbb{C}^\infty : v \in \ell\right\},$$

whose fibre over the line $\ell \in \mathbb{C}P^\infty$ is the line ℓ itself, viewed as a copy of $\mathbb{C}$.

[9] The symbol $\approx$ denotes homotopy of maps.

$k \mapsto P_s(k)$; also, pick pair-wise disjoint open balls U_i around K_i (in particular, each U_i contains no singular point other than K_i). Smoothen $\{P_s(k)\}$ into $\{P_s^\mu(k)\}$ as explained in Section 3.1, and compute the M vorticity integers $N_i \in \mathbb{Z}$ as in (3.3); this involves the choice of a smoothing parameter $\mu \in [-\mu_0, \mu_0]$, and for simplicity we choose the same sufficiently small $\mu_0 > 0$ for all singular points. Call $\mathcal{L}_s$ the line bundle associated to such smoothed family of projectors; it is a vector bundle over $\left(\mathbb{T}_2^* \times [-\mu_0, \mu_0]\right) \setminus \bigcup_{i=1}^M C_i$, where $C_i := U_i \times (-\mu_0, \mu_0)$. The above arguments now show that we can find a bundle $\widehat{\mathcal{L}}_s$, defined on $\left(\mathbb{T}_2^* \times [-\mu_0, \mu_0]\right) \setminus \left(S \times \{\mu = 0\}\right)$, such that $\widehat{\mathcal{L}}_s$ resticts to $\mathcal{L}_s$ whenever the latter is defined, while it coincides with $\mathcal{P}_{n_v^{(i)}, s}$ on $\left(U_i \times [-\mu_0, \mu_0]\right) \setminus \left\{\left(k = K_i, \mu = 0\right)\right\}$, where $n_v^{(i)} := sN_i$. Thus, deformations of families of rank-1 singular projectors with M singular points are uniquely determined by M-tuples of integers, their local vorticities. ♢

5 Decrease of Wannier functions in graphene

In this Section, we will use the n-canonical eigenvectors $\phi_{n,\pm}(q)$, that were explicitly computed via the canonical models presented in Section , to extract the rate of decay of the Wannier functions of graphene. Actually, we can prove a more general result, under the following

Assumption 5.1. We consider a periodic Schrödinger operator, *i. e.* an operator in the form $H_\Gamma = -\Delta + V_\Gamma$, acting in $L^2(\mathbb{R}^2)$, where V_Γ is real-valued, Δ-bounded with relative bound zero, and periodic with respect to a lattice $\Gamma \subset \mathbb{R}^2$. For a Bloch band E_s of H_Γ, we assume that:

- (i) E_s intersects the Bloch band E_{s-1}[10] at finitely many points $\{K_1, \ldots, K_M\}$, *i. e.* $E_s(k_0) = E_{s-1}(k_0) =: E_0$ for every $k_0 \in \{K_1, \ldots, K_M\}$;
- (ii) for every $k_0 \in \{K_1, \ldots, K_M\}$ there exist constants $r, v_+, v_- > 0$ and $m \in \{1, 2\}$, possibly depending on k_0, such that for $|q| < r$

$$\begin{aligned} E_s(k_0 + q) - E_0 &= v_+ |q|^m + \mathcal{O}(|q|^{m+1}), \\ E_{s-1}(k_0 + q) - E_0 &= -v_- |q|^m + \mathcal{O}(|q|^{m+1}); \end{aligned} \tag{5.1}$$

- (iii) the following *semi-gap condition* holds true:

$$\inf_{k \in \mathbb{T}_2^*} \{|E_s(k) - E_i(k)| : i \neq s,\, i \neq s-1\} =: g > 0;$$

- (iv) the dimension of the eigenspace corresponding to the eigenvalue $E_s(k)$ (resp. $E_{s-1}(k)$) is 1 for every $k \in \mathbb{T}_2^* \setminus \{K_1, \ldots, K_M\}$;
- (v) there exists a deformation $H^\mu(k)$ of the fibre Hamiltonian $H(k)$, as in (2.1), such that, if $P_*(k)$ denotes the spectral projection of $H(k)$ onto the eigenvalues $\{E_s(k), E_{s-1}(k)\}$, then for all $k_0 \in \{K_1, \ldots, K_M\}$ the operator $P_*(k_0) H^\mu(k) P_*(k_0)$ is close, in the norm-resolvent sense, to[11] $P_*(k_0) H_m^\mu(k) P_*(k_0)$, where $H_m^\mu(k)$

[10] All the following statements remain true, with only minor modifications in the proofs, if E_{s-1} is replaced by E_{s+1}.
[11] With abuse of notation, we denote

is as in (3.25) with $n = m$ and $e(q) = |q|^m$, for the same m as in item ((*ii*)) and uniformly for $|k - k_0| < r$ and $\mu \in [-\mu_0, \mu_0]$.

♢

Condition ((*i*)) corresponds to considering a semimetallic solid. Condition ((*ii*)) characterises the local behaviour of the eigenvalues; while some of our results hold true for any $m \in \mathbb{N}^\times$, we need the assumption $m \in \{1,2\}$ in order to prove Theorem 5.2. Condition ((*iii*)) guarantees that the Bloch bands not involved in the relevant intersection do not interfere with the local structure of the eigenprojectors. Condition ((*iv*)) excludes permanent degeneracy of the eigenvalues. Lastly, condition ((*v*)) corresponds to the assumption that the tight-binding Hamiltonian $H^\mu_m(k)$ is an accurate approximation, in the norm-resolvent sense, of the original continuous Hamiltonian. Notice that we crucially assume $d = 2$.

It is usually accepted that Assumption 5.1 holds true for (monolayer and bilayer) graphene (with $M = 2$), since conditions ((*i*)), ((*ii*)) and ((*iii*)) can be explicitly checked to hold within the tight-binding approximation, and these conditions are expected to be stable under approximations. Recently, C. Fefferman and M. Weinstein [11] provided sufficient conditions on V_Γ yielding (i) and (ii) with $m = 1$. Hereafter, the indices $\{s, s-1\}$ will be replaced by $\{+,-\}$ to streamline the notation.

We recall that the Wannier function depends on a choice of the phase for the Bloch function ψ_+ (or, equivalently, its periodic part u_+) according to the following definition.

Definition 5.1. The **Wannier function** $w_+ \in L^2(\mathbb{R}^2)$ corresponding to the Bloch function ψ_+ for the Bloch band E_+ is

$$w_+(x) := \frac{1}{|\mathbb{B}|^{1/2}} \int_{\mathbb{B}} \mathrm{d}k\, \psi_+(k,x) = \frac{1}{|\mathbb{B}|^{1/2}} \int_{\mathbb{B}} \mathrm{d}k\, \mathrm{e}^{\mathrm{i}k\cdot x} u_+(k,[x]) \tag{5.2}$$

where $\mathbb{B}$ is the fundamental unit cell for Γ^*, and $[x] = x \bmod \Gamma$. ♢

Thus w_+ is nothing but the Bloch-Floquet anti-transform of the Bloch function ψ_+ (see Section 2.1). Recall also that the decay rate of the Wannier function as $|x| \to \infty$ is related to the regularity of the corresponding Bloch function, see *e.g.* [23, Section 2.2] or [35, Equation (2.5)]. In particular, if the Bloch function can be chosen to be C^∞-smooth, then the associated Wannier function decays at infinity faster than the inverse of any polynomial.

Since the Wannier function is defined by integration over $\mathbb{B}$, the smoothness of $k \mapsto \psi_+(k,\cdot)$ can be analysed separately in different regions of the Brillouin zone. The problem is therefore reduced to a local analysis of the Bloch functions around the intersection points, as detailed in the next Subsection.

$$P_*(k_0) H^\mu_m(k) P_*(k_0) := \sum_{a,b \in \{s,s-1\}} |u_a(k_0)\rangle \left(H^\mu_m(k)\right)_{a,b} \langle u_b(k_0)|$$

with respect to an orthonormal basis $\{u_s(k_0), u_{s-1}(k_0)\}$ of $\operatorname{Ran} P_*(k_0)$.

5.1 Reduction to a local problem around the intersection points

First, notice that the Bloch function relative to the Bloch band E_+ is unique, up to the choice of a k-dependent phase: we assume that such a choice has been performed[12], and denote the corresponding Bloch function by $\psi_+(k)$. Now, let $U = U_{k_0} := \{k \in \mathbb{B} : |k - k_0| < r\}$ be the neighbourhood of the intersection point $k_0 \in \{K_1, \dots, K_M\}$ for which expansion (5.1) holds, and let $\widetilde{\chi}_U(k)$ be a smoothed characteristic function for U, namely a smooth function supported in U which is identically 1 on a smaller disc $D \subset U$ of radius $\rho < r$. We assume that such smoothed characteristic functions are radially symmetric, *i. e.* $\widetilde{\chi}_U(k_0 + q) = \widetilde{\chi}(|q|)$. Then the Bloch function ψ_+ may be written as

$$\psi_+(k) = \sum_{i=1}^{M} \widetilde{\chi}_{U_{K_i}}(k)\psi_+(k) + \left(1 - \sum_{i=1}^{M} \widetilde{\chi}_{U_{K_i}}(k)\right)\psi_+(k).$$

The summands in the first term, call them $\psi_U(k) = \psi_{U_{K_i}}(k)$, contain all the information regarding the crossing of the two energy bands at the points in $\{K_1, \dots, K_M\}$. On the other hand, since the Bloch bands intersect *only* at these points (Assumption 5.1((i))), then the last term, call it $\widetilde{\psi}(k)$, can be assumed to be smooth. As the Wannier transform (5.2) is linear, the Wannier function $w_+(x)$ corresponding to the Bloch function $\psi_+(k)$ via (5.2) splits as

$$w_+(x) = \sum_{i=1}^{M} w_{U_{K_i}}(x) + \widetilde{w}(x)$$

with an obvious meaning of the notation. In the next Subsection we will prove (see Theorem 5.1) that each of the functions $w_{U_{K_i}}$ has a power-law decay at infinity. Moreover, since $k \mapsto \widetilde{\psi}(k)$ is smooth, we can make the reminder term $\widetilde{w}$ decay as fast as the inverse of a polynomial of arbitrary degree, by choosing $\widetilde{\chi}$ sufficiently regular. Consequently we get that the asymptotic behaviour of the true Wannier function w_+ is determined by that of the functions $w_{U_{K_i}}$.

In the following, we will concentrate on one intersection point $k_0 \in \{K_1, \dots, K_M\}$, and calculate the rate of decay at infinity of the function w_U. Let us also notice that, for reasons similar to the above, the behaviour of w_U at infinity does not depend on the particular choice of the cutoff function $\widetilde{\chi}_U$, provided it is sufficiently regular. Indeed, if $\widetilde{\chi}_U$ and $\widetilde{\chi}'_U$ are two different cutoffs, both satisfying the above conditions, then their difference $\widetilde{\chi}''_U := \widetilde{\chi}_U - \widetilde{\chi}'_U$ is supported away from the intersection point k_0. This means that the corresponding $\psi''_U(k) = \widetilde{\chi}''_U(k)\psi_+(k)$ is regular, and this in turn implies that w''_U decays fast at infinity. For this reason, we are allowed to choose a simple form for the function $\widetilde{\chi}_U$: in particular, we will choose $\widetilde{\chi}(|q|)$ to be polynomial in $|q|$ (of sufficiently high degree N) for $|q| \in (\rho, r)$, *i. e.*

$$\widetilde{\chi}(|q|) = \begin{cases} 1 & \text{if } 0 \le |q| \le \rho, \\ \sum_{i=0}^{N} \alpha_i |q|^i & \text{if } \rho < |q| < r, \\ 0 & \text{if } |q| \ge r. \end{cases} \tag{5.3}$$

[12] The decay rate at infinity of Wannier functions may *a priori* depend on such a choice, but this does not happen provided the change of phase is sufficiently smooth, as detailed in Remark 5.1.

The coefficients α_i are chosen in order to guarantee that $\widetilde{\chi}$ is as smooth as required. In particular, having $\widetilde{\chi} \in C^p([0,+\infty))$ requires $N \geq 2p-1$.

5.2 Asymptotic decrease of the *n*-canonical Wannier function

We proceed to determine the rate of decay of w_U, extracting it from the models which were illustrated in Section 3.2. Clearly

$$w_U(x) = \frac{1}{|\mathbb{B}|^{1/2}} \int_{\mathbb{B}} \mathrm{d}k\, \psi_U(k,x) = \frac{1}{|\mathbb{B}|^{1/2}} \int_U \mathrm{d}k\, \mathrm{e}^{\mathrm{i}k\cdot x} \widetilde{\chi}_U(k)\, u_+(k,[x]). \tag{5.4}$$

We claim that its asymptotic behaviour is the same as that of the *n-canonical Wannier function*

$$w_{\mathrm{can}}(x) := \frac{1}{|\mathbb{B}|^{1/2}} \int_U \mathrm{d}k\, \mathrm{e}^{\mathrm{i}k\cdot x} \widetilde{\chi}_U(k) \phi_n(k,[x]) = \frac{\mathrm{e}^{\mathrm{i}k_0\cdot x}}{|\mathbb{B}|^{1/2}} \int_U \mathrm{d}q\, \mathrm{e}^{\mathrm{i}q\cdot x} \widetilde{\chi}(|q|) \phi_n(q,[x]) \tag{5.5}$$

where n is the vorticity of the family of projectors $\left\{P_+^\mu(k)\right\}_{k\in R\setminus\{k_0\},\mu\in[-\mu_0,\mu_0]}$ corresponding to the deformed fibre Hamiltonian $H^\mu(k)$, as in Assumption 5.1((v)) (here $R \subset \mathbb{B}$ is a contractible region containing U but not intersecting any of the chosen balls centered at the other intersection points), and

$$\phi_n(q,[x]) := \phi_{n,+}(q)_1\, u_+(k_0,[x]) + \phi_{n,+}(q)_2\, u_-(k_0,[x]) \tag{5.6}$$

with $\phi_{n,+}(q) = \left(\phi_{n,+}(q)_1, \phi_{n,+}(q)_2\right)$ as in (3.22). We will motivate why the vorticity of $\left\{P_+^\mu(k)\right\}$ is non-zero in Subsection . To prove this claim, we will establish the following two main results of this Section.

Theorem 5.1. *Let w_{can} be the n-canonical Wannier function defined as in* (5.5)*, with $n \neq 0$. Then there exist two positive constants $R, c > 0$ such that*

$$|w_{\mathrm{can}}(x)| \leq \frac{c}{|x|^2} \quad \textit{if} \quad |x| \geq R. \tag{5.7}$$

The proof of the previous Theorem is postponed to Subsection .

While the proof of Theorem 5.1 does not require restrictions on the value of m in Assumption 5.1((ii)), it is crucial that $m \in \{1,2\}$ for the techniques employed in our proof of Theorem 5.2. In the following we will denote by $|X|^\alpha$ the operator acting on a suitable domain in $L^2(\mathbb{R}^2)$ by $(|X|^\alpha w)(x) := |x|^\alpha w(x)$.

Theorem 5.2. *There exists a choice of the Bloch function ψ_+ such that the following holds: For w_U and w_{can} defined as in* (5.4) *and* (5.5)*, respectively, and $m \in \{1,2\}$ as in Equation* (5.1)*, one has*

$$|X|^s (w_U - w_{\mathrm{can}}) \in L^2(\mathbb{R}^2)$$

for $s \geq 0$ depending on m as follows:

- *if $m = 1$, for all $s < 2$;*
- *if $m = 2$, for all $s < 1$.*

The proof of the previous Theorem is postponed to Subsection .

By combining the above two Theorems with the fact that the decay at infinity of the true Wannier function w_+ is equal to the one of w_U, as was shown in the previous Subsection, we deduce at once the following

Theorem 5.3. *Consider an operator $H_\Gamma = -\Delta + V_\Gamma$ acting in $L^2(\mathbb{R}^2)$ and a Bloch band E_s satisfying Assumption 5.1. Then there exists a choice of the Bloch function relative to the Bloch band E_s such that the corresponding Wannier function $w_+ \in L^2(\mathbb{R}^2)$ satisfies the following L^2-decay condition:*

$$|X|^\alpha w_+ \in L^2(\mathbb{R}^2) \quad \text{for every } 0 \le \alpha < 1. \tag{5.8}$$

Proof. Fix $0 \le \alpha < 1$. The L^2-norm of the function $|X|^\alpha w_+$ can be estimated by

$$\begin{aligned} \left\| |X|^\alpha w_+ \right\|^2_{L^2(\mathbb{R}^2)} &= \int_{\mathbb{R}^2} \mathrm{d}x\, |x|^{2\alpha} |w_+(x)|^2 \le \\ &\le \int_{\mathbb{R}^2} \mathrm{d}x\, |x|^{2\alpha} |w_+(x) - w_{\mathrm{can}}(x)|^2 + \int_{\mathbb{R}^2} \mathrm{d}x\, |x|^{2\alpha} |w_{\mathrm{can}}(x)|^2. \end{aligned} \tag{5.9}$$

In order to give a bound to the first integral, we use the result of Theorem 5.2. Firstly we write

$$\begin{aligned} \int_{\mathbb{R}^2} \mathrm{d}x\, |x|^{2\alpha} |w_+(x) - w_{\mathrm{can}}(x)|^2 = \int_{D_1} \mathrm{d}x\, |x|^{2\alpha} |w_+(x) - w_{\mathrm{can}}(x)|^2 + \\ + \int_{\mathbb{R}^2 \setminus D_1} \mathrm{d}x\, |x|^{2\alpha} |w_+(x) - w_{\mathrm{can}}(x)|^2 \end{aligned}$$

where $D_1 \subset \mathbb{R}^2$ is the ball of radius 1 around the origin. The first term on the right-hand side of the above equality is finite, because the function $w_+ - w_{\mathrm{can}}$ is in $L^2(\mathbb{R}^2)$ (hence *a fortiori* in $L^2(D_1)$) and $|x|^{2\alpha} \le 1$ for $x \in D_1$. For $x \in \mathbb{R}^2 \setminus D_1$ and $\alpha \in [0,1)$, by Theorem 5.2 we conclude that

$$\int_{\mathbb{R}^2 \setminus D_1} \mathrm{d}x\, |x|^{2\alpha} |w_+(x) - w_{\mathrm{can}}(x)|^2 \le \left\| |X|^\alpha (w_+ - w_{\mathrm{can}}) \right\|^2_{L^2(\mathbb{R}^2)}$$

is finite.

To show that also the second summand in (5.9) is finite, we use instead Theorem 5.1. Write

$$\int_{\mathbb{R}^2} \mathrm{d}x |x|^{2\alpha} |w_{\mathrm{can}}(x)|^2 = \int_{D_R} \mathrm{d}x |x|^{2\alpha} |w_{\mathrm{can}}(x)|^2 + \int_{\mathbb{R}^2 \setminus D_R} \mathrm{d}x |x|^{2\alpha} |w_{\mathrm{can}}(x)|^2.$$

Again by the fact that the Wannier function w_{can} is in $L^2(\mathbb{R}^2)$, it follows that the first integral on the right-hand side is finite. As for the second summand, we use the estimate provided by Equation (5.7); thus we have

$$\int_{\mathbb{R}^2 \setminus D_R} \mathrm{d}x |x|^{2\alpha} |w_{\mathrm{can}}(x)|^2 \le \mathrm{const} \cdot \int_R^\infty \mathrm{d}|x|\, |x|\, |x|^{2\alpha} |x|^{-4} \tag{5.10}$$

and this last integral is convergent if and only if $\alpha < 1$. □

Proof of Theorem 5.1

We proceed to the proof of Theorem 5.1, establishing the rate of decay at infinity of the n-canonical Wannier function w_{can} (corresponding to the n-canonical eigenvector for an eigenvalue crossing). For later convenience, we will prove a slightly more general result, concerning the Wannier function associated to a Bloch function which is obtained from the n-canonical eigenvector by multiplication times q_j, $j \in \{1,2\}$.

Proposition 5.1. *Define*

$$w_{n,p}(x) := \frac{\mathrm{e}^{\mathrm{i}k_0\cdot x}}{|\mathbb{B}|^{1/2}} \int_U \mathrm{d}q\, \mathrm{e}^{\mathrm{i}q\cdot x} q_j^p \widetilde{\chi}(|q|) \phi_n(q,[x])$$

where $j \in \{1,2\}$, $p \in \{0,1\}$, *and* $\phi_n(q,[x])$ *is as in* (5.6). *Then there exist two positive constants* $R, c > 0$ *such that*

$$\left| w_{n,p}(x) \right| \le \frac{c}{|x|^{p+2}} \quad \text{for } |x| \ge R.$$

Notice that the exponent in the power-law asymptotics for $w_{n,p}$ is *independent* on n (but the prefactor c will depend on it, as will be apparent from the proof). The statement of Theorem 5.1 regarding the decay rate of w_{can} is a particular case of the above, namely when $p = 0$.

Proof. For notational simplicity, we set $j = 1$, the case $j = 2$ being clearly analogous. Without loss of generality, we also assume that $n > 0$. We choose Cartesian coordinates in $\mathbb{R}^2$ such that $x = (0, |x|)$, and consequently $q \cdot x = -2\pi |q|\,|x| \sin\theta_q$. Since the n-canonical eigenfunction is

$$\phi_{n,+}(q) = \mathrm{e}^{\mathrm{i}n\theta_q/2} \begin{pmatrix} \cos(n\theta_q/2) \\ \sin(n\theta_q/2) \end{pmatrix},$$

we can write

$$w_{n,p}(x) = \frac{\mathrm{e}^{\mathrm{i}k_0\cdot x}}{|\mathbb{B}|^{1/2}} \left[w_{\cos,p}(x)\, u_+(k_0,[x]) + w_{\sin,p}(x)\, u_-(k_0,[x]) \right] \tag{5.11}$$

where

$$w_{\cos,p}(x) := \int_0^r \mathrm{d}|q|\, |q|^{p+1} \widetilde{\chi}(|q|) \int_0^{2\pi} \mathrm{d}\theta_q\, \mathrm{e}^{-\mathrm{i}2\pi|q|\,|x|\sin\theta_q} \cos(\theta_q)^p \mathrm{e}^{\mathrm{i}n\theta_q/2} \cos\left(\frac{n}{2}\theta_q\right),$$
$$w_{\sin,p}(x) := \int_0^r \mathrm{d}|q|\, |q|^{p+1} \widetilde{\chi}(|q|) \int_0^{2\pi} \mathrm{d}\theta_q\, \mathrm{e}^{-\mathrm{i}2\pi|q|\,|x|\sin\theta_q} \cos(\theta_q)^p \mathrm{e}^{\mathrm{i}n\theta_q/2} \sin\left(\frac{n}{2}\theta_q\right).$$

The function $x \mapsto u_\pm(k_0,[x])$ is Γ-periodic, and as a consequence of its definition (2.2) it is in the Sobolev space $W^{2,2}(\mathbb{T}_Y^2)$, hence continuous; consequently, it is a bounded function. Thus, the upper bound on $\left| w_{n,p} \right|$ is completely determined by that on the functions $w_{\cos,p}$ and $w_{\sin,p}$.

Notice that for $p \in \{0,1\}$

$$\cos(\theta_q)^p \mathrm{e}^{\mathrm{i}n\theta_q/2} \cos\left(\frac{n}{2}\theta_q\right) = \frac{1}{4}\left(\mathrm{e}^{\mathrm{i}(n+p)\theta_q} + \mathrm{e}^{\mathrm{i}(n-p)\theta_q} + \mathrm{e}^{\mathrm{i}p\theta_q} + \mathrm{e}^{-\mathrm{i}p\theta_q}\right),$$
$$\cos(\theta_q)^p \mathrm{e}^{\mathrm{i}n\theta_q/2} \sin\left(\frac{n}{2}\theta_q\right) = \frac{1}{4\mathrm{i}}\left(\mathrm{e}^{\mathrm{i}(n+p)\theta_q} + \mathrm{e}^{\mathrm{i}(n-p)\theta_q} - \mathrm{e}^{\mathrm{i}p\theta_q} - \mathrm{e}^{-\mathrm{i}p\theta_q}\right),$$

so that we can write

$$w_{\cos,p}(x) = \frac{1}{4}\left(I_{n+p,p}(|x|) + I_{n-p,p}(|x|) + I_{p,p}(|x|) + I_{-p,p}(|x|)\right),$$
$$w_{\sin,p}(x) = \frac{1}{4\mathrm{i}}\left(I_{n+p,p}(|x|) + I_{n-p,p}(|x|) - I_{p,p}(|x|) - I_{-p,p}(|x|)\right),$$

where

$$I_{\ell,p}(|x|) := \int_0^r \mathrm{d}|q|\,|q|^{p+1}\widetilde{\chi}(|q|) \int_0^{2\pi} \mathrm{d}\theta_q\, \mathrm{e}^{\mathrm{i}(\ell\theta_q - 2\pi|q||x|\sin\theta_q)} =$$
$$= \frac{1}{(2\pi|x|)^{p+2}} \int_0^{2\pi r|x|} \mathrm{d}z\, z^{p+1}\widetilde{\chi}\left(\frac{z}{2\pi|x|}\right) \int_0^{2\pi} \mathrm{d}\theta_q\, \mathrm{e}^{\mathrm{i}(\ell\theta_q - z\sin\theta_q)},$$

with the change of variables $z = 2\pi|q||x|$.

Now, by definition [26]

$$\frac{1}{2\pi}\int_0^{2\pi} \mathrm{d}\theta_q\, \mathrm{e}^{\mathrm{i}(\ell\theta_q - z\sin\theta_q)} = \frac{1}{2\pi}\int_0^{2\pi} \mathrm{d}\theta_q\, \cos\left(\ell\theta_q - z\sin\theta_q\right) =: J_\ell(z) \tag{5.12}$$

is the Bessel function of order ℓ: thus, the functions $w_{\cos,p}$ and $w_{\sin,p}$ are combinations of integrals of the Bessel functions, which explicitly look like

$$I_{\ell,p}(|x|) = \frac{1}{(2\pi)^{p+1}}\,|x|^{-p-2} \int_0^{2\pi r|x|} \mathrm{d}z\, z^{p+1}\widetilde{\chi}\left(\frac{z}{2\pi|x|}\right) J_\ell(z).$$

In order to evaluate these integrals and establish their asymptotic properties, we split

$$I_{\ell,p}(|x|) = I^{(1)}_{\ell,p}(|x|) + I^{(2)}_{\ell,p}(|x|),$$

where

$$I^{(1)}_{\ell,p}(|x|) := \frac{1}{(2\pi)^{p+1}}\,|x|^{-p-2} \int_0^{2\pi\rho|x|} \mathrm{d}z\, z^{p+1} J_\ell(z),$$
$$I^{(2)}_{\ell,p}(|x|) := \frac{1}{(2\pi)^{p+1}}\,|x|^{-p-2} \int_{2\pi\rho|x|}^{2\pi r|x|} \mathrm{d}z\, z^{p+1}\widetilde{\chi}\left(\frac{z}{2\pi|x|}\right) J_\ell(z).$$

Notice that the function $\widetilde{\chi}$ does not appear in the integral $I^{(1)}_{\ell,p}$, since it is constantly equal to 1 for $0 \le |q| < \rho$ (compare (5.3)).

We now use the fact [26, Sec. 2.5, Eqn. (6)] that for large real $t \to \infty$

$$\int_0^t \mathrm{d}z\, z^\mu J_\nu(z) = \frac{2^\mu \Gamma\left(\frac{\nu+\mu+1}{2}\right)}{\Gamma\left(\frac{\nu-\mu+1}{2}\right)} - \left(\frac{2}{\pi t}\right)^{1/2} t^\mu h(t),$$

whenever $\Re(\nu+\mu) > -1$, where $h(t) = f(t)\cos\theta(t) + g(t)\sin\theta(t)$ with

$$\theta(t) = t - \nu\frac{\pi}{2} + \frac{\pi}{4}, \quad f(t) = 1 + \mathcal{O}(t^{-2}), \quad g(t) = \mathcal{O}(t^{-1}).$$

This allows to immediately compute the asymptotic rate of $I^{(1)}_{\ell,p}(|x|)$:

$$\begin{aligned} I^{(1)}_{\ell,p}(|x|) &= \frac{2^{p+1}\Gamma\left(\frac{\ell+p+2}{2}\right)}{\Gamma\left(\frac{\ell-p}{2}\right)} \frac{1}{(2\pi)^{p+1}} |x|^{-p-2} - \\ &\quad - \frac{1}{(2\pi)^{p+1}} |x|^{-p-2} \left(\frac{2}{\pi\cdot 2\pi\rho|x|}\right)^{1/2} (2\pi\rho|x|)^{p+1} h(2\pi\rho|x|) = \\ &= \frac{\Gamma\left(\frac{\ell+p+2}{2}\right)}{\Gamma\left(\frac{\ell-p}{2}\right)\pi^{p+1}} |x|^{-p-2} - \frac{\rho^{p+(1/2)}}{\pi} |x|^{-3/2} h(2\pi\rho|x|). \end{aligned}$$

We now compute also the asymptotics of $I^{(2)}_{\ell,p}(|x|)$ for large $|x|$. We use the explicit polynomial form (5.3) for the cutoff function $\widetilde{\chi}$ in the interval (ρ, r), thus obtaining

$$\begin{aligned} I^{(2)}_{\ell,p}(|x|) &= \frac{1}{(2\pi)^{p+1}} |x|^{-p-2} \left(\int_0^{2\pi r|x|} - \int_0^{2\pi\rho|x|}\right) \mathrm{d}z\, z^{p+1} \left(\sum_{i=0}^{N} \alpha_i \frac{z^i}{(2\pi|x|)^i}\right) J_\ell(z) = \\ &= 2\pi \sum_{i=0}^{N} \frac{\alpha_i}{(2\pi|x|)^{p+i+2}} \left(\int_0^{2\pi r|x|} - \int_0^{2\pi\rho|x|}\right) \mathrm{d}z\, z^{p+i+1} J_\ell(z) = \\ &= 2\pi \sum_{i=0}^{N} \frac{\alpha_i}{(2\pi|x|)^{p+i+2}} \left[-\left(\frac{2}{\pi\cdot 2\pi r|x|}\right)^{1/2} (2\pi r|x|)^{p+i+1} h(2\pi r|x|) - (r \leftrightarrow \rho)\right] = \\ &= \frac{r^{p+(1/2)}}{\pi} \left(-\sum_{i=0}^{N} \alpha_i\, r^i\right) |x|^{-3/2} h(2\pi r|x|) + \frac{\rho^{p+(1/2)}}{\pi} \left(\sum_{i=0}^{N} \alpha_i\, \rho^i\right) |x|^{-3/2} h(2\pi\rho|x|) = \\ &= \frac{\rho^{p+(1/2)}}{\pi} |x|^{-3/2} h(2\pi\rho|x|) \end{aligned}$$

where in the last equality we used the fact that $\widetilde{\chi}(\rho) = 1$ and $\widetilde{\chi}(r) = 0$.

From these computations, we deduce that[13]

$$I_{\ell,p}(|x|) = \frac{\Gamma\left(\frac{\ell+p+2}{2}\right)}{\Gamma\left(\frac{\ell-p}{2}\right)\pi^{p+1}} |x|^{-p-2} + \mathcal{O}(|x|^{-p-j}) \quad \text{for all } j \in \mathbb{N}^\times.$$

[13] The prefactor can be computed using the factorial relation $\Gamma(z+1) = z\Gamma(z)$: one obtains

$$\frac{\Gamma\left(\frac{\ell+p+2}{2}\right)}{\Gamma\left(\frac{\ell-p}{2}\right)\pi^{p+1}} = \begin{cases} \dfrac{\ell}{2\pi} & \text{if } p = 0, \\[2ex] \dfrac{\ell^2-1}{4\pi^2} & \text{if } p = 1. \end{cases}$$

We conclude that the upper bound on the rate of decay at infinity of both $w_{\cos,p}$ and $w_{\sin,p}$ (and hence that of the Wannier functions $w_{n,p}$) is given by a multiple of $|x|^{-p-2}$, for both $p = 0$ and $p = 1$ and independently of $n \in \mathbb{Z}$. □

Notice that with the above proof we actually have a stronger control on the asymptotic behaviour of the function $w_{n,p}$ than what stated in Proposition 5.1: Indeed, from (5.11) we see that $w_{n,p}$ is a combination of functions which behave asymptotically as $|x|^{-p-2}$ (up to arbitrarily higher order terms), times a Γ-periodic function of x.

5.3 *Asymptotic decrease of the true Wannier function*

In this Subsection, we will prove Theorem 5.2. The importance of this result lies in the fact that we can deduce from it an upper bound on the decay rate at infinity of the true Wannier function in the continuous model of (monolayer and bilayer) graphene, as in Theorem 5.3. Indeed, what we will show in the following is that all the singularity of the Bloch function $u_+(k) \in \mathcal{H}_{\mathrm{f}}$ at the intersection point k_0 is encoded in its components along the vectors $u_+(k_0)$ and $u_-(k_0)$ in $\mathcal{H}_{\mathrm{f}}$. This is essentially a consequence of Assumption 5.1((iii)), namely of the fact that all Bloch bands not involved in the intersection at k_0 are well separated from the intersecting ones.

True Bloch bundle vs. stratified Bloch bundle

Let us briefly summarise the geometric results of Section 4, in order to specify them to the case under study; we will use all the notation of that Section. Assume that $r > 0$ is so small that the ball of radius $2r$ is all contained in R. Denote as above by $\{P_+(k) := |u_+(k)\rangle \langle u_+(k)|\}_{k \in R \setminus k_0}$ the family of projectors corresponding to the Bloch band E_+; we use it as our Datum 3.1, so we smoothen it via a parameter $\mu \in [-\mu_0, \mu_0]$ and calculate the vorticity $n \in \mathbb{Z}$ using the eigenprojectors of the deformation $H^{\mu}(k)$ appearing in Assumption 5.1((v)). Theorem 4.1 then establishes the existence of a vector bundle $\widehat{\mathcal{L}}$ on $\widehat{B}$ such that:

- outside of a cylinder C' of radius $r + r' < 2r$ centered at the singular point ($k = k_0, \mu = 0$), the bundle $\widehat{\mathcal{L}}$ *coincides* with the bundle $\mathcal{L}_+$, which is associated to the smoothed family of projectors $\{P_+^{\mu}(k)\}$;
- inside a smaller pointed cylinder $\mathring{C}_1$ of radius $r_1 := r - r' > 0$ centered at the singular point ($k = k_0, \mu = 0$), the bundle $\widehat{\mathcal{L}}$ *coincides* with the n-canonical stratified Bloch bundle $\mathcal{P}_n = \mathcal{P}_{n,+}$;
- inside the tubular neighbourhood T of width r' of the cylindrical surface $\mathcal{C} = \partial C$, the bundle $\widehat{\mathcal{L}}$ is constructed extending the isomorphism of Hermitian bundles

  $$\mathcal{L}_+\big|_{\mathcal{C}} \simeq \mathcal{P}_n\big|_{\mathcal{C}} \tag{5.13}$$

  (see Lemma 4.1).

On the other hand, as $\mathring{C}$ is a deformation retract of $\mathcal{C}$, the isomorphism (5.13) extends to an isomorphism

$$\mathcal{L}_+\big|_{\overset{\circ}{C}} \simeq \mathcal{P}_n\big|_{\overset{\circ}{C}} \tag{5.14}$$

which, together with the first items of the list above, allows us to conclude that *the bundle $\widehat{\mathcal{L}}$ constructed via Theorem 4.1 is isomorphic to the Bloch bundle $\mathcal{L}_+$ as bundles on the whole $\widehat{B}$.*

We now want to translate the information contained in the latter isomorphism in terms of the associated families of projectors, and of the "sections" of these bundles (*i. e.* Bloch functions). In order to do so, we first show that the vorticity n of the family $\{P_+(k)\}$ equals $m \in \{1,2\}$ as in Assumption 5.1((ii)), so that in particular it is non-zero. Indeed, consider the deformation $H^\mu(k)$ of the fibre Hamiltonian $H(k) = (-\mathrm{i}\nabla_y + k)^2 + V_\Gamma(y)$, as in Assumption 5.1($(v)$), and a circle Λ_* in the complex plane enclosing only the eigenvalues $\left\{E^\mu_+(k), E^\mu_-(k)\right\}$ for $|k-k_0|$ and μ sufficiently small. Then the Riesz integral

$$P^\mu_*(k) := \frac{\mathrm{i}}{2\pi}\oint_{\Lambda_*} \mathrm{d}z\,\left(H^\mu(k) - z\mathbb{1}\right)^{-1}$$

defines a smooth family of projectors over $C = U \times (-\mu_0, \mu_0)$ (see [35, Prop. 2.1] for a detailed proof), such that $P^{\mu=0}_*(k) = P_*(k)$. By using again the Riesz formula with a different contour $\Lambda^\mu(k)$ enclosing only the eigenvalue $E^\mu_+(k)$ (compare the proof of Proposition 5.2 below), we can realise $P^\mu_+(k)$ as a subprojector of $P^\mu_*(k)$. Denoting $\Pi := P_*(k_0)$, we then have

$$\begin{aligned}
\left\|\Pi P^\mu_+(k)\Pi - \Pi P^\mu_{m,+}(k)\Pi\right\|_{\mathcal{B}(\mathcal{H}_\mathrm{f})} &= \left\|P^\mu_+(k) - P^\mu_{m,+}(k)\right\|_{\mathcal{B}(\operatorname{Ran}\Pi)} = \\
&= \left\|\frac{\mathrm{i}}{2\pi}\oint_{\Lambda^\mu(k)} \mathrm{d}z\left[\left(H^\mu(k) - z\mathbb{1}\right)^{-1} - \left(H^\mu_m(k) - z\mathbb{1}\right)^{-1}\right]\right\|_{\mathcal{B}(\operatorname{Ran}\Pi)} = \\
&\le \frac{1}{2\pi}\,|\Lambda^\mu(k)|\,\left\|\left(H^\mu(k) - z\mathbb{1}\right)^{-1} - \left(H^\mu_m(k) - z\mathbb{1}\right)^{-1}\right\|_{\mathcal{B}(\operatorname{Ran}\Pi)}
\end{aligned}$$

where $H_m(k)$ is as in (3.25) (with $n = m$ and $e(q) = |q|^m$) and $P^\mu_{m,+}(q)$ is its eigenprojector. The norm on the right-hand side of the above inequality is uniformly bounded by Assumption 5.1((v)), say by $\delta > 0$, and the length of the circle $\Lambda^\mu(k)$ can be made to shrink as $|q|^m$ when $|q| \to 0$. Thus we deduce that

$$\left\|P^\mu_+(k) - P^\mu_{n,+}(k)\right\|_{\mathcal{B}(\operatorname{Ran}\Pi)} \le \mathrm{const}|q|^m\delta, \tag{5.15}$$

and the right-hand side of the above inequality can be made smaller than 1. By Lemma 3.1, we then have

$$n_\mathrm{v}(P_+) = n_\mathrm{v}(P_{m,+}) = m \in \{1,2\}$$

by Assumption 5.1((ii)).

The above estimate gives the existence of a Kato-Nagy unitary $V^\mu(k)$, as in (3.7), such that

$$\Pi\,P^\mu_+(k)\,\Pi = V^\mu(k)\,P^\mu_{m,+}(k)\,V^\mu(k)^{-1}.$$

This can be restated in terms of the existence of a Bloch function u^μ_+ (*i. e.* an eigenfunction of P^μ_+) such that

$$\Pi u_+^\mu(k) = V^\mu(k)\phi_n^\mu(k) \quad \text{for } (k,\mu) \in \mathring{C}, \tag{5.16}$$

where

$$\phi_n^\mu(q,[x]) := \phi_{m,+}^\mu(q)_1\, u_+(k_0,[x]) + \phi_{m,+}^\mu(q)_2\, u_-(k_0,[x])$$

with $\phi_{m,+}^\mu(q) = \big(\phi_{m,+}^\mu(q)_1, \phi_{m,+}^\mu(q)_2\big)$ as in (3.16). Moreover, combining the definition (3.7) of $V^\mu(k)$ and the estimate (5.15), one easily checks that $V^\mu(k)$ actually extends smoothly to the whole cylinder C, in particular at $(k = k_0, \mu = 0)$.

We restrict our attention to the slice $\mu = 0$. Denote by w_{eff} the Wannier function associated via (5.2) to $U \ni k \mapsto \Pi\, u_+(k) =: u_{\mathrm{eff}}(k)$. Arguing as in Section 5.1, one deduces that the asymptotic decay of w_{eff} is determined by the integration of u_{eff} on U in (5.2). Then the equality (5.16) implies that

$$\begin{aligned} |\mathbb{B}|^{1/2}\, w_{\mathrm{eff}}(x) &\asymp \int_U \mathrm{d}q\, \mathrm{e}^{\mathrm{i}q\cdot x}\, \widetilde{\chi}(|q|)\Pi u_+(k_0+q,[x]) = \\ &= \sum_{b\in\{+,-\}} \left[\int_U \mathrm{d}q\, \mathrm{e}^{\mathrm{i}q\cdot x} \left(\sum_{a\in\{1,2\}} V(k_0+q)_{a,b}\, \widetilde{\chi}(|q|)\phi_{m,+}(q,[x])_a \right) \right] u_b(k_0,[x]). \end{aligned}$$

As was already noticed, the functions $u_\pm(k_0,\cdot)$ do not contribute to the decay at infinity of w_{eff}. On the other hand, by Taylor expansion at k_0 we can write

$$V(k_0+q)_{a,b} = V(k_0)_{a,b} + \sum_{j=1}^{2} q_j \frac{\partial V}{\partial q_j}(k_0)_{a,b} + \sum_{j,\ell=1}^{2} q_j\, q_\ell R_{j,\ell}(q) \tag{5.17}$$

where the remainder $R_{j,\ell}$ is C^∞-smooth on U. Consequently, we get

(5.18)

$$\begin{aligned} \int_U \mathrm{d}q\, \mathrm{e}^{\mathrm{i}q\cdot x} V(k_0+q)_{a,b}\widetilde{\chi}(|q|)\phi_{m,+}(q,[x])_a &= V(k_0)_{a,b}\left(\int_U \mathrm{d}q\, \mathrm{e}^{\mathrm{i}q\cdot x}\, \widetilde{\chi}(|q|)\phi_{m,+}(q,[x])_a \right) + \\ &+ \sum_{j=1}^{2} \frac{\partial V}{\partial q_j}(k_0)_{a,b} \left(\int_U \mathrm{d}q\, \mathrm{e}^{\mathrm{i}q\cdot x}\, q_j \widetilde{\chi}(|q|)\phi_{m,+}(q,[x])_a \right) + \\ &+ \sum_{j,\ell=1}^{2} \int_U \mathrm{d}q\, \mathrm{e}^{\mathrm{i}q\cdot x}\, q_j q_l R_{j,\ell}(q)\widetilde{\chi}(|q|)\phi_{m,+}(q,[x])_a. \end{aligned}$$

The terms in brackets in the first and second summand have already been estimated in Proposition 5.1, and so are known to produce the rate of decay at infinity of $|x|^{-2}$ and $|x|^{-3}$, respectively. As for the third summand, we preliminarly notice that the function

$$S(q) := q_j q_l R_{j,\ell}(q)\widetilde{\chi}(|q|)\phi_{m,+}(q,[x])_a$$

is in $W^{2,\infty}(U)$. Indeed, the map $q \mapsto R_{j,\ell}(q)\widetilde{\chi}(|q|)$ is smooth and bounded, while for all $r,s \in \{1,2\}$

$$\frac{\partial^2}{\partial q_r \partial q_s}\big(q_j q_\ell \phi_{m,+}(q,[x])_a\big)$$

is in $L^\infty(U)$, since $\phi_{m,+}(q,[x])_a$ is homogeneous of order zero in q.
We can now proceed to an integration by parts: observe in fact that

$$-x_r\, x_s \int_U \mathrm{d}q\, \mathrm{e}^{\mathrm{i}q\cdot x}\, S(q) = \int_U \mathrm{d}q\, \frac{\partial^2}{\partial q_r \partial q_s}\left(\mathrm{e}^{\mathrm{i}q\cdot x}\right) S(q) = \\ = \int_U \mathrm{d}q\, \mathrm{e}^{\mathrm{i}q\cdot x}\, \frac{\partial^2 S}{\partial q_r \partial q_s}(q).$$

The boundary terms vanish because $\widetilde{\chi}$ is zero on ∂U. By what we have shown above, we obtain that

$$\left| x_r\, x_s \int_U \mathrm{d}q\, \mathrm{e}^{\mathrm{i}q\cdot x}\, S(q) \right| \le |U| \left\| \frac{\partial^2 S}{\partial q_r \partial q_s} \right\|_\infty < +\infty,$$

so that the third summand in (5.18) decays faster than $|x|^{-2}$ at infinity. We conclude that the asymptotic behaviour of w_{eff} is that of $|x|^{-2}$.

Remark 5.1 (Invariance of the decay rate of Wannier functions). Given Theorem 5.2, whose proof will be completed in the next Subsection, the above argument shows also that the decay rate of the Wannier function w_+ is not affected by a change of phase in the corresponding Bloch function ψ_+, provided the phase is at least of class C^2. Indeed, we already know that the decay rate of w_+ depends only on the local behaviour of ψ_+ around the intersection point. The exchange of $\psi_+(k)$ with $\mathrm{e}^{\mathrm{i}\theta(k)}\psi_+(k)$, for $k \in U$, is then equivalent to the exchange of $\phi_{m,+}(k)$ with $\mathrm{e}^{\mathrm{i}\theta(k)}\phi_{m,+}(k)$. This exchange is implemented by the action of the unitary diagonal operator $V(k) = \mathrm{e}^{\mathrm{i}\theta(k)}\mathbb{1} \in U(2)$: if the dependence of $\theta(k)$ on $k \in U$ is C^2, then it is possible to perform a Taylor expansion as in (5.17), so that the above argument applies. ♢

Proof of Theorem 5.2

Finally, we proceed to show that the decay of w_{eff}, the Wannier function corresponding to $\Pi u_+(k)$, and of w_U, the Wannier function corresponding to the restriction to U of $u_+(k)$, are the same. This is achieved by showing that their difference, which is the Wannier function associated to $(\mathbb{1}-\Pi)u_+(k) =: u_{\mathrm{rem}}(k)$, decays sufficiently fast at infinity (*i. e.* at least faster than $|x|^{-2}$); this in turn will be proved by showing that $u_{\mathrm{rem}}(k)$ is sufficiently smooth, say of class $W^{s,2}$ for some positive s. Indeed, in view of the results relating regularity of Bloch functions and asymptotic properties of the corresponding Wannier functions (compare [35, Equation (2.5)]), we have that

$$\text{if } u_{\mathrm{rem}} \in W^{s,2}(U;\mathcal{H}_{\mathrm{f}}) \text{ then } |X|^s\,(w_U - w_{\mathrm{eff}}) \in L^2(\mathbb{R}^2). \tag{5.19}$$

Before establishing the Sobolev regularity of u_{rem}, we need to prove some estimates on the derivatives of the projector $P_+(k)$, and correspondingly on those of the Bloch function $u_+(k)$.

Proposition 5.2. *Let* $\{P_+(k)\}_{k\in\mathring{U}}$ *be the family of eigenprojectors for the Hamiltonian* $H_\Gamma = -\Delta + V_\Gamma$ *as in Assumption 5.1. Let* $m \in \{1,2\}$ *be as in* (5.1)*. Then, for all choices of multi-indices* $I \in \{1,2\}^N$, $N \in \mathbb{N}$, *there exists a constant* $C_N > 0$ *such that*

$$\left\|\partial_I^N P_+(k)\right\|_{\mathcal{B}(\mathcal{H}_{\mathrm{f}})} \le \frac{C_N}{|q|^{Nm}} \qquad \text{for all } k = k_0 + q, \quad 0 < |q| < r. \tag{5.20}$$

Proof. We will explicitly prove the validity of estimates of the form (5.20) for $N \le 2$, as these are the only cases which will be needed later in the proof of Theorem 5.2. Using similar techniques, one can prove the result for arbitrary N.

The projector $P_+(k)$ can be computed by means of the Riesz integral formula, namely

$$P_+(k) = \frac{\mathrm{i}}{2\pi} \oint_{\Lambda(k)} \mathrm{d}z\, (H(k) - z\mathbb{1})^{-1},$$

where $H(k) = (-\mathrm{i}\nabla_y + k)^2 + V_\Gamma$ is the fibre Hamiltonian (2.1), and $\Lambda(k)$ is a circle in the complex plane, enclosing only the eigenvalue $E_+(k)$. We choose $\Lambda(k)$ with center on the real axis, passing through $E_0 = E_+(k_0)$ and having diameter $d(q) = 2v_+|q|^m$, where v_+ and m are the constants appearing in Assumption 5.1((ii)); in particular, the length of the circle $\Lambda(k)$ is proportional to $|q|^m$. Hereafter we assume, without loss of generality, that $E_0 = 0$ and that r is so small that $2v_+r^m < (g/3)$, where g is as in Assumption 5.1((iii)).

Recall that $\kappa \mapsto H(\kappa)$, $\kappa \in \mathbb{C}^2$, defines an analytic family in the sense of Kato (see Section 2.1). In particular, in view of [40, Thm. VI.4] one can compute the derivatives of $H(k)$ and of its spectral projection using either weak or strong limits with the same result. As a consequence, one obtains

$$\partial_j P_+(k) = -\frac{\mathrm{i}}{2\pi} \oint_{\Lambda(k)} \mathrm{d}z\, (H(k) - z\mathbb{1})^{-1} \partial_j H(k) (H(k) - z\mathbb{1})^{-1}. \tag{5.21}$$

Notice that the dependence of the contour of integration on k does not contribute to the above derivative, because the region contained between two close circles $\Lambda(k)$ and $\Lambda(k+h)$ does not contain any point in the spectrum of $H(k)$.

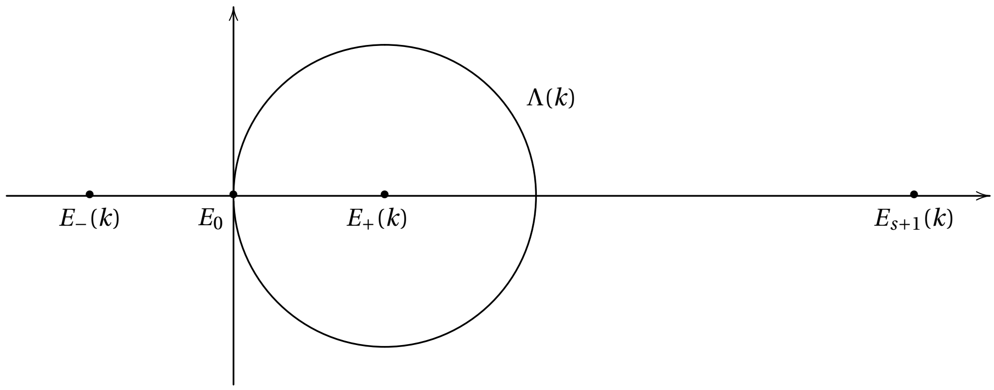


Fig. 4 The integration countour $\Lambda(k)$

By the explicit expression of $H(k)$ given above, we deduce that

$$\partial_j H(k) = 2\left(-\mathrm{i}\frac{\partial}{\partial y_j} + k_j\right) =: D_j(k).$$

Moreover, the resolvent of $H(k)$ is a bounded operator, whose norm equals

$$\left\|(H(k) - z\mathbb{1})^{-1}\right\|_{\mathcal{B}(\mathcal{H}_\mathrm{f})} = \frac{1}{\operatorname{dist}(z, \sigma(H(k)))}$$

where $\sigma(H(k))$ is the spectrum of the fibre Hamiltonian. As z runs on the circle $\Lambda(k)$, the distance on the right-hand side of the above equality is minimal when z is real, and the minimum is attained at the closest eigenvalue of $H(k)$, namely the selected Bloch band $E_+(k)$ or the eigenvalue $E_-(k)$. By Assumption 5.1((*ii*)), we conclude in both cases that

$$\left\| (H(k) - z\mathbb{1})^{-1} \right\|_{\mathcal{B}(\mathcal{H}_\mathrm{f})} \le \frac{c}{|q|^m} \tag{5.22}$$

for some constant $c > 0$. In order to go further in our estimate, we need the following result.

Lemma 5.1. *There exists a constant $C > 0$ such that*

$$\left\| \partial_j H(k)(H(k) - z\mathbb{1})^{-1} \right\|_{\mathcal{B}(\mathcal{H}_\mathrm{f})} \le \frac{C}{|q|^m}$$

uniformly in $z \in \Lambda(k)$, for any $k \in \mathring{U}$.

Remark 5.2. Notice that the operator $\partial_j H(k)(H(k) - z\mathbb{1})^{-1}$ is indeed a bounded operator on $\mathcal{H}_\mathrm{f}$. This is because the range of the resolvent $(H(k) - z\mathbb{1})^{-1}$ is the domain $\mathcal{D} = W^{2,2}(\mathbb{T}^2_Y)$ of $H(k)$, and $k \mapsto H(k)$ is strongly differentiable, so that $\partial_j H(k)$ is well-defined on $\mathcal{D}$. ♢

Proof of Lemma 5.1. We recall [41, Chap. XII, Problem 11] that, if H_0 is a self-adjoint operator and V, W are symmetric, then

$$W << H_0 \text{ and } V << H_0 \quad \Longrightarrow \quad W << H_0 + V, \tag{5.23}$$

where the notation $B << A$ means that B is A-bounded with relative bound zero. Since $\mathrm{i}\partial/\partial y_j << -\Delta$ and $V_\Gamma << -\Delta$ by Assumption 5.1, by iterating (5.23) we obtain

$$\mathrm{i}\frac{\partial}{\partial y_j} << -\Delta + 2\mathrm{i}k \cdot \nabla_y + |k|^2 \mathbb{1} + V_\Gamma = H(k),$$

so that $D_j(k) << H(k)$. By definition of relative boundedness, this means that for any $a > 0$ there exists $b > 0$ such that

$$\|D_j(k)\psi\|^2 \le a^2 \|H(k)\psi\|^2 + b^2 \|\psi\|^2$$

for any ψ in the domain of $H(k)$.

Fix $a > 0$. Then, by [2, Lemma 2.40 and Eqn. (2.110)], if $z_0 = \mathrm{i}b/a$ one has

$$\begin{aligned} \|D_j(k)(H(k) - z\mathbb{1})^{-1}\|_{\mathcal{B}(\mathcal{H}_\mathrm{f})} &\le \left\| D_j(k)\,(H(k) - z_0\mathbb{1})^{-1} \right\|_{\mathcal{B}(\mathcal{H}_\mathrm{f})} + \\ &+ |z - z_0| \left\| D_j(k)\,(H(k) - z_0\mathbb{1})^{-1} \right\|_{\mathcal{B}(\mathcal{H}_\mathrm{f})} \left\| (H(k) - z\mathbb{1})^{-1} \right\|_{\mathcal{B}(\mathcal{H}_\mathrm{f})} \le \\ &\le a + |z - z_0|\; a\,\frac{c}{|q|^m} \end{aligned}$$

where we have used also Equation (5.22). As z varies in the circle $\Lambda(k)$, whose radius is proportional to $|q|^m \ll 1$, we can estimate

$$|z - z_0| \le \frac{b}{a} + 1 \quad \text{for every } z \in \Lambda(k), \text{ uniformly in } k \in \mathring{U}.$$

As a consequence, there exists a constant $C > 0$ such that

$$\left\| D_j(k)(H(k) - z\mathbb{1})^{-1} \right\|_{\mathcal{B}(\mathcal{H}_f)} \le a + c\frac{a+b}{|q|^m} \le \frac{C}{|q|^m},$$

yielding the claim. □

Plugging the result of this Lemma and Equation (5.22) into (5.21), and taking into account the fact that the length of $\Lambda(k)$ is proportional to $|q|^m$, we obtain that

$$\left\| \partial_j P_+(k) \right\|_{\mathcal{B}(\mathcal{H}_f)} \le \frac{C_1}{|q|^m}.$$

The second derivatives of $P_+(k)$ can be computed similarly, again by means of the Riesz formula (5.21) and taking into account Remark 5.2: we obtain

$$\begin{aligned}\partial^2_{j,\ell} P_+(k) = \frac{\mathrm{i}}{2\pi} \oint_{\Lambda(k)} \mathrm{d}z \, \Big[&(H(k) - z\mathbb{1})^{-1} \left(\partial_j H(k) (H(k) - z\mathbb{1})^{-1} \right) \cdot \\ &\cdot \left(\partial_\ell H(k)(H(k) - z\mathbb{1})^{-1} \right) + (j \leftrightarrow \ell) + \\ &- (H(k) - z\mathbb{1})^{-1} \partial^2_{j,\ell} H(k)(H(k) - z\mathbb{1})^{-1} \Big].\end{aligned}$$

Notice that $\partial^2_{j,\ell} H(k) = \delta_{j,\ell} \mathbb{1}_{\mathcal{H}_f}$, so that the last term in the above sum is easily estimated by $|q|^{-m}$. Again by (5.22) and Lemma 5.1 we obtain that the first two terms are bounded by a constant multiple of $|q|^{-2m}$. We conclude that

$$\left\| \partial^2_{j,\ell} P_+(k) \right\|_{\mathcal{B}(\mathcal{H}_f)} \le \frac{C_2}{|q|^{2m}},$$

uniformly in $k \in \mathring{U}$. □

From the above estimates on the derivatives of $P_+(k)$, we can deduce analogous estimates for the derivatives of the Bloch function $u_+(k)$.

Proposition 5.3. *Let $\{P_+(k)\}_{k \in \mathring{U}}$ and $m \in \{1,2\}$ be as in the hypotheses of Proposition 5.2. There exists a function $k \mapsto u_+(k) \in \mathcal{H}_f$ such that $P_+(k)u_+(k) = u_+(k)$ and, for all choices of multi-indices $I \in \{1,2\}^N$, $N \in \mathbb{N}$, there exists a constant $C'_N > 0$ such that*

$$\left\| \partial^N_I u_+(k) \right\|_{\mathcal{H}_f} \le \frac{C'_N}{|q|^{Nm}} \qquad \text{for all } k = k_0 + q, \quad 0 < |q| < r. \tag{5.24}$$

Proof. Again we will prove this statement only for $N \le 2$, the general case being completely analogous. Fix any point $k_* \in \mathring{U}$ and $\delta < 1$: then, by continuity of the map $k \mapsto P_+(k)$ away from k_0, there exists a neighbourhood $U_* \ni k_*$ such that $\|P_+(k) - P_+(k_*)\|_{\mathcal{B}(\mathcal{H}_f)} \le \delta < 1$ for all $k \in U_*$. The Kato-Nagy formula (3.7) then provides a unitary operator $W(k)$ which intertwines $P_+(k_*)$ and $P_+(k)$, in the sense that

$P_+(k) = W(k)P_+(k_*)W(k)^{-1}$. Choose any $u_* \in \operatorname{Ran} P_+(k_*)$ with $\|u_*\|_{\mathcal{H}_f} = 1$. Then, by setting $u_+(k) := W(k)u_*$ one obtains a unit vector in $\operatorname{Ran} P_+(k)$, and moreover

$$\left\|\partial_I^N u_+(k)\right\|_{\mathcal{H}_f} \le \left\|\partial_I^N W(k)\right\|_{\mathcal{B}(\mathcal{H}_f)}.$$

Hence, if we prove that the Kato-Nagy unitary W satisfies estimates of the form (5.20), we can deduce that also (5.24) holds.

Set $Q(k) := (P_+(k) - P_+(k_*))^2$, and notice that by hypothesis $\|Q(k)\| \le \delta^2$. Recall that the Kato-Nagy unitary is given by the formula

$$W(k) = G(Q(k))\,(P_+(k)P_+(k_*) + (\mathbb{1} - P_+(k))(\mathbb{1} - P_+(k_*))),$$

where $G(Q(k))$ is the function $G(z) := (1-z)^{-1/2}$ evaluated on the self-adjoint operator $Q(k)$ by functional calculus. The function G admits a power series expansion

$$G(z) = \sum_{n=0}^{\infty} g_n z^n$$

which is absolutely convergent and term-by-term differentiable for $|z| \le \delta < 1$ (compare (3.8)).

Differentiating the above expression for $W(k)$ with the use of the Leibniz rule for bounded-operator-valued functions, we obtain

$$\begin{aligned}\partial_j W(k) = {} & G(Q(k))\left(\partial_j P_+(k)\right)(2P_+(k_*) - \mathbb{1}) + \\ & + \left(\partial_j G(Q(k))\right)(P_+(k)P_+(k_*) + (\mathbb{1} - P_+(k))(\mathbb{1} - P_+(k_*))).\end{aligned}$$

As for the first summand, it follows from the properties of functional calculus that the term $G(Q(k))$ is bounded in norm by $G(\delta^2)$, while $2P_+(k_*) - \mathbb{1}$ has norm at most equal to 3. In the second summand, instead, the operator $(P_+(k)P_+(k_*) + (\mathbb{1} - P_+(k))(\mathbb{1} - P_+(k_*)))$ is clearly uniformly bounded in U_*, while the norm of $\partial_j G(Q(k))$ can be estimated by

$$\left\|\partial_j G(Q(k))\right\| \le \left(\sum_{n=0}^{\infty} n|g_n|\delta^{2(n-1)}\right)\left\|\partial_j Q(k)\right\|.$$

The term in brackets is finite because also the power series for the derivative of $G(z)$ is absolutely convergent. Moreover, we have that

$$\partial_j Q(k) = (P_+(k) - P_+(k_*))\left(\partial_j P_+(k)\right) + \left(\partial_j P_+(k)\right)(P_+(k) - P_+(k_*))$$

from which we deduce that

$$\left\|\partial_j Q(k)\right\| \le 2\delta \left\|\partial_j P_+(k)\right\|.$$

In conclusion, using (5.20) we obtain that

$$\left\|\partial_j W(k)\right\| \le \text{const} \cdot \left\|\partial_j P_+(k)\right\| \le \frac{C_1'}{|q|^m}.$$

The second derivatives of $W(k)$ can be treated similarly, by using again Leibniz rule. One has

$$\begin{aligned}\partial^2_{j,\ell} W(k) = G(Q(k)) \left(\partial^2_{j,\ell} P_+(k)\right) (2P_+(k_*) - \mathbb{1}) + \\ + \left(\partial_j G(Q(k))\right) (\partial_\ell P_+(k)) (2P_+(k_*) - \mathbb{1}) + (j \leftrightarrow \ell) + \\ + \left(\partial^2_{j,\ell} G(Q(k))\right) (P_+(k) P_+(k_*) + (\mathbb{1} - P_+(k))(\mathbb{1} - P_+(k_*))) .\end{aligned}$$

The terms on the first two lines can be estimated as was done above by a multiple of $|q|^{-2m}$. For the one on the third line, we notice that

$$\begin{aligned}\left\| \partial^2_{j,\ell} G(Q(k)) \right\| \le \left(\sum_{n=0}^{\infty} n(n-1) |g_n| \delta^{2(n-2)} \right) \left\| \partial_j Q(k) \right\| \, \| \partial_\ell Q(k) \| + \\ + \left(\sum_{n=0}^{\infty} n |g_n| \delta^{2(n-1)} \right) \left\| \partial^2_{j,\ell} Q(k) \right\|\end{aligned}$$

where the series in brackets are finite, due to the absolute convergence of the power series for the derivatives of $G(z)$. From the fact that

$$\begin{aligned}\partial^2_{j,\ell} Q(k) = (P_+(k) - P_+(k_*)) \left(\partial^2_{j,\ell} P_+(k)\right) + \left(\partial^2_{j,\ell} P_+(k)\right) (P_+(k) - P_+(k_*)) + \\ + \left(\partial_j P_+(k)\right) (\partial_\ell P_+(k)) + (\partial_\ell P_+(k)) \left(\partial_j P_+(k)\right)\end{aligned}$$

we derive that

$$\left\| \partial^2_{j,\ell} Q(k) \right\| \le 2\delta \left\| \partial^2_{j,\ell} P_+(k) \right\| + 2 \left\| \partial_j P_+(k) \right\| \, \| \partial_\ell P_+(k) \| .$$

Putting all the pieces together, we conclude that

$$\left\| \partial^2_{j,\ell} W(k) \right\| \le \mathrm{const} \cdot \left\| \partial^2_{j,\ell} P_+(k) \right\| + \mathrm{const} \cdot \left\| \partial_j P_+(k) \right\| \, \| \partial_\ell P_+(k) \| \le \frac{C_2'}{|q|^{2m}}$$

as wanted. □

With the help of the estimates (5.24), we can establish the Sobolev regularity of the function $u_{\mathrm{rem}}(k)$.

Proposition 5.4. *Let u_+ be as constructed in Proposition 5.3 and $m \in \{1,2\}$ as in (5.1). Define $u_{\mathrm{rem}}(k) := (\mathbb{1} - \Pi) u_+(k)$. Then*

- *if $m = 1$, one has $u_{\mathrm{rem}} \in W^{s,2}(U; \mathcal{H}_{\mathrm{f}})$ for all $s < 2$;*
- *if $m = 2$, one has $u_{\mathrm{rem}} \in W^{s,2}(U; \mathcal{H}_{\mathrm{f}})$ for all $s < 1$.*

Proof. We begin with the following simple observation: as $P_+(k)$ is a subprojector of $P_*(k)$, we have that

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

and consequently, as $u_+(k)$ is an eigenvector for $P_+(k)$, that

$$u_{\mathrm{rem}}(k) = (P_*(k) - \Pi) u_+(k).$$

From this, we deduce that

$$\partial_j u_{\mathrm{rem}}(k) = \partial_j P_*(k)\, u_+(k) + (P_*(k) - \Pi)\, \partial_j u_+(k).$$

The first summand is bounded in norm, because $P_*(k)$ is smooth in k and $u_+(k)$ has unit norm. As for the second summand, we know by (5.24) that

$$\left\| \partial_j u_+(k) \right\| \leq \frac{C_1'}{|q|^m}.$$

Moreover, by the smoothness of the map $k \mapsto P_*(k)$ and the definition of $\Pi = P_*(k_0)$, we deduce the Lipschitz estimate

$$\|P_*(k) - \Pi\| \leq L|q| \tag{5.25}$$

for some constant $L > 0$. In conclusion, we get that

$$\left\| \partial_j u_{\mathrm{rem}}(k) \right\| \leq \mathrm{const} \cdot |q|^{-m+1}.$$

Thus, if $m = 1$, then $\partial_j u_{\mathrm{rem}}$ is bounded, and hence the function u_{rem} is in $W^{1,\infty}(U; \mathcal{H}_{\mathrm{f}})$. Instead, if $m = 2$, then we can deduce that u_{rem} is in $W^{1,p}(U; \mathcal{H}_{\mathrm{f}})$ for all $p < 2$. Denoting by $\left\{ F^s_{p,q} \right\}$ the scale of Triebel-Lizorkin spaces (see *e.g.* [43]) one has that $W^{1,p} = F^1_{p,p} \subseteq F^1_{p,\infty}$ is continuously embedded in $F^s_{2,2} = W^{s,2}$ for $s = 1 - d(1/p - 1/2)$, in view of [43, Theorem 2.2.3]. Thus, up to a continuous embedding, u_{rem} is in $W^{s,2}(U; \mathcal{H}_{\mathrm{f}})$ for every $s < 1$, yielding the claim for $m = 2$.

As for the second derivative

$$\partial^2_{j,\ell} u_{\mathrm{rem}}(k) = \partial^2_{j,\ell} P_*(k)\, u_+(k) + \left\{ \partial_j P_*(k)\, \partial_\ell u_+(k) + (j \leftrightarrow \ell) \right\} + (P_*(k) - \Pi) \partial^2_{j,\ell} u_+(k),$$

we get that the first term is again bounded; the terms in brackets can be estimated by (5.24) with a multiple of $|q|^{-m}$; and the last summand, again by (5.24) and the Lipschitz estimate (5.25), is bounded in norm by a multiple of $|q|^{-2m+1}$. For $m = 1$, these two powers of $|q|$ coincide, and we conclude that u_{rem} is in $W^{2,p}(U; \mathcal{H}_{\mathrm{f}})$ for all $p < 2$. Again by the interpolation methods of [43, Theorem 2.2.3], we deduce that up to a continuous embedding u_{rem} is in $W^{s,2}(U; \mathcal{H}_{\mathrm{f}})$ for all $s < 2$, when $m = 1$. □

The above result allows us to finally conclude the proof of Theorem 5.2. Indeed, by the considerations at the beginning of this Subsection (see Equation (5.19)) we have that

$$|X|^s (w_U - w_{\mathrm{eff}}) \in L^2(\mathbb{R}^2) \qquad \begin{cases} \text{if } m = 1, \text{ for all } 0 \leq s < 2 \\ \text{if } m = 2, \text{ for all } 0 \leq s < 1 \end{cases}$$

which is exactly the statement of Theorem 5.2.

A Distributional Berry curvature for eigenvalue intersections

Is there a way to define the Berry curvature also for singular families of projectors, *i. e.* in presence of an eigenvalue intersection? Strictly speaking, notions like "connection" and "curvature" make sense only in the case of smooth vector bundles, as they are defined through differential forms. The eigenspace bundle for an eigenvalue intersection, on the other hand, is singular at the intersection point $q = 0$ – see for example (3.13). Thus, in order to define a curvature also in the latter case, we have to "pay a toll": this amounts to using differential forms intepreted in a *distributional sense.*

We make this last statement more rigorous, at least for the canonical families of projectors presented in Section 3.2. We want to recover the Berry curvature for eigenvalue intersections from its analogue for avoided crossings, defining for all test functions $f \in C_0^\infty(U)$

$$\omega_{n,\pm}[f] := \lim_{\mu\downarrow 0} \omega^\mu_{n,\pm}[f] + \lim_{\mu\uparrow 0} \omega^\mu_{n,\pm}[f], \tag{A.1}$$

where $T[f]$ denotes the action of the distribution T on the test function f.

The distributions on the right-hand side of (A.1) are the ones obtained from the Berry curvature (compare Equation (3.27))

$$\omega^\mu_{n,\pm}(q) = \pm\frac{n}{2}\left[\partial_{|q|}\left(\frac{\mu}{\sqrt{|q|^2+\mu^2}}\right)\mathrm{d}|q|\wedge \mathrm{d}\theta_q - \partial_\mu\left(\frac{\mu}{\sqrt{|q|^2+\mu^2}}\right)\mathrm{d}\theta_q\wedge \mathrm{d}\mu\right].$$

Explicitly, when these act on a μ-independent test function, the term containing $\mathrm{d}\mu$ does not contribute, yielding to

$$\omega^\mu_{n,\pm}[f] = \pm\frac{n}{2}\int_U \partial_{|q|}\left(\frac{\mu}{\sqrt{|q|^2+\mu^2}}\right) f(|q|,\theta_q)\,\mathrm{d}|q|\wedge \mathrm{d}\theta_q. \tag{A.2}$$

The right-hand side of this equality changes sign according to whether μ is positive or negative, but still the two limits for $\mu\downarrow 0$ and $\mu\uparrow 0$ in (A.1) give the same result, because the change in sign is compensated by the different orientation of the "top" and "bottom" caps of the cylinder $\mathcal{C}$, that are approaching the plane $\mu = 0$ (compare Figure 1). Hence,

$$\omega_{n,\pm}[f] = \lim_{\mu\downarrow 0} \pm n \int_U \partial_{|q|}\left(\frac{\mu}{\sqrt{|q|^2+\mu^2}}\right) f(|q|,\theta_q)\,\mathrm{d}|q|\wedge \mathrm{d}\theta_q.$$

We may assume that f is a radial-symmetric test function[1], *i. e.* $f = f(|q|)$. We thus have

$$\frac{1}{2\pi}\,\omega^{\mu}_{n,\pm}[f] = \pm n \int_0^r \mathrm{d}|q|\,\partial_{|q|}\left(\frac{\mu}{\sqrt{|q|^2+\mu^2}}\right) f(|q|). \tag{A.3}$$

Notice that

$$\partial_{|q|}\left(\frac{\mu}{\sqrt{|q|^2+\mu^2}}\right) = -\frac{1}{\mu}\,\frac{|q|/\mu}{\left[1+(|q|/\mu)^2\right]^{3/2}} = j_\mu(-|q|),$$

where

$$j_\mu(|q|) = \frac{1}{\mu}\,j\left(\frac{|q|}{\mu}\right), \quad j(|q|) := \frac{|q|}{\left(1+|q|^2\right)^{3/2}}.$$

Consider for a moment the variable $|q|$ as varying on the whole real axis, and define

$$J(|q|) := -j(|q|)\chi_{(-\infty,0]}(|q|)$$

where $\chi_{(-\infty,0]}$ is the characteristic function of the negative axis. The function J then satisfies

$$J(|q|) \geq 0 \text{ for all } |q| \in \mathbb{R}, \quad \text{and} \quad \int_{-\infty}^{+\infty} \mathrm{d}|q|\,J(|q|) = 1.$$

These two properties allow one to construct the so-called *approximate identities* (compare [46, Theorem 1.18]), namely the functions

$$J_\mu(|q|) := \frac{1}{\mu}\,j\left(\frac{|q|}{\mu}\right),$$

which are known to satisfy

---

[1] Indeed, if $\widetilde{f}$ is in $C_0^\infty(U)$ and

$$T^{\mu}_{n,\pm}(|q|) := \pm n\,\partial_{|q|}\left(\frac{\mu}{\sqrt{|q|^2+\mu^2}}\right),$$

then we have

$$\omega^{\mu}_{n,\pm}[\widetilde{f}] = \int_U T^{\mu}_{n,\pm}(|q|)\widetilde{f}(|q|,\theta_q)\,\mathrm{d}|q| \wedge \mathrm{d}\theta_q = \int_0^r \mathrm{d}|q|\,T^{\mu}_{n,\pm}(|q|)\int_0^{2\pi} \mathrm{d}\theta_q \widetilde{f}(|q|,\theta_q).$$

Set

$$f(|q|) := \int_0^{2\pi} \mathrm{d}\theta_q \widetilde{f}(|q|,\theta_q).$$

Then f is a C^∞ function, because $\widetilde{f}$ is smooth and integration is performed on the compact set S^1; moreover, the support of f is contained in a ball of radius $\widetilde{r}$ around $q = 0$, where

$$\widetilde{r} := \max_{q \in \operatorname{supp}\widetilde{f}} |q|.$$

By definition $\widetilde{r} < r$, because $\widetilde{f}$ has compact support in U; hence also f is compactly supported in the same ball.

$$\lim_{\mu\downarrow 0}(J_\mu * F)(t) = \lim_{\mu\downarrow 0}\int_{-\infty}^{+\infty} \mathrm{d}|q|\, J_\mu(t-|q|)F(|q|) = F(t)$$

for every compactly-supported function F and all $t \in \mathbb{R}$. Applying this to the function $F(|q|) = f(|q|)\chi_{(0,+\infty)}(|q|)$ (*i. e.* extending f to zero for negative $|q|$), we obtain that

$$\begin{aligned} f(0) = F(0) &= \lim_{\mu\downarrow 0}\int_{-\infty}^{+\infty} \mathrm{d}|q|\, J_\mu(-|q|)F(|q|) = \\ &= \lim_{\mu\downarrow 0}\int_{-\infty}^{+\infty} \mathrm{d}|q| \left(-\frac{1}{\mu} j\left(-\frac{|q|}{\mu}\right)\chi_{(-\infty,0]}\left(-\frac{|q|}{\mu}\right)\right)\chi_{[0,+\infty)}(|q|)f(|q|) = \\ &= -\lim_{\mu\downarrow 0}\int_{0}^{+\infty} j_\mu(-|q|)f(|q|). \end{aligned}$$

In the last of the above equalities we have used the fact that as $\mu > 0$

$$\chi_{(-\infty,0]}\left(-\frac{|q|}{\mu}\right) = \chi_{(-\infty,0]}(-|q|) = \chi_{[0,+\infty)}(|q|).$$

Now it suffices to observe that on the right-hand side of (A.3) we have the expression

$$\int_0^r \mathrm{d}|q|\, \partial_{|q|}\left(\frac{\mu}{\sqrt{|q|^2+\mu^2}}\right) f(|q|) = \int_0^{+\infty} \mathrm{d}|q|\, j_\mu(-|q|)f(|q|)$$

because, as f has compact support in U, integration on $[0,r]$ or on $[0,+\infty)$ in the $|q|$-variable yields the same result. When μ approaches 0 from above, we thus obtain

$$\frac{1}{2\pi}\omega_{n,\pm}[f] = \lim_{\mu\downarrow 0}\frac{1}{2\pi}\omega^{\mu}_{n,\pm}[f] = \mp n f(0).$$

In conclusion, as a distribution $\omega_{n,\pm}$ is a multiple of the Dirac delta “function”:

$$\frac{1}{2\pi}\omega_{n,\pm} = \mp n\delta_0.$$

In other words, the curvature of the (singular, hence ill-defined!) eigenspace “bundle” for an eigenvalue intersection is all concentrated at the intersection point $q = 0$. Moreover, we can define a Chern number for this eigenspace “bundle” $\mathcal{P}^0_{n,\pm}$, with abuse of notation, by posing

$$\mathrm{ch}_1\left(\mathcal{P}^0_{n,\pm}\right) = \frac{1}{2\pi}\int_U \omega_{n,\pm} = \mp n\int_U \delta_0 = \mp n.$$

References

1. AGRACHEV, A.A. : Space of Symmetric Operators with Multiple Ground States, (Russian) *Funktsional. Anal. i Prilozhen.* **45** (2011), no. 4, 1–15. Translation in *Funct. Anal. Appl.* **45** (2011), no. 4, 241—251.
2. AMREIN, W.O. : Hilbert space methods in Quantum Mechanics. EPFL Press, Lausanne, 2009.

3. BELLISSARD, J.; SCHULZ-BALDES, H.; VAN ELST, A. : The Non Commutative Geometry of the Quantum Hall Effect, *J. Math. Phys.* **35** (1994), 5373–5471.
4. BENA, C.; MONTAMBAUX, G. : Remarks on the tight-binding model of graphene, *New Journal of Physics* **11** (2009), 095003.
5. BROUDER, CH.; PANATI, G.; CALANDRA, M.; MOUROUGANE,CH.; MARZARI, N.: Exponential localization of Wannier functions in insulators, *Phys. Rev. Lett.* **98** (2007), 046402.
6. CASTRO NETO, A.H.; GUINEA, F.; PERES, N.M.R.; NOVOSELOV, K.S.; GEIM, A.K. : The electronic properties of graphene, *Rev. Mod. Phys.* **81** (2009), 109–162.
7. DES CLOIZEAUX, J. : Energy bands and projection operators in a crystal: Analytic and asymptotic properties, *Phys. Rev.* **135** (1964), A685–A697.
8. DES CLOIZEAUX, J. : Analytical properties of n-dimensional energy bands and Wannier functions, *Phys. Rev.* **135** (1964), A698–A707.
9. DUBROVIN, B.A.; NOVIKOV, S.P.; FOMENKO, A.T. : Modern Geometry – Methods and Applications. Part II: The Geometry and Topology of Manifolds. No. 93 in Graduate Texts in Mathematics. Springer-Verlag, New York, 1985.
10. FERMANIAN KAMMERER, C.; LASSER, C. : Wigner measures and codimension two crossings, *J. Math. Phys.* **44** (2003), 507–527.
11. FEFFERMAN, C.L.; WEINSTEIN, M.I. : Waves in Honeycomb Structures, preprint arXiv:1212.6684 (2012).
12. GOERBIG, M.O. : Electronic properties of graphene in a strong magnetic field, preprint arXiv:1004.3396v4 (2011).
13. GRAF, G.M. : Aspects of the Integer Quantum Hall Effect, *Proceedings of Symposia in Pure Mathematics* **76** (2007), 429–442.
14. HAGEDORN, G.A. : Classification and normal forms for quantum mechanical eigenvalue crossings, *Astérisque* **210** (1992), 115–134.
15. HAGEDORN, G.A. : Classification and normal forms for avoided crossings of quantum mechanical energy levels, *Jour. Phys. A* **31** (1998), 369–383.
16. HAINZL, C.; LEWIN, M.; SPARBER, C. : Ground state properties of graphene in Hartree-Fock theory, *J. Math. Phys.* **53** (2012), 095220.
17. HALDANE, F.D.M. : Model for a Quantum Hall effect without Landau levels: condensed-matter realization of the "parity anomaly", *Phys. Rev. Lett.* **61** (1988), 2017.
18. HASAN, M.Z.; KANE, C.L. : Colloquium: Topological Insulators, *Rev. Mod. Phys.* **82** (2010), 3045–3067.
19. KANE, C.L.; MELE, E.J. : $\mathbb{Z}_2$ Topological Order and the Quantum Spin Hall Effect, *Phys. Rev. Lett.* **95** (2005), 146802.
20. KATO, T. : Perturbation theory for linear operators. Springer, Berlin, 1966.
21. KING-SMITH, R.D. ; VANDERBILT, D. : Theory of polarization of crystalline solids, *Phys. Rev.* **B 47** (1993), 1651–1654.
22. KOHN, W. : Analytic Properties of Bloch Waves and Wannier Functions, *Phys. Rev.* **115** (1959), 809.
23. KUCHMENT, P. : Floquet Theory for Partial Differential Equations. Operator Theory: Advances and Applications, vol. 60. Birkhäuser, 1993.
24. LEE, J.M. : Introduction to Smooth Manifolds. No. 218 in Graduate Text in Mathematics. Springer, 2003.
25. LEPORI, L.; MUSSARDO, G.; TROMBETTONI, A. : $(3+1)$ Massive Dirac Fermions with Ultracold Atoms in Optical Lattices, *EPL (Europhysics Letters)* **92** (2010), 50003.
26. LUKE, Y.L. : Integrals of Bessel Functions. McGraw-Hill, 1962.
27. MC CANN, E.; FALKO, V. I. : Landau-level degeneracy and quantum Hall effect in a graphite bilayer, *Phys. Rev. Letters* **96** (2006), 086805.
28. MARZARI, N.; MOSTOFI, A.A.; YATES, J.R.; SOUZA, I.; VANDERBILT, D. : Maximally localized Wannier functions: Theory and applications, *Rev. Mod. Phys.* **84** (2012), 1419.
29. MARZARI, N.; VANDERBILT, D. : Maximally localized generalized Wannier functions for composite energy bands, *Phys. Rev. B* **56** (1997), 12847–12865.
30. MILNOR, J.W.; STASHEFF, J.D. : Characteristic Classes. No. 76 in Annals of Mathematical Studies. Princeton Univesity Press, 1974.
31. MIN, H.; MACDONALD, A.H. : Chiral decomposition in the electronic structure of graphene multilayers, *Phys. Rev. B* **77** (2008), 155416.
32. NENCIU, G. : Existence of the exponentially localized Wannier functions, *Commun. Math. Phys.* **91** (1983), 81–85.

33. NENCIU, G. : Dynamics of band electrons in electric and magnetic fields: Rigorous justification of the effective Hamiltonians, *Rev. Mod. Phys.* **63** (1991), 91–127.
34. NOVOSELOV, K. S.; MCCANN, E.; MOROZOV, S.V.; FALKO, V.I.; KATSNELSON, M.I.; GEIM, A.K.; SCHEDIN, F.; JIANG, D. : Unconventional quantum Hall effect and Berry's phase of 2π in bilayer graphene, *Nature Phys.* **2** (2006), 177.
35. PANATI, G.; PISANTE, A. : Bloch bundles, Marzari-Vanderbilt functional and maximally localized Wannier functions, *Commun. Math. Phys.* **322**, Issue 3 (2013), 835-875.
36. PANATI, G.; SPARBER, C.; TEUFEL, S. : Geometric currents in piezoelectricity, *Arch. Rat. Mech. Anal.* **91** (2009), 387–422.
37. PANATI, G.; SPOHN, H.; TEUFEL, S. : Effective dynamics for Bloch electrons: Peierls substitution and beyond, *Commun. Math. Phys.* **242** (2003), 547–578.
38. PANATI, G.: Triviality of Bloch and Bloch-Dirac bundles, *Ann. Henri Poincaré* **8** (2007), 995–1011.
39. PARK, C.-H.; MARZARI, N. : Berry phase and pseudospin winding number in bilayer graphene, *Phys. Rev. B* **84** (2011), 1 – 5.
40. REED, M.; SIMON, B. : Methods of Modern Mathematical Physics, vol. I: Functional Analysis, revised and enlarged edition. Academic Press, 1980.
41. REED, M.; SIMON, B. : Methods of Modern Mathematical Physics, vol. IV: Analysis of Operators. Academic Press, 1978.
42. RESTA, R. : Theory of the electric polarization in crystals, *Ferroelectrics* **136** (1992), 51–75.
43. RUNST, T.; SICKEL, W. : Sobolev Spaces of Fractional Order, Nemytskij Operators, and Nonlinear Partial Differential Equations. Walter de Gruyter, 1996.
44. SOLUYANOV, A.A.; VANDERBILT, D. : Wannier representation of $\mathbb{Z}_2$ topological insulators, *Phys. Rev. B* **85** (2012), 115415.
45. STEENROD, N. : The Topology of Fibre Bundles. Princeton University Press, 1960.
46. STEIN, E.M.; WEISS, G. : Introduction to Fourier Analysis on Euclidean Spaces. Princeton University Press, 1971.
47. TARRUEL, L.; GREIF, D.; UEHLINGER, TH.; JOTZU, G.; ESSLINGER, T. : Creating, moving and merging Dirac points with a Fermi gas in a tunable honeycomb lattice, *Nature* **483** (2012), 302–305.
48. THOULESS D.J.; KOHMOTO, M.; NIGHTINGALE, M.P.; DE NIJS, M. : Quantized Hall conductance in a two-dimensional periodic potential, *Phys. Rev. Lett.* **49** (1982), 405–408.
49. VOISIN, C. : Hodge Theory and Complex Algebraic Geometry I. No. 76 in Cambridge Studies in Advanced Mathematics. Cambridge University Press, 2002.
50. VON NEUMANN, J.; WIGNER, E. : On the behaviour of eigenvalues in adiabatic processes, *Phys. Z.* **30** (1929), 467. Republished in: Hettema, H. (ed.), Quantum Chemistry: Classic Scientific Papers. World Scientific Series in 20th Century Chemistry, vol. 8. World Scientific, 2000.
51. WALLACE, P.R. : The band theory of graphite, *Phys. Rev.* **71** (1947), 622–634.
52. WANNIER, G.H. : The structure of electronic excitation levels in insulating crystals, *Phys. Rev.* **52** (1937), 191–197.
53. XIAO, D.; CHANG, M.-C.; NIU, Q. : Berry phase effects on electronic properties, *Rev. Mod. Phys.* **82** (2010), 1959–2007.
54. ZHU, S.L.; WANG, B.; DUAN, L.M. : Simulation and detection of Dirac fermions with cold atoms in an optical lattice, *Phys. Rev. Lett.* **98** (2007), 260402.

Part II
Topological Insulators

We reproduce here the content of the paper

FIORENZA, D.; MONACO, D.; PANATI, G. : Construction of real-valued localized composite Wannier functions for insulators, *Ann. Henri Poincaré* (2015), DOI 10.1007/s00023-015-0400-6.

and the preprint

FIORENZA, D.; MONACO, D.; PANATI, G. : $\mathbb{Z}_2$ invariants of topological insulators as geometric obstructions, available at arXiv:1408.1030.

Construction of real-valued localized composite Wannier functions for insulators

Domenico Fiorenza, Domenico Monaco, and Gianluca Panati

Abstract We consider a real periodic Schrödinger operator and a physically relevant family of $m \geq 1$ Bloch bands, separated by a gap from the rest of the spectrum, and we investigate the localization properties of the corresponding composite Wannier functions. To this aim, we show that in dimension $d \leq 3$ there exists a global frame consisting of smooth quasi-Bloch functions which are both periodic and time-reversal symmetric. Aiming to applications in computational physics, we provide a constructive algorithm to obtain such Bloch frame. The construction yields the existence of a basis of composite Wannier functions which are real-valued and almost-exponentially localized.
The proof of the main result exploits only the fundamental symmetries of the projector on the relevant bands, allowing applications, beyond the model specified above, to a broad range of gapped periodic quantum systems with a time-reversal symmetry of bosonic type.

Key words: Periodic Schrödinger operators, Wannier functions, Bloch frames.

1 Introduction

The existence of an orthonormal basis of well-localized Wannier functions is a crucial issue in solid-state physics [30]. Indeed, such a basis is the key tool to obtain effective tight-binding models for a linear or non-linear Schrödinger dynamics [41, 42, 20, 21, 53], it allows computational methods whose cost scales linearly with the size of the confining box [13], it is useful in the rigorous analysis of perturbed

Domenico Fiorenza
Dipartimento di Matematica, "La Sapienza" Università di Roma, Piazzale Aldo Moro 2, 00185 Rome, Italy
e-mail: fiorenza@mat.uniroma1.it

Domenico Monaco
SISSA, Via Bonomea 265, 34136 Trieste, Italy
e-mail: dmonaco@sissa.it

Gianluca Panati
Dipartimento di Matematica, "La Sapienza" Università di Roma, Piazzale Aldo Moro 2, 00185 Rome, Italy
e-mail: panati@mat.uniroma1.it

periodic Hamiltonians [3, 28, 9], and it is crucial in the modern theory of polarization of crystalline solids [46, 26, 39] and in the pioneering research on topological insulators [17, 47, 43, 44, 49, 50]

In the case of a single isolated Bloch band, which does not touch any other Bloch band, the rigorous proof of the existence of exponentially localized Wannier functions goes back to the work of W. Kohn [27], who provided a proof in dimension $d = 1$ for an even potential. The latter assumption was later removed by J. de Cloizeaux [6], who also gave a proof valid for any $d > 1$ under the assumption that the periodic potential is centro-symmetric [5, 6]. The first proof under generic assumptions, again for any $d > 1$, was provided by G. Nenciu [32], and few years later a simpler proof appeared [18].

In real solids, Bloch bands intersect each other. Therefore, as early suggested [1, 6], it is more natural to focus on a family of m Bloch bands which is separated by a gap from the rest of the spectrum, as *e. g.* the family of all the Bloch bands below the Fermi energy in an insulator or a semiconductor. Accordingly, the notion of Bloch function is weakened to that of *quasi-Bloch function* and, correspondingly, one considers *composite Wannier functions* (Definition 2.1). In the multi-band case, the existence of exponentially localized composite Wannier functions is subtle, since it might be topologically obstructed. A proof of existence was provided in [34, 33] for $d = 1$, while a proof in the case $d \leq 3$ required more abstract bundle-theoretic methods [2, 37], both results being valid for any number of bands $m \in \mathbb{N}$. In the 1-dimensional case generalizations to non-periodic gapped systems are also possible [35], as well as extensions to quasi-1-dimensional systems [8].

Beyond the abstract existence results, computational physics strived for an explicit construction. On the one hand, Marzari and Vanderbilt [29] suggested a shift to a variational viewpoint, which is nowadays very popular in computational solid-state physics. They introduced a suitable localization functional, defined on a set of composite Wannier functions, and argued that the corresponding minimizers are expected to be exponentially localized. They also noticed that, for $d = 1$, the minimizers are indeed exponentially localized in view of the relation between the composite Wannier functions and the eigenfunctions of the reduced position operator [25, 35]. For $d > 1$, the exponential localization of the minimizers follows instead from deeper properties of the localization functional [38], if $d \leq 3$ and some technical hypotheses are satisfied. Moreover, there is numerical evidence that the minimizers are *real-valued* functions, but a mathematical proof of this fact is still missing [29, 2].

On the other hand, researchers are also working to obtain an explicit algorithm yielding composite Wannier functions which are both real-valued and well-localized [7]. As a predecessor in this direction, we mention again the result in [18], which provides an explicit proof in the single-band case, *i. e.* for $m = 1$, through the construction of time-reversal symmetric Bloch functions (see below for detailed comments).

In this paper, following the second route, we provide an explicitly constructive algorithm to obtain, for any $d \leq 3$ and $m \in \mathbb{N}$, composite Wannier functions which are *real-valued* and *almost-exponentially localized*, in the sense that they decay faster than the inverse of any polynomial (Theorem 3.2). The latter result follows from a more general theorem (Theorem 3.1), which applies to a broad range of gapped periodic quantum systems with a time-reversal symmetry of *bosonic* (or *even*) type (see Assumption 3.1). Under such assumption, we explicitly construct a smooth frame of eigenfunctions of the relevant projector (*i. e.* quasi-Bloch functions in the application to Schrödinger operators) which are both pseudo-periodic and time-reversal symmetric, in the sense of Definition 3.1. Since the result is proved in a general setting, we foresee possible applications to periodic Pauli or Dirac operators, as well as to tight-binding models as *e. g.* the one proposed by Haldane [15]. Despite of the apparent similarity, the case of systems with *fermionic* (or *odd*) time-reversal symmetry, relevant in the context of topological insulators [16], is radically different, as emphasized in [51, 14, 10], see Remark 3.1.

We conclude the Introduction with few comments about the relation between our constructive algorithm and the proofs of some previous results.
The proof provided by Helffer and Sjöstrand for $m = 1$ and $d \in \mathbb{N}$ [18], is explicitly constructive and yields real-valued Wannier functions. However, the proof has not a direct generalization to the case $m > 1$ for a very subtle reason, which is occasionally overlooked even by experts. We illustrate the crucial difficulty in the simplest case, by considering a unitary matrix $U(k_1) \in \mathcal{U}(\mathbb{C}^m)$ depending continuously on a parameter $k_1 \in \mathbb{T}^1 = \mathbb{R}/2\pi\mathbb{Z}$. When mimicking the proof in [18], one defines (*e. g.* via spectral calculus) the unitary $U(k_1)^{k_2}$, for $k_2 \in [0, 1/2]$, which is well-defined whenever a determination of the complex logarithm has been chosen in such a way that the branch-cut does not touch the (point) spectrum of $U(k_1)$. As $k_1 \in \mathbb{T}^1$ varies, the branch-cut must vary accordingly, and it might happen that the branch-cut for $k_1 = 2\pi$ equals the one for $k_1 = 0$ after a complete wind (or more) in the complex plane. In such eventuality, the rest of the argument fails. In [32], a similar difficulty appears.[1] As far as we know, there is no direct way to circumvent this kind of difficulty. For this reason, in this paper we develop a radically different tecnique.

The paper is organized as follows. In Section 2 we consider a real periodic Schrödinger operator and we show that, for a gapped system as *e. g.* an insulator, the orthogonal projector on the Bloch states up to the gap satisfies some natural properties (Proposition 2.1). Generalizing from the specific example, the abstract version of these properties becomes our starting point, namely Assumption 3.1. In Section 3 we state our main results, and we shortly comment on the structure of the proof, which is the content of Section 4. Finally, a technical result concerning the smoothing of a continuous symmetric Bloch frame to obtain a smooth symmetric Bloch frame, which holds true in any dimension and might be of independent interest, is provided in Section 5.

Acknowledgments. We are indebted to A. Pisante for many useful comments. G.P. is grateful to H. Cornean and G. Nenciu for useful discussions, and to H. Spohn and S. Teufel for stimulating his interest in this problem during the preparation of [40]. We are grateful to the *Institut Henri Poincaré* for the kind hospitality in the framework of the trimester "Variational and Spectral Methods in Quantum Mechanics", organized by M. J. Esteban and M. Lewin.
This project was supported by the National Group for Mathematical Physics (INdAM-GNFM) and from MIUR (Project PRIN 2012).

[1] We cite textually from [32]: *Unfortunately, we have been unable to prove that* $T(\mathbf{z}^{q-1})$ *admits an analytic and periodic logarithm [. . .], and therefore we shall follow a slightly different route.*

2 From Schrödinger operators to covariant families of projectors

The dynamics of a particle in a crystalline solid can be modeled by use of a *periodic Schrödinger operator*

$$H_\Gamma = -\Delta + V_\Gamma \qquad \text{acting in } L^2(\mathbb{R}^d),$$

where the potential V_Γ is periodic with respect to a lattice (called the *Bravais lattice* in the physics literature)

$$\Gamma := \mathrm{Span}_{\mathbb{Z}}\{a_1,\dots,a_d\} \simeq \mathbb{Z}^d \subset \mathbb{R}^d, \qquad \text{with } \{a_1,\dots,a_d\} \text{ a basis in } \mathbb{R}^d.$$

Assuming that

$$V_\Gamma \in L^2_{\mathrm{loc}}(\mathbb{R}^d) \text{ for } d \le 3, \qquad \text{or} \qquad V_\Gamma \in L^p_{\mathrm{loc}}(\mathbb{R}^d) \text{ with } p > d/2 \text{ for } d \ge 4, \tag{2.1}$$

the operator H_Γ is self-adjoint on the domain $H^2(\mathbb{R}^d)$ [45, Theorem XIII.96].

In order to simplify the analysis of such operators, one looks for a convenient representation which (partially) diagonalizes simultaneously both the Hamiltonian and the lattice translations. This is provided by the (*modified*) *Bloch-Floquet transform*, defined on suitable functions $w \in C_0(\mathbb{R}^d) \subset L^2(\mathbb{R}^d)$ as

$$(\mathcal{U}_{\mathrm{BF}}\, w)(k,y) := \frac{1}{|\mathbb{B}|^{1/2}} \sum_{\gamma\in\Gamma} \mathrm{e}^{-\mathrm{i}k\cdot(y+\gamma)}\, w(y+\gamma), \qquad y \in \mathbb{R}^d,\ k \in \mathbb{R}^d. \tag{2.2}$$

Here $\mathbb{B}$ is the fundamental unit cell for the dual lattice $\Gamma^* := \mathrm{Span}_{\mathbb{Z}}\{b_1,\dots,b_d\} \subset \mathbb{R}^d$, determined by the basis $\{b_1,\dots,b_d\}$ which satisfies $b_i \cdot a_j = 2\pi\delta_{ij}$, namely

$$\mathbb{B} := \left\{ k = \sum_{j=1}^d k_j b_j \in \mathbb{R}^d : -1/2 \le k_j \le 1/2 \right\}.$$

From (2.2), one immediately reads the (pseudo-)periodicity properties

$$\begin{aligned} \big(\mathcal{U}_{\mathrm{BF}}\, w\big)(k, y+\gamma) &= \big(\mathcal{U}_{\mathrm{BF}}\, w\big)(k,y) && \text{for all } \gamma \in \Gamma, \\ \big(\mathcal{U}_{\mathrm{BF}}\, w\big)(k+\lambda, y) &= \mathrm{e}^{-\mathrm{i}\lambda\cdot y}\big(\mathcal{U}_{\mathrm{BF}}\, w\big)(k,y) && \text{for all } \lambda \in \Gamma^*. \end{aligned} \tag{2.3}$$

The function $\big(\mathcal{U}_{\mathrm{BF}}\, w\big)(k,\cdot)$, for fixed $k \in \mathbb{R}^d$, is thus periodic, so it can be interpreted as an element in the Hilbert space $\mathcal{H}_{\mathrm{f}} := L^2(\mathbb{T}^d_Y)$, where $\mathbb{T}^d_Y = \mathbb{R}^d/\Gamma$ is the torus obtained by identifying opposite faces of the fundamental unit cell for Γ, given by

$$Y := \left\{ y = \sum_{j=1}^d y_j a_j \in \mathbb{R}^d : -1/2 \le y_j \le 1/2 \right\}.$$

Following [40], we reinterpret (2.3) in order to emphasize the role of covariance with respect to the action of the relevant symmetry group. Setting

$$\big(\tau(\lambda)\psi\big)(y) := \mathrm{e}^{-\mathrm{i}\lambda\cdot y}\psi(y), \qquad \text{for } \psi \in \mathcal{H}_{\mathrm{f}},$$

one obtains a unitary representation $\tau : \Gamma^* \to \mathcal{U}(\mathcal{H}_f)$ of the group of translations by vectors of the dual lattice. One can then argue that $\mathcal{U}_{BF}$ establishes a unitary transformation $\mathcal{U}_{BF} : L^2(\mathbb{R}^d) \to \mathcal{H}_\tau$, where $\mathcal{H}_\tau$ is the Hilbert space

$$\mathcal{H}_\tau := \left\{\phi \in L^2_{\mathrm{loc}}(\mathbb{R}^d, \mathcal{H}_f) : \ \phi(k+\lambda) = \tau(\lambda)\,\phi(k)\ \forall \lambda \in \Gamma^*, \text{ for a.e. } k \in \mathbb{R}^d\right\}$$

equipped with the inner product

$$\langle \phi, \psi \rangle_{\mathcal{H}_\tau} = \int_{\mathbb{B}} \langle \phi(k), \psi(k) \rangle_{\mathcal{H}_f}\, \mathrm{d}k.$$

Moreover, the inverse transformation $\mathcal{U}_{BF}^{-1} : \mathcal{H}_\tau \to L^2(\mathbb{R}^d)$ is explicitely given by

$$\left(\mathcal{U}_{BF}^{-1}\phi\right)(x) = \frac{1}{|\mathbb{B}|^{1/2}} \int_{\mathbb{B}} \mathrm{d}k\, \mathrm{e}^{\mathrm{i}k\cdot x} \phi(k, x).$$

In view of the identification

$$\mathcal{H}_\tau \simeq \int_{\mathbb{B}}^{\oplus} \mathrm{d}k\, \mathcal{H}_f,$$

we see that the Schrödinger operator H_Γ becomes a fibered operator in the Bloch-Floquet representation, *i. e.*

$$\mathcal{U}_{BF}\, H_\Gamma\, \mathcal{U}_{BF}^{-1} = \int_{\mathbb{B}}^{\oplus} \mathrm{d}k\, H(k), \qquad \text{where} \qquad H(k) = \left(-\mathrm{i}\nabla_y + k\right)^2 + V_\Gamma(y).$$

The fiber operator $H(k)$, $k \in \mathbb{R}^d$, acts on the k-independent domain $H^2(\mathbb{T}^d_Y) \subset \mathcal{H}_f$, where it defines a self-adjoint operator. Moreover, it has compact resolvent, and thus pure point spectrum. We label its eigenvalues, accumulating at infinity, in increasing order, as $E_0(k) \le E_1(k) \le \cdots \le E_n(k) \le E_{n+1}(k) \le \cdots$, counting multiplicities. The functions $\mathbb{R}^d \ni k \mapsto E_n(k) \in \mathbb{R}$ are called *Bloch bands*. Since the fiber operator $H(k)$ is τ*-covariant*, in the sense that

$$H(k+\lambda) = \tau(\lambda)^{-1}\, H(k)\, \tau(\lambda), \qquad \lambda \in \Gamma^*,$$

Bloch bands are actually periodic functions of $k \in \mathbb{R}^d$, *i. e.* $E_n(k+\lambda) = E_n(k)$ for all $\lambda \in \Gamma^*$, and hence are determined by the values attained at points $k \in \mathbb{B}$.

A solution $u_n(k)$ to the eigenvalue problem

$$H(k)\, u_n(k) = E_n(k)\, u_n(k), \qquad u_n(k) \in \mathcal{H}_f, \qquad \|u_n(k)\|_{\mathcal{H}_f} = 1,$$

constitutes the (periodic part of the) n*-th Bloch function*, in the physics terminology. Assuming that, for fixed $n \in \mathbb{N}$, the eigenvalue $E_n(k)$ is non-degenerate for all $k \in \mathbb{R}^d$, the function $u_n : y \mapsto u_n(k, y)$ is determined up to the choice of a k-dependent phase, called the *Bloch gauge*.

By definition, the **Wannier function** w_n corresponding to the Bloch function $u_n \in \mathcal{H}_\tau$ is the preimage, via Bloch-Floquet transform, of the Bloch function, *i. e.*

$$w_n(x) := \left(\mathcal{U}_{\mathrm{BF}}^{-1} u_n\right)(x) = \frac{1}{|\mathbb{B}|^{1/2}} \int_{\mathbb{B}} \mathrm{d}k\, \mathrm{e}^{\mathrm{i}k\cdot x} u_n(k,x). \tag{2.4}$$

Localization (*i. e.* decay at infinity) of the Wannier function $w = w_n$ and smoothness of the associated Bloch function $u = u_n$ are related by the following statement, that can be checked easily from the definition (2.2) of the Bloch-Floquet transform (see [38, Sec. 2] for details):

$$\begin{aligned} w \in H^s(\mathbb{R}^d),\ s \in \mathbb{N} &\Longleftrightarrow u \in L^2(\mathbb{B}, H^s(\mathbb{T}_Y^d)), \\ \langle x\rangle^r w \in L^2(\mathbb{R}^d),\ r \in \mathbb{N} &\Longleftrightarrow u \in \mathcal{H}_\tau \cap H^r_{\mathrm{loc}}(\mathbb{R}^d, \mathcal{H}_{\mathrm{f}}), \end{aligned} \tag{2.5}$$

where we used the Japanese bracket notation $\langle x\rangle = (1 + |x^2|)^{1/2}$. A Wannier function such that $\langle x\rangle^r w \in L^2(\mathbb{R}^d)$ for all $r \in \mathbb{N}$ will be called **almost-exponentially localized**.

As mentioned in the Introduction, to deal with real solids, where generically the Bloch bands intersect each other, a multi-band theory becomes necessary. Many of the above statements can be formulated even in the case when more than one Bloch band is considered. Let $\sigma_*(k)$ be the set $\{E_i(k) : n \le i \le n + m - 1\}$, $k \in \mathbb{B}$, corresponding to a family of m Bloch bands. Usually, in the applications, $\sigma_*(k)$ consists of some Bloch bands which are physically relevant, as *e. g.* the bands below the Fermi energy in insulators and semiconductors. Assume the following *gap condition*:

$$\inf_{k\in\mathbb{B}} \operatorname{dist}\big(\sigma_*(k), \sigma(H(k)) \setminus \sigma_*(k)\big) > 0. \tag{2.6}$$

The relevant object to consider in this case is then the *spectral projector* $P_*(k)$ on the set $\sigma_*(k)$, which in the physics literature reads

$$P_*(k) = \sum_{n\in\mathcal{I}_*} |u_n(k)\rangle \langle u_n(k)|,$$

where the sum runs over all the bands in the relevant family, *i. e.* over the set $\mathcal{I}_* = \{n \in \mathbb{N} : E_n(k) \in \sigma_*(k)\}$. As proved in [38, Prop. 2.1], elaborating on a longstanding tradition of related results [45, 33], the projector $P_*(k)$ satisfies the properties listed in the following Proposition.

Proposition 2.1. *Let $P_*(k) \in \mathcal{B}(\mathcal{H}_{\mathrm{f}})$ be the spectral projector of $H(k)$ corresponding to the set $\sigma_*(k) \subset \mathbb{R}$. Assume that σ_* satisfies the gap condition* (2.6). *Then the family $\{P_*(k)\}_{k\in\mathbb{R}^d}$ has the following properties:*

(p_1) *the map $k \mapsto P_*(k)$ is smooth from $\mathbb{R}^d$ to $\mathcal{B}(\mathcal{H}_{\mathrm{f}})$ (equipped with the operator norm);*

(p_2) *the map $k \mapsto P_*(k)$ is τ-covariant, i. e.*

$$P_*(k+\lambda) = \tau(\lambda)\, P_*(k)\, \tau(\lambda)^{-1} \qquad \forall k \in \mathbb{R}^d, \quad \forall \lambda \in \Gamma^*;$$

(p_3) *there exists an antiunitary operator[2] C acting on $\mathcal{H}_{\mathrm{f}}$ such that*

$$P_*(-k) = C\, P_*(k)\, C^{-1} \qquad \textit{and} \qquad C^2 = 1.$$

[2] By *antiunitary* operator we mean a surjective antilinear operator $C : \mathcal{H} \to \mathcal{H}$, such that $\langle C\phi, C\psi\rangle_{\mathcal{H}} = \langle \psi, \phi\rangle_{\mathcal{H}}$ for any $\phi, \psi \in \mathcal{H}$.

The antiunitary operator C appearing in (p_3) is explicitly given by the complex conjugation in $\mathcal{H}_{\mathrm{f}} = L^2(\mathbb{T}^d_Y)$ and, in particular, one has $C\tau(\lambda) = \tau(-\lambda)C$ for all $\lambda \in \Gamma^*$.

In the multi-band case, it is convenient [1, 5] to relax the notion of Bloch function and to consider *quasi-Bloch functions*, defined as elements $\phi \in \mathcal{H}_\tau$ such that

$$P_*(k)\phi(k) = \phi(k), \qquad \|\phi(k)\|_{\mathcal{H}_{\mathrm{f}}} = 1, \qquad \text{for a.e. } k \in \mathbb{B}.$$

A *Bloch frame* is, by definition, a family of quasi-Bloch functions $\{\phi_a\}_{a=1,\dots,m}$, constituting an orthonormal basis of $\operatorname{Ran} P_*(k)$ at a.e. $k \in \mathbb{B}$.
In this context, a non-abelian Bloch gauge appears, since whenever $\{\phi_a\}$ is a Bloch frame, then one obtains another Bloch frame $\{\widetilde{\phi}_a\}$ by setting

$$\widetilde{\phi}_a(k) = \sum_{b=1}^{m} \phi_b(k)\, U_{ba}(k) \qquad \text{for some unitary matrix } U(k).$$

Equipped with this terminology, we rephrase a classical definition [6] as follows:

Definition 2.1 (Composite Wannier functions). The *composite Wannier functions* $\{w_1,\dots,w_m\} \subset L^2(\mathbb{R}^d)$ associated to a Bloch frame $\{\phi_1,\dots,\phi_m\} \subset \mathcal{H}_\tau$ are defined as

$$w_a(x) := \left(\mathcal{U}_{\mathrm{BF}}^{-1}\phi_a\right)(x) = \frac{1}{|\mathbb{B}|^{1/2}} \int_{\mathbb{B}} \mathrm{d}k\, \mathrm{e}^{\mathrm{i}k\cdot x}\phi_a(k,x).$$

◊

An orthonormal basis of $\mathcal{U}_{\mathrm{BF}}^{-1} \operatorname{Ran} P_*$ is readily obtained by considering the translated

$$w_{\gamma,a}(x) := w_a(x-\gamma).$$

In view of the orthogonality of the trigonometric polynomials, the set $\{w_{\gamma,a}\}_{\gamma\in\Gamma, 1\le a\le m}$ is an orthonormal basis of $\mathcal{U}_{\mathrm{BF}}^{-1} \operatorname{Ran} P_*$, which we refer to as a *composite Wannier basis*. The mentioned Bloch gauge freedom implies that the latter basis is not unique, and its properties (*e. g.* localization) will in general depend on the choice of a Bloch gauge.

As emphasized in the Introduction, the existence of an orthonormal basis of well-localized Wannier functions is a crucial issue in solid-state physics. In view of (2.5), the existence of a composite Wannier basis consisting of almost-exponentially localized functions is equivalent to the existence of a C^∞-smooth Bloch frame for $\{P_*(k)\}_{k\in\mathbb{R}^d}$. The existence of the latter might be *a priori* obstructed since, as noticed by several authors [27, 5, 33], there might be competition between the smoothness of the function $k \mapsto \phi_a(k)$ and its pseudo-periodicity properties, here encoded in the fact that $\phi_a \in \mathcal{H}_\tau$ must satisfy (2.3). *A posteriori*, it has been proved that, as a consequence of the time-reversal symmetry of the system, encoded in property (p_3), such obstruction is absent, yielding the existence of a C^∞-smooth (actually, analytic) Bloch frame for any $d \le 3$ and $m \in \mathbb{N}$ [37, 2]. The result in [37], however, neither provides explicitly such Bloch frame, nor it guarantees that it is time-reversal symmetric. In the next Sections, we tackle these problems in a more general framework.

3 Assumptions and main results

Abstracting from the case of periodic Schrödinger operators, we state our results in a general setting. Our assumptions are designed to rely only on two fundamental symmetries of the system, namely covariance with respect to translations by vectors in the dual lattice and a time-reversal symmetry of bosonic type, *i. e.* with a time-reversal operator Θ satisfying $\Theta^2 = \mathbb{1}$ (see Remark 3.1 for the fermionic case). In view of that, the following abstract results apply both to continuous models, as *e. g.* the real Schrödinger operators considered in the previous Section, and to discrete models, as *e. g.* the Haldane model [15].

In the following, 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 $\Lambda \simeq \mathbb{Z}^d \subset \mathbb{R}^d$ which, in the application to Schrödinger operators, is identified with the dual (or reciprocal) lattice Γ^*.

Assumption 3.1. We consider a family of orthogonal projectors $\{P(k)\}_{k \in \mathbb{R}^d} \subset \mathcal{B}(\mathcal{H})$ satisfying the following assumptions:

(P_1) *smoothness*: the map $\mathbb{R}^d \ni k \mapsto P(k) \in \mathcal{B}(\mathcal{H})$ is C^∞-smooth;

(P_2) τ*-covariance*: the map $k \mapsto P(k)$ is covariant with respect to a unitary representation[3] $\tau : \Lambda \to \mathcal{U}(\mathcal{H})$, $\lambda \mapsto \tau(\lambda) \equiv \tau_\lambda$, in the sense that

$$P(k+\lambda) = \tau_\lambda \, P(k) \, \tau_\lambda^{-1} \quad \text{for all } k \in \mathbb{R}^d, \, \lambda \in \Lambda;$$

(P_3) *time-reversal symmetry*: there exists an antiunitary operator Θ acting on $\mathcal{H}$, called the *time-reversal operator*, such that

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

Moreover, we assume the following

(P_4) *compatibility condition*: for all $\lambda \in \Lambda$ one has $\Theta \, \tau_\lambda = \tau_\lambda^{-1} \, \Theta$.

◊

It follows from the assumption (P_1) that the rank m of the projector $P(k)$ is constant in k. We will assume that $m < +\infty$. Proposition 2.1 guarantees that the above assumptions are satisfied by the spectral projectors $\{P_*(k)\}_{k \in \mathbb{R}^d}$ corresponding to an isolated family of Bloch bands of a *real* periodic Schrödinger operator.

Definition 3.1 (Symmetric Bloch frame). Let $\mathcal{P} = \{P(k)\}_{k \in \mathbb{R}^d}$ be a family of projectors satisfying Assumption 3.1. A **local Bloch frame** for $\mathcal{P}$ on a region $\Omega \subset \mathbb{R}^d$ is a map

$$\begin{aligned} \Phi : \Omega &\longrightarrow \mathcal{H} \oplus \ldots \oplus \mathcal{H} = \mathcal{H}^m \\ k &\longmapsto (\phi_1(k), \ldots, \phi_m(k)) \end{aligned}$$

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

such that for a.e. $k \in \Omega$ the set $\{\phi_1(k), \ldots, \phi_m(k)\}$ is an orthonormal basis spanning $\operatorname{Ran} P(k)$. If $\Omega = \mathbb{R}^d$ we say that Φ is a **global Bloch frame**. Moreover, we say that a (global) Bloch frame is

(F_0) *continuous* if the map $\phi_a : \mathbb{R}^d \to \mathcal{H}^m$ is continuous for all $a \in \{1, \ldots, m\}$;
(F_1) *smooth* if the map $\phi_a : \mathbb{R}^d \to \mathcal{H}^m$ is C^∞-smooth for all $a \in \{1, \ldots, m\}$;
(F_2) τ*-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

$$\phi_a(-k) = \Theta \phi_a(k) \quad \text{for all } k \in \mathbb{R}^d,\ a \in \{1, \ldots, m\}.$$

A global Bloch frame is called **symmetric** if satisfies both (F_2) and (F_3). ◊

Theorem 3.1 (Abstract result). *Assume $d \le 3$. Let $\mathcal{P} = \{P(k)\}_{k \in \mathbb{R}^d}$ be a family of orthogonal projectors satisfying Assumption 3.1, with finite rank $m \in \mathbb{N}$. Then there exists a global* **smooth symmetric Bloch frame** *for $\mathcal{P}$. Moreover, the proof is explicitly constructive.*

As mentioned in Section 1, the relevance of Theorem 3.1 is twofold. On the one hand, it provides the first constructive proof, for $m > 1$ and $d > 1$, of the existence of smooth τ-equivariant Bloch frames, thus providing an explicit algorithm to obtain an almost-exponentially localized composite Wannier basis. On the other hand, the fact that such smooth Bloch frame also satisfies (F_3) implies the existence of *real-valued* localized composite Wannier functions, a fact indirectly conjectured in the literature about optimally localized Wannier functions, and confirmed by numerical evidence [29, Section V.B]. We summarize these consequences in the following statement.

Theorem 3.2 (Application to Schrödinger operators). *Assume $d \le 3$. Consider a real periodic Schrödinger operator in the form $H_\Gamma = -\Delta + V_\Gamma$, with V_Γ satisfying* (2.1), *acting on $H^2(\mathbb{R}^d) \subset L^2(\mathbb{R}^d)$. Let $\mathcal{P}_* = \{P_*(k)\}_{k \in \mathbb{R}^d}$ be the set of spectral projectors corresponding to a family of m Bloch bands satisfying condition* (2.6)*. Then one constructs an orthonormal basis $\{w_{\gamma,a}\}_{\gamma \in \Gamma, 1 \le a \le m}$ of $\mathcal{U}_{\mathrm{BF}}^{-1} \operatorname{Ran} P_*$ consisting of composite Wannier functions such that:*

(i) *each function $w_{\gamma,a}$ is* ***real-valued****, and*
(ii) *each function $w_{\gamma,a}$ is* ***almost-exponentially localized****, in the sense that*

$$\int_{\mathbb{R}^d} \langle x \rangle^{2r} |w_{\gamma,a}(x)|^2 \mathrm{d}x < +\infty \qquad \text{for all } r \in \mathbb{N}.$$

Proof. In view of Proposition 2.1, the family $\mathcal{P}_* = \{P_*(k)\}_{k \in \mathbb{R}^d}$ satisfies Assumption 3.1. Thus, by Theorem 3.1, there exists a global smooth symmetric Bloch frame in the sense of Definition 3.1. In view of (F_1) and (F_2), each ϕ_a is an element of $\mathcal{H}_\tau \cap C^\infty(\mathbb{R}^d, \mathcal{H}_{\mathrm{f}})$, and thus Φ is a smooth Bloch frame in the sense of Section 2.

By (2.5), the corresponding Wannier functions $w_a := \mathcal{U}_{\mathrm{BF}}^{-1} \phi_a$ satisfy $\langle x \rangle^r w_a \in L^2(\mathbb{R}^d)$ for all $r \in \mathbb{N}$. Then the set of all the translated functions $\{w_{\gamma,a}\}$, with $w_{\gamma,a}(x) = w_a(x - \gamma)$, provides a composite Wannier basis consisting of almost-exponentially localized functions, as stated in (ii).

Moreover, Φ satisfies (F_3) which in this context reads $\phi_a(-k) = C\phi_a(k) = \overline{\phi_a}(k)$, since C is just complex conjugation in $L^2(\mathbb{T}^d_Y)$. By Definition 2.1, one concludes that

$$\overline{w_a}(x) = \frac{1}{|\mathbb{B}|^{1/2}} \int_{\mathbb{B}} \mathrm{d}k\, \mathrm{e}^{-\mathrm{i}k\cdot x}\, \overline{\phi_a}(k,x) = \frac{1}{|\mathbb{B}|^{1/2}} \int_{\mathbb{B}} \mathrm{d}k\, \mathrm{e}^{\mathrm{i}(-k)\cdot x}\, \phi_a(-k,x) = w_a(x),$$

which yields property (i) and concludes the proof. □

We sketch the structure of the proof of Theorem 3.1, provided in Sections 4 and 5. First, one easily notices that, in view of properties (F_2) and (F_3), a global symmetric Bloch frame $\Phi : \mathbb{R}^d \to \mathcal{H}^m$ is completely specified by the values it assumes on the *effective unit cell*

$$\mathbb{B}_{\mathrm{eff}} := \left\{ k = \sum_j k_j e_j \in \mathbb{B} : k_1 \geq 0 \right\}.$$

Indeed, every point $k \in \mathbb{R}^d$ can be written (with an a.e.-unique decomposition) as $k = (-1)^s k' + \lambda$, for some $k' \in \mathbb{B}_{\mathrm{eff}}$, $\lambda \in \Lambda$ and $s \in \{0,1\}$. Then the symmetric Bloch frame Φ satisfies $\Phi(k) = \tau_\lambda \Theta^s \Phi(k')$ for $k' \in \mathbb{B}_{\mathrm{eff}}$. Viceversa, a local Bloch frame $\Phi_{\mathrm{eff}} : \mathbb{B}_{\mathrm{eff}} \to \mathcal{H}^m$ can be canonically extended to a global symmetric Bloch frame Φ by posing

$$\Phi(k) = \tau_\lambda \Theta^s \Phi_{\mathrm{eff}}(k') \qquad \text{for } k = (-1)^s k' + \lambda. \tag{3.1}$$

However, to obtain a global *continuous* Bloch frame, the map $\Phi_{\mathrm{eff}} : \mathbb{B}_{\mathrm{eff}} \to \mathcal{H}^m$ must satisfy some non-trivial “gluing conditions” on the boundary $\partial\mathbb{B}_{\mathrm{eff}}$, involving vertices, edges (for $d \geq 2$), faces (for $d \geq 3$), and so on. In Section 4, we investigate in detail such conditions, showing that it is always possible to construct a local continuous Bloch frame $\Phi_{\mathrm{eff}} : \mathbb{B}_{\mathrm{eff}} \to \mathcal{H}^m$ satisfying them, provided $d \leq 3$. More specifically, we assume as given a continuous Bloch frame $\Psi : \mathbb{B}_{\mathrm{eff}} \to \mathcal{H}^m$, called *the input frame*, which does not satisfy any special condition on the boundary of $\mathbb{B}_{\mathrm{eff}}$, as *e. g.* the outcome of numerical computations in solid-state physics. Then we explicitly construct a unitary matrix $U_{\mathrm{eff}}(k)$ such that the “corrected” frame

$$\Phi_{\mathrm{eff}}(k)_a := \sum_{b=1}^m \Psi_b(k)\, U_{\mathrm{eff}}(k)_{ba}$$

is still continuous and satisfies all the relevant symmetry conditions on $\partial\mathbb{B}_{\mathrm{eff}}$. Then, formula (3.1) will provide a global *continuous symmetric* Bloch frame Φ.
A naïf smoothing procedure, based on the Steenrod’s Approximation Theorem, starting from Φ would yield a global smooth τ-equivariant Bloch frame which, in general, does not satisfies property (F_3). For this reason, we develop in Section 5 a new symmetry-preserving smoothing algorithm which, starting from a global continuous symmetric Bloch frame, produces a global *smooth symmetric* Bloch frame arbitrarily close to the former one (Theorem 5.1). The latter procedure, which holds true in any dimension, yields the global smooth symmetric Bloch frame whose existence is claimed in Theorem 3.1.

Remark 3.1 (Systems with fermionic time-reversal symmetry). Our results heavily rely on the fact that we consider a *bosonic* (or even) time-reversal (TR) symmetry.

In other instances, as in the context of TR-symmetric topological insulators [16], and specifically in the Kane-Mele model [22], assumption (P_3) is replaced by

($P_{3,-}$) *fermionic time-reversal symmetry*: there exists an antiunitary operator Θ acting on $\mathcal{H}$ such that

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

Then the statement analogous to Theorem 3.1 is false: there might be topological obstruction to the existence of a continuous symmetric Bloch frame [11, 14]. One proves [14, 10] that such obstruction is classified by a $\mathbb{Z}_2$ topological invariant for $d = 2$, and by four $\mathbb{Z}_2$ invariants for $d = 3$, and that the latter equal the indices introduced by Fu, Kane and Mele [11, 12]. However, if one does not require time-reversal symmetry but only τ-equivariance, then a global smooth Bloch frame does exist even in the fermionic case, as a consequence of the vanishing of the first Chern class and of the result in [37], see [31] for a detailed review. ♢

4 Proof: Construction of a smooth symmetric Bloch frame

In this Section, we provide an explicit algorithm to construct a global smooth symmetric Bloch frame, as claimed in Theorem 3.1.

Our general strategy will be the following. We consider a local continuous (resp. smooth)[4] Bloch frame $\Psi : \mathbb{B}_{\text{eff}} \to \mathcal{H}^m$, which always exists since $\mathbb{B}_{\text{eff}}$ is contractible and no special conditions on the boundary are imposed.[5] We look for a unitary-matrix-valued map $U : \mathbb{B}_{\text{eff}} \to \mathcal{U}(\mathbb{C}^m)$ such that the modified local Bloch frame

$$\Phi_a(k) = \sum_{b=1}^{m} \Psi_b(k) U_{ba}(k), \quad U(k) \in \mathcal{U}(\mathbb{C}^m) \tag{4.1}$$

satisfies (F_2) and (F_3) on the boundary $\partial\mathbb{B}_{\text{eff}}$. The latter requirement corresponds to conditions on the values that U assumes on the vertices, edges and faces of $\partial\mathbb{B}_{\text{eff}}$, according to the dimension. These conditions will be investigated in the next Subsections, after a preliminary characterization of the relevant symmetries.

[4] A smooth input frame Ψ is required only to write an explicit formula for the continuous extension from the boundary $\partial\mathbb{B}_{\text{eff}}$ to the whole $\mathbb{B}_{\text{eff}}$, as detailed in Remarks 4.2 and 4.3. At a first reading, the reader might prefer to focus on the case of a continuous input frame.

[5] Moreover, a smooth Ψ can be explicitly constructed by using the intertwining unitary by Kato and Nagy [24, Sec. I.6.8] on finitely-many sufficiently small open sets covering $\mathbb{B}_{\text{eff}}$. In the applications to computational physics, Ψ corresponds to the outcome of the numerical diagonalisation of the Hamiltonian at fixed crystal momentum, followed by a choice of quasi-Bloch functions and by a standard routine which corrects the phases to obtain a (numerically) continuous (resp. smooth) Bloch frame on $\mathbb{B}_{\text{eff}}$.

4.1 The relevant group action

Properties (P_2) and (P_3) are related to some fundamental automorphisms of $\mathbb{R}^d$, namely the maps c and t_λ defined by

$$c(k) = -k \qquad \text{and} \qquad t_\lambda(k) = k + \lambda \quad \text{for } \lambda \in \Lambda. \tag{4.2}$$

Since $c\, t_\lambda = t_{-\lambda} c$ and $c^2 = t_0$, one concludes that the relevant symmetries are encoded in the group

$$G_d := \{t_\lambda, t_\lambda c\}_{\lambda \in \Lambda} \subset \mathrm{Aut}(\mathbb{R}^d). \tag{4.3}$$

We notice that, assuming also (P_4), the action of G_d on $\mathbb{R}^d$ can be lifted to an action on $\mathbb{R}^d \times \mathrm{Fr}(m, \mathcal{H})$, where $\mathrm{Fr}(m, \mathcal{H})$ is the set of orthonormal m-frames in $\mathcal{H}$. To streamline the notation, we denote by $\Phi = (\phi_1, \dots, \phi_m)$ an element of $\mathrm{Fr}(m, \mathcal{H})$. Any bounded linear or antilinear operator $A : \mathcal{H} \to \mathcal{H}$ acts on frames componentwise, *i. e.* we set

$$A\Phi := (A\phi_1, \dots, A\phi_m).$$

Moreover, the space $\mathrm{Fr}(m, \mathcal{H})$ carries a free right action[6] of the group $\mathcal{U}(\mathbb{C}^m)$, denoted by

$$(\Phi \triangleleft U)_b := \sum_{a=1}^{m} \phi_a U_{ab}.$$

A similar notation appears in [14]. Notice that, by the antilinearity of the time-reversal operator Θ, one has

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

A lift of the G_d action from $\mathbb{R}^d$ to $\mathbb{R}^d \times \mathrm{Fr}(m, \mathcal{H})$ is obtained by considering, as generators, the automorphisms C and T_λ, defined by

$$C(k, \Phi) = (c(k), \Theta\Phi) \qquad T_\lambda(k, \Phi) = (t_\lambda(k), \tau_\lambda \Phi) \tag{4.4}$$

for any $(k, \Phi) \in \mathbb{R}^d \times \mathrm{Fr}(m, \mathcal{H})$. The relation $t_\lambda\, c = c\, t_{-\lambda}$ implies that, for every $\lambda \in \Lambda$, one has to impose the relation

$$\begin{aligned} T_\lambda C(k, \Phi) &= C T_{-\lambda}(k, \Phi) && \forall (k, \Phi) \in \mathbb{R}^d \times \mathrm{Fr}(m, \mathcal{H}) \\ \textit{i. e. } \tau_\lambda \Theta \Phi &= \Theta \tau_{-\lambda} \Phi && \forall \Phi \in \mathrm{Fr}(m, \mathcal{H}), \end{aligned}$$

which holds true in view of (P_4). Thus the action of G_d is lifted to $\mathbb{R}^d \times \mathrm{Fr}(m, \mathcal{H})$.

Given a family of projectors $\mathcal{P}$ satisfying (P_2), (P_3) and (P_4), it is natural to consider the set of global Bloch frames for $\mathcal{P}$, here denoted by $\mathrm{Fr}(\mathcal{P})$. Notice that

$$\mathrm{Fr}(\mathcal{P}) \subset \left\{ f : \mathbb{R}^d \to \mathrm{Fr}(m, \mathcal{H}) \right\} \subset \mathbb{R}^d \times \mathrm{Fr}(m, \mathcal{H}).$$

[6] This terminology means that $\Phi \triangleleft \mathbb{I} = \Phi$, $(\Phi \triangleleft U_1) \triangleleft U_2 = \Phi \triangleleft (U_1 U_2)$ and that if $\Phi \triangleleft U_1 = \Phi \triangleleft U_2$ then $U_1 = U_2$, for all $\Phi \in \mathrm{Fr}(m, \mathcal{H})$ and $U_1, U_2 \in \mathcal{U}(\mathbb{C}^m)$.

It is easy to check that the action of G_d, previously extended to $\mathbb{R}^d \times \mathrm{Fr}(m, \mathcal{H})$, restricts to $\mathrm{Fr}(\mathcal{P})$. Indeed, whenever Φ is an orthonormal frame for $\operatorname{Ran} P(k)$ one has that

$$\begin{aligned} P(t_\lambda(k))\tau_\lambda\Phi &= \tau_\lambda P(k)\tau_\lambda^{-1}\tau_\lambda\Phi = \tau_\lambda P(k)\Phi = \tau_\lambda\Phi, \\ P(c(k))\Theta\Phi &= \Theta P(k)\Theta^{-1}\Theta\Phi = \Theta P(k)\Phi = \Theta\Phi, \end{aligned}$$

yielding that $\tau_\lambda\Phi$ is an orthonormal frame in $\operatorname{Ran}(P(t_\lambda(k)))$ and $\Theta\Phi$ is an orthonormal frame in $\operatorname{Ran}(P(c(k)))$.

4.2 Solving the vertex conditions

The relevant vertex conditions are associated to those points $k \in \mathbb{R}^d$ which have a non-trivial stabilizer with respect to the action of G_d, namely to the points in the set

$$V_d = \left\{ k \in \mathbb{R}^d : \exists\, g \in G_d, g \neq \mathbb{1} : g(k) = k \right\}. \tag{4.5}$$

Since $G_d = \{t_\lambda, t_\lambda c\}_{\lambda\in\Lambda}$ and t_λ acts freely on $\mathbb{R}^d$, the previous definition reads

$$\begin{aligned} V_d &= \left\{ k \in \mathbb{R}^d : \exists \lambda \in \Lambda : \ t_\lambda c(k) = k \right\} \\ &= \left\{ k \in \mathbb{R}^d : \exists \lambda \in \Lambda : -k + \lambda = k \right\} = \{1/2\lambda\}_{\lambda\in\Lambda}, \end{aligned}$$

i. e. V_d consists of those points[7] which have half-integer coordinates with respect to the basis $\{e_1, \dots, e_d\}$. For convenience, we set $k_\lambda := 1/2\lambda$.

If Φ is a symmetric Bloch frame, then conditions (F_2) and (F_3) imply that

$$\Phi(k_\lambda) = \Phi(t_\lambda c(k_\lambda)) = \tau_\lambda\Theta\Phi(k_\lambda) \qquad k_\lambda \in V_d. \tag{4.6}$$

We refer to (4.6) as the **vertex condition at the point** $k_\lambda \in V_d$. For a generic Bloch frame Ψ, instead, $\Psi(k_\lambda)$ and $\tau_\lambda\Theta\Psi(k_\lambda)$ are different. Since they both are orthonormal frames in $\operatorname{Ran} P(k_\lambda)$, there exists a unique unitary matrix $U_{\mathrm{obs}}(k_\lambda) \in \mathcal{U}(\mathbb{C}^m)$ such that

$$\Psi(k_\lambda) \triangleleft U_{\mathrm{obs}}(k_\lambda) = \tau_\lambda\Theta\Psi(k_\lambda), \qquad \lambda \in \Lambda. \tag{4.7}$$

The obstruction unitary $U_{\mathrm{obs}}(k_\lambda)$ must satisfy a compatibility condition. Indeed, by applying $\tau_\lambda\Theta$ to both sides of (4.7) one obtains

$$\begin{aligned} \tau_\lambda\Theta\left(\Psi(k_\lambda) \triangleleft U_{\mathrm{obs}}(k_\lambda)\right) &= \tau_\lambda\Theta\tau_\lambda\Theta\Psi(k_\lambda) \\ &= \tau_\lambda\tau_{-\lambda}\Theta^2\Psi(k_\lambda) = \Psi(k_\lambda) \end{aligned}$$

where assumption (P_4) has been used. On the other hand, the left-hand side also reads

[7] In the context of topological insulators, such points are called *time-reversal invariant momenta* (TRIMs) in the physics literature.

$$\begin{aligned}\tau_\lambda\Theta\left(\Psi(k_\lambda)\triangleleft U_{\rm obs}(k_\lambda)\right) &= (\tau_\lambda\Theta\Psi(k_\lambda))\triangleleft\overline{U_{\rm obs}}(k_\lambda) = \\ &= \Psi(k_\lambda)\triangleleft\Big(U_{\rm obs}(k_\lambda)\,\overline{U_{\rm obs}}(k_\lambda)\Big).\end{aligned}$$

By the freeness of the action of $\mathcal{U}(\mathbb{C}^m)$ on frames, one concludes that

$$U_{\rm obs}(k_\lambda) = U_{\rm obs}(k_\lambda)^{\mathsf{T}} \tag{4.8}$$

where M^{T} denotes the transpose of the matrix M.

The value of the unknown U, appearing in (4.1), at the point $k_\lambda \in V_d$ is constrained by the value of the obstruction matrix $U_{\rm obs}(k_\lambda)$. Indeed, from (4.6) and (4.1) it follows that for every $\lambda \in \Lambda$

$$\begin{aligned}\Psi(k_\lambda)\triangleleft U(k_\lambda) = \Phi(k_\lambda) &= \tau_\lambda\Theta\,\Phi(k_\lambda) \\ &= \tau_\lambda\Theta\left(\Psi(k_\lambda)\triangleleft U(k_\lambda)\right) \\ &= (\tau_\lambda\Theta\Psi(k_\lambda))\triangleleft\overline{U}(k_\lambda) \\ &= \Psi(k_\lambda)\triangleleft U_{\rm obs}(k_\lambda)\overline{U}(k_\lambda).\end{aligned}$$

By the freeness of the $\mathcal{U}(\mathbb{C}^m)$-action, we obtain the condition[8]

$$U_{\rm obs}(k_\lambda) = U(k_\lambda)U(k_\lambda)^{\mathsf{T}}. \tag{4.9}$$

The existence of a solution $U(k_\lambda) \in \mathcal{U}(\mathbb{C}^m)$ to equation (4.9) is granted by the following Lemma, which can be applied to $V = U_{\rm obs}(k_\lambda)$ in view of (4.8).

Lemma 4.1 (Solution to the vertex equation). *Let $V \in \mathcal{U}(\mathbb{C}^m)$ be such that $V^{\mathsf{T}} = V$. Then there exists a unitary matrix $U \in \mathcal{U}(\mathbb{C}^m)$ such that $V = U\,U^{\mathsf{T}}$.*

Proof. Since $V \in \mathcal{U}(\mathbb{C}^m)$ is normal, it can be unitarily diagonalised. Hence, there exists a unitary matrix $W \in \mathcal{U}(\mathbb{C}^m)$ such that

$$V = W\mathrm{e}^{\mathrm{i}M}W^*$$

where $M = \mathrm{diag}(\mu_1,\dots,\mu_m)$ and each μ_j is chosen so that[9] $\mu_j \in [0,2\pi)$. We set

$$U = W\mathrm{e}^{\mathrm{i}M/2}W^*.$$

Since $V^{\mathsf{T}} = V$ one has $\overline{W}\mathrm{e}^{\mathrm{i}M}W^{\mathsf{T}} = W\mathrm{e}^{\mathrm{i}M}W^*$, yielding

$$\mathrm{e}^{\mathrm{i}M}W^{\mathsf{T}}W = W^{\mathsf{T}}W\mathrm{e}^{\mathrm{i}M},$$

i. e. the matrix $\mathrm{e}^{\mathrm{i}M}$ commutes with $A := W^{\mathsf{T}}W$. Thus also $\mathrm{e}^{\mathrm{i}M/2}$ commutes with A (since each μ_j is in $[0,2\pi)$), hence one has

---

[8] The presence of the transpose in condition (4.9) might appear unnatural in the context of our Assumptions. A more natural reformulation of condition (4.9), involving an orthogonal structure canonically associated to Θ, will be discussed in a forthcoming paper [4].

[9] The latter condition is crucial: it expresses the fact that the arguments of the eigenvalues $\{\omega_1,\dots,\omega_m\}$ of V are "synchronized", *i. e.* they are computed by using the same branch of the complex logarithm.

$$UU^{\mathsf{T}} = W e^{iM/2} A^{-1} e^{iM/2} A W^{*} = W e^{iM} W^{*} = V.$$

□

In view of (4.8), we have the following

Corollary 4.1. *For every $k_\lambda \in V_d$ there exists a unitary matrix $U(k_\lambda)$ such that $U_{\mathrm{obs}}(k_\lambda) = U(k_\lambda)U(k_\lambda)^{\mathsf{T}}$. In particular, the Bloch frame $\Phi(k_\lambda) = \Psi(k_\lambda) \triangleleft U(k_\lambda)$ satisfies the vertex condition* (4.6) *at the point $k_\lambda \in V_d$.*

4.3 Construction in the 1-dimensional case

In the 1-dimensional case, the boundary of $\mathbb{B}_{\mathrm{eff}}$ consists of two vertices $v_0 = 0$ and $v_1 = k_{e_1}$. Given, as an input, a continuous Bloch frame $\Psi : \mathbb{B}_{\mathrm{eff}} \to \mathcal{H}^m$, equation (4.7) provides, for each vertex, an obstruction matrix $U_{\mathrm{obs}}(v_i)$. In view of Corollary 4.1, one obtains a unitary $U(v_i)$ which solves equation (4.9) for $k_\lambda = v_i$, $i \in \{0,1\}$.

Since $\mathcal{U}(\mathbb{C}^m)$ is a path-connected manifold, there exists a smooth path $W : [0,1/2] \to \mathcal{U}(\mathbb{C}^m)$ such that $W(0) = U(v_0)$ and $W(1/2) = U(v_1)$. Moreover, the path W can be explicitly constructed, as detailed in the following Remark.

Remark 4.1 (Interpolation of unitaries). The problem of constructing a smooth interpolation between two unitaries U_1 and U_2 in $\mathcal{U}(\mathbb{C}^m)$ has an easy explicit solution. First, by left multiplication times U_1^{-1}, the problem is equivalent to the construction of a smooth interpolation between $\mathbb{I}$ and $U_1^{-1}U_2 =: U_* \in \mathcal{U}(\mathbb{C}^m)$. Since U_* is normal, there exists a unitary matrix S_* such that $S_* U_* S_*^{-1} = e^{iD}$, with $D = \mathrm{diag}(\delta_1, \dots, \delta_m)$ a diagonal matrix. Then the map $t \mapsto W(t) := S_*^{-1} e^{i2tD} S_*$ is an explicit smooth interpolation between $W(0) = \mathbb{I}$ and $W(1/2) = U_*$. ◊

We define a local continuous Bloch frame $\Phi_{\mathrm{eff}} : \mathbb{B}_{\mathrm{eff}} \to \mathcal{H}^m$ by setting

$$\Phi_{\mathrm{eff}}(k) = \Psi(k) \triangleleft W(k), \qquad k \in \mathbb{B}_{\mathrm{eff}}.$$

Notice that Φ_{eff} satisfies, in view of the construction above, the vertex conditions

$$\Phi_{\mathrm{eff}}(0) = \Theta\Phi_{\mathrm{eff}}(0) \quad \text{and} \quad \Phi_{\mathrm{eff}}(k_{e_1}) = \tau_{e_1}\Theta\Phi_{\mathrm{eff}}(k_{e_1}), \tag{4.10}$$

which are special cases of condition (4.6). We extend Φ_{eff} to a global Bloch frame $\Phi : \mathbb{R}^1 \to \mathcal{H}^m$ by using equation (3.1). We claim that Φ is a *continuous* symmetric Bloch frame. Indeed, it satisfies (F_2) and (F_3) in view of (3.1) and it is continuous since Φ_{eff} satisfies (4.10). On the other hand, Φ is in general non-smooth at the vertices in V_1. By using the symmetry-preserving smoothing procedure, as stated in Proposition 5.1, we obtain a global smooth symmetric Bloch frame Φ_{sm}. This concludes the proof of Theorem 3.1 for $d = 1$.

4.4 Construction in the 2-dimensional case

The reduced unit cell $\mathbb{B}_{\mathrm{eff}}$ contains exactly six elements in V_2. In adapted coordinates, so that (k_1, k_2) represents the point $k_1 e_1 + k_2 e_2$ for $\Lambda = \mathrm{Span}_{\mathbb{Z}}\{e_1, e_2\}$, they are labelled as follows (Figure 1):

$$v_1 = (0,0), \quad v_2 = \left(0, -\frac{1}{2}\right), \quad v_3 = \left(\frac{1}{2}, -\frac{1}{2}\right), \qquad (4.11)$$
$$v_4 = \left(\frac{1}{2}, 0\right), \quad v_5 = \left(\frac{1}{2}, \frac{1}{2}\right), \quad v_6 = \left(0, \frac{1}{2}\right).$$

The oriented segment joining v_i to v_{i+1} (with $v_7 \equiv v_1$) is labelled by E_i.

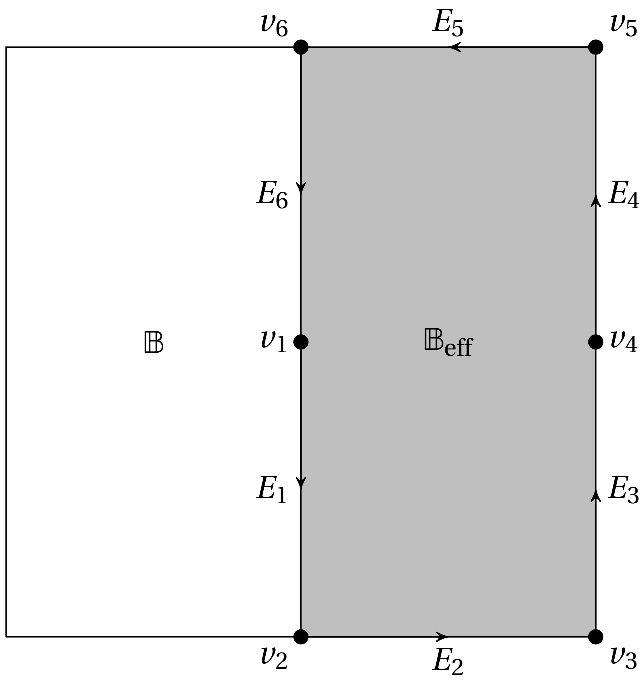


Fig. 1 The effective unit cell (shaded area), its vertices and its edges. We use adapted coordinates (k_1, k_2) such that $k = k_1 e_1 + k_2 e_2$.

We start from a local continuous (resp. smooth) Bloch frame $\Psi : \mathbb{B}_{\rm eff} \to \mathcal{H}^m$. Given Ψ, the obstruction matrix defined in (4.7) yields, via Corollary 4.1, a unitary matrix $U(v_i)$ solving equation (4.9), for $i \in \{1, \dots, 4\}$.

Construction of the frame on the 1-skeleton

As in the 1-dimensional case, we exploit the constructive existence of a smooth path $W_i : [0, 1/2] \to \mathcal{U}(\mathbb{C}^m)$ such that $W_i(0) = U(v_i)$ and $W_i(1/2) = U(v_{i+1})$, for $i \in \{1,2,3\}$. These $\mathcal{U}(\mathbb{C}^m)$-valued paths are concatenated by setting

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

so to obtain a piecewise-smooth map $\widetilde{U} : E_1 \cup E_2 \cup E_3 \to \mathcal{U}(\mathbb{C}^m)$. Let

$$\widetilde{\Phi}(k) := \Psi(k) \triangleleft \widetilde{U}(k) \qquad \text{for } k \in E_1 \cup E_2 \cup E_3.$$

We extend the map $\widetilde{\Phi}$ to a continuous (resp. piecewise-smooth) symmetric Bloch frame $\widehat{\Phi}$ on $\partial\mathbb{B}_{\text{eff}}$ by imposing properties (F_2) and (F_3), *i. e.* by setting

$$\widehat{\Phi}(k) := \begin{cases} \widetilde{\Phi}(k) & \text{if } k \in E_1 \cup E_2 \cup E_3 \\ \tau_{e_1}\Theta\widetilde{\Phi}(t_{e_1}c(k)) & \text{if } k \in E_4 \\ \tau_{e_2}\widetilde{\Phi}(t_{e_2}^{-1}(k)) & \text{if } k \in E_5 \\ \Theta\widetilde{\Phi}(c(k)) & \text{if } k \in E_6. \end{cases} \tag{4.12}$$

By construction $\widehat{\Phi}$ satisfies all the *edge symmetries* for a symmetric Bloch frame Φ listed below:

$$\begin{aligned} \Phi(c(k)) &= \Theta\Phi(k) && \text{for } k \in E_1 \cup E_6 \\ \Phi(t_{e_2}(k)) &= \tau_{e_2}\Phi(k) && \text{for } k \in E_2 \\ \Phi(t_{e_1}c(k)) &= \tau_{e_1}\Theta\Phi(k) && \text{for } k \in E_3 \cup E_4 \\ \Phi(t_{e_2}^{-1}(k)) &= \tau_{e_2}^{-1}\Phi(k) && \text{for } k \in E_5. \end{aligned} \tag{4.13}$$

The map $\widehat{\Phi} : \partial\mathbb{B}_{\text{eff}} \to \mathcal{H}^m$ is continuous (resp. piecewise-smooth), since $\widetilde{\Phi}$ is continuous (resp. piecewise-smooth) and satisfies by construction the vertex conditions at v_i for $i \in \{1,4\}$.

Extension to the 2-torus

Since both $\widehat{\Phi}(k)$ and the input frame $\Psi(k)$ are orthonormal frames in $\operatorname{Ran} P(k)$, for every $k \in \partial\mathbb{B}_{\text{eff}}$, there exists a unique unitary matrix $\widehat{U}(k)$ such that

$$\widehat{\Phi}(k) = \Psi(k) \triangleleft \widehat{U}(k) \qquad \text{for } k \in \partial\mathbb{B}_{\text{eff}}. \tag{4.14}$$

Explicitly, $\widehat{U}(k)_{ab} = \langle \psi_a(k), \widehat{\phi}_b(k) \rangle$, which also show that the map $\widehat{U}$ is continuous (resp. piecewise-smooth) on $\partial\mathbb{B}_{\text{eff}}$.

We look for a continuous extension $U_{\text{eff}} : \mathbb{B}_{\text{eff}} \to \mathcal{U}(\mathbb{C}^m)$ of $\widehat{U}$, such that $\Phi_{\text{eff}} := \Psi \triangleleft U_{\text{eff}}$ satisfies the edge symmetries (4.13). Noticing that $\partial\mathbb{B}_{\text{eff}}$ is homeomorphic to a circle S^1, we use some well-known facts in algebraic topology: if X is a topological space, then a continuous map $f : S^1 \to X$ extends to a continuous map $F : D^2 \to X$, where D^2 is the 2-dimensional disc enclosed by the circle S^1, if and only if its homotopy class $[f]$ is the trivial element in $\pi_1(X)$. Since, in our case, the space X is the group $\mathcal{U}(\mathbb{C}^m)$, we also use the fact that the exact sequence of groups

$$1 \longrightarrow \mathcal{SU}(\mathbb{C}^m) \longrightarrow \mathcal{U}(\mathbb{C}^m) \xrightarrow{\det} U(1) \longrightarrow 1$$

induces an isomorphism $\pi_1(\mathcal{U}(\mathbb{C}^m)) \simeq \pi_1(U(1))$. On the other hand, the degree homomorphism

$$\deg : \pi_1(U(1)) \xrightarrow{\sim} \mathbb{Z}, \quad [\varphi : S^1 \to U(1)] \longmapsto \frac{1}{2\pi i}\oint_{S^1} \varphi(z)^{-1}\partial_z\varphi(z)\,\mathrm{d}z \tag{4.15}$$

establishes an isomorphism of groups $\pi_1(U(1)) \simeq \mathbb{Z}$. We conclude that a continuous map $f : \partial\mathbb{B}_{\text{eff}} \to \mathcal{U}(\mathbb{C}^m)$ can be continuously extended to $F : \mathbb{B}_{\text{eff}} \to \mathcal{U}(\mathbb{C}^m)$ if and only if $\deg([\det f]) \in \mathbb{Z}$ is zero.

The following Lemma is the crucial step in the 2-dimensional construction. It shows that, even if $\deg([\det \widehat{U}]) = r \neq 0$, it is always possible to construct a continuous map $X : \partial\mathbb{B}_{\text{eff}} \to \mathcal{U}(\mathbb{C}^m)$ such that $\deg([\det \widehat{U} X]) = 0$ and $\widehat{\Phi} \triangleleft X$ still satisfies the edge symmetries.[10]

Lemma 4.2 (Solution to the face-extension problem). *Let $r \in \mathbb{Z}$. There exists a piecewise-smooth map $X : \partial\mathbb{B}_{\text{eff}} \to \mathcal{U}(\mathbb{C}^m)$ such that:*

(i) $\deg([\det X]) = -r$;
(ii) *if a Bloch frame Φ satisfies the edge symmetries* (4.13)*, the frame $\Phi \triangleleft X$ also does;*
(iii) $X(k) \neq \mathbb{1}$ *only for $k \in E_3 \cup E_4$.*

Property (iii) will not be used in this Section, but it will be useful to solve the 3-dimensional problem.

Proof. First, we translate (ii) into an explicit condition on X. For $k \in E_1 \cup E_6$, condition (ii) means that for every Φ such that $\Phi(-k) = \Theta\Phi(k)$ one has that

$$\begin{gathered}(\Phi \triangleleft X)(-k) = \Theta\,(\Phi \triangleleft X)(k)\\ \Updownarrow\\ \Phi(-k) \triangleleft X(-k) = \Theta\,(\Phi(k) \triangleleft X(k))\\ \Updownarrow\\ (\Theta\Phi(k)) \triangleleft X(-k) = (\Theta\Phi(k)) \triangleleft \overline{X}(k),\end{gathered}$$

yielding the explicit condition

$$X(-k) = \overline{X}(k), \quad k \in E_1 \cup E_6. \tag{4.16}$$

Similarly, one obtains

$$X(t_{e_1} c(k)) = \overline{X}(k) \qquad \text{for } k \in E_3 \cup E_4 \tag{4.17}$$

$$X(t_{e_2}(k)) = X(k) \qquad \text{for } k \in E_2 \tag{4.18}$$

$$X(t_{e_2}^{-1}(k)) = X(k) \qquad \text{for } k \in E_5. \tag{4.19}$$

Thus condition (ii) on X is equivalent to the relations (4.16), (4.17), (4.18) and (4.19).

We now exhibit a map $X : \partial\mathbb{B}_{\text{eff}} \to \mathcal{U}(\mathbb{C}^m)$ which satisfies the previous relations, and such that $\deg([\det X]) = -r$. Define $\xi : \partial\mathbb{B}_{\text{eff}} \to \mathbb{C}$ by

$$\xi(k) := \begin{cases} \mathrm{e}^{-\mathrm{i}2\pi r(k_2+1/2)} & \text{for } k \in E_3 \cup E_4 \\ 1 & \text{otherwise,} \end{cases} \tag{4.20}$$

and set $X(k) := \operatorname{diag}(\xi(k), 1, \dots, 1) \in \mathcal{U}(\mathbb{C}^m)$ for $k \in \partial\mathbb{B}_{\text{eff}}$. The map X is clearly piecewise-smooth. Then, one easily checks that:

(i) $\deg([\det X]) = -r$, since $\deg([\det X]) = \deg([\xi]) = -r$.

[10] This is a special feature of systems with *bosonic* TR-symmetry: if assumption (P_3) is replaced by ($P_{3,-}$), the analogous statement does not hold true [10].

(ii) X trivially satisfies relations (4.16), (4.18) and (4.19), since $X(k) \equiv \mathbb{I}$ for $k \in E_1 \cup E_2 \cup E_5 \cup E_6$. It also satisfies relation (4.17). Indeed, let $k = (1/2, k_2) \in E_3 \cup E_4$. Since $t_{e_1} c(k) = (1/2, -k_2)$, one has

$$X(t_{e_1} c(k)) = X(1/2, -k_2) = \mathrm{diag}(\xi(1/2, -k_2), 1, \dots, 1) = \mathrm{diag}(\overline{\xi(1/2, k_2)}, 1, \dots, 1) = \overline{X}(k).$$

(iii) property (iii) is satisfied by construction.

□

Set $r := \deg([\det \widehat{U}])$. In view of Lemma 4.2, the continuous (resp. piecewise-smooth) map $U := \widehat{U} X : \partial\mathbb{B}_{\mathrm{eff}} \to \mathcal{U}(\mathbb{C}^m)$ satisfies $\deg([\det U]) = 0$ and hence extends to a continuous (resp. piecewise-smooth) map $U_{\mathrm{eff}} : \mathbb{B}_{\mathrm{eff}} \to \mathcal{U}(\mathbb{C}^m)$. Moreover, the extension procedure is explicitely constructive whenever U is piecewise-smooth, as detailed in Remark 4.2. By setting $\Phi_{\mathrm{eff}}(k) := \Psi(k) \triangleleft U_{\mathrm{eff}}(k)$, we obtain a continuous symmetric Bloch frame on the whole reduced unit cell $\mathbb{B}_{\mathrm{eff}}$, which moreover satisfies the edge symmetries (4.13) in view of item (ii) in Lemma 4.2. Then formula (3.1) defines a global symmetric Bloch frame Φ, which is continuous in view of the fact that Φ_{eff} satisfies (4.13). The symmetry-preserving smoothing procedure (Proposition 5.1) yields a global smooth symmetric Bloch frame, arbitrarily close to Φ. This concludes the proof of Theorem 3.1 for $d = 2$.

Remark 4.2 (Explicit extension to the whole effective cell, $d = 2$). We emphasize that the extension of the *piecewise-smooth* map $U : \partial\mathbb{B}_{\mathrm{eff}} \to \mathcal{U}(\mathbb{C}^m)$, with $\deg[\det U] = 0$, to a continuous (actually, piecewise-smooth) map $U_{\mathrm{eff}} : \mathbb{B}_{\mathrm{eff}} \to \mathcal{U}(\mathbb{C}^m)$ is explicit. For notational convenience, we use the shorthand $\mathcal{U}(m) \equiv \mathcal{U}(\mathbb{C}^m)$.

First notice that the problem of constructing a continuous extension of U can be decomposed into two simpler problems, since $\mathcal{U}(m) \approx \mathcal{U}(1) \times \mathcal{SU}(m)$ (as topological spaces), where the identification is provided *e. g.* by the map

$$W \mapsto (\det W, W^\flat) \in \mathcal{U}(1) \times \mathcal{SU}(m) \qquad \text{with } W^\flat = \mathrm{diag}(\det W^{-1}, 1, \dots, 1) W.$$

Thus the problem is reduced to exhibit a continuous extension of (a) the map $f : k \mapsto \det U(k) \in \mathcal{U}(1)$, and (b) the map $f^\flat : k \mapsto U^\flat(k) \in \mathcal{SU}(m)$.

As for problem (a), let $f : \partial\mathbb{B}_{\mathrm{eff}} \to \mathcal{U}(1)$ be a degree-zero piecewise-smooth function. Then, a piecewise-smooth extension $F : \mathbb{B}_{\mathrm{eff}} \to \mathcal{U}(1)$ is constructed as follows. Let $\theta_0 \in \mathbb{R}$ be such that $f(0, -1/2) = \mathrm{e}^{\mathrm{i}2\pi\theta_0}$. Define the piecewise-smooth function $\varphi : [0, 3] \to \mathcal{U}(1)$ as

$$\varphi(t) = \begin{cases} f(t, -1/2) & \text{if } 0 \le t \le 1/2 \\ f(1/2, -1 + t) & \text{if } 1/2 \le t \le 3/2 \\ f(2 - t, 1/2) & \text{if } 3/2 \le t \le 2 \\ f(0, 5/2 - t) & \text{if } 2 \le t \le 3 \end{cases} \tag{4.21}$$

and set

$$\theta(t) = \theta_0 + \frac{1}{2\pi\mathrm{i}} \int_0^t \varphi(\tau)^{-1} \varphi'(\tau) \mathrm{d}\tau, \qquad \text{for } t \in [0, 3].$$

By the Cauchy integral formula, $\theta(3) = \theta(0) + \deg(f) = \theta(0) = \theta_0$. Moreover,

$$e^{i2\pi\theta(t)} = \varphi(t)$$

for every $t \in [0,3]$. Then, one can choose $F(k_1, k_2) = e^{i2\pi\omega(k_1,k_2)}$, where

$$\omega(k_1,k_2) := \begin{cases} -2k_2\,\theta\left(\frac{k_2-2k_1+1/2}{4k_2}\right) & \text{if } k_2 \le -|2k_1-1/2|, \\ (4k_1-1)\,\theta\left(1+\frac{k_2}{4k_1-1}\right) & \text{if } -|2k_1-1/2| \le k_2 \le |2k_1-1/2|, \text{ with } k_1 \ge 1/4, \\ 2k_2\,\theta\left(2-\frac{k_2+2k_1-1/2}{4k_2}\right) & \text{if } k_2 \ge |2k_1-1/2|, \\ (-4k_1+1)\,\theta\left(\frac{5}{2}-\frac{k_2}{-4k_1+1}\right) & \text{if } -|2k_1-1/2| \le y \le |2k_1-1/2|, \text{ with } k_1 \le 1/4. \end{cases}$$

Note that ω is continuous at $(1/4,0)$ with $\omega(1/4,0) = 0$, since θ is continuous on $[0,3]$ and so there exist a $|\theta|_{\max} \in \mathbb{R}$ such that $|\theta(t)| \le |\theta|_{\max}$ for any $t \in [0,3]$.

As for problem (b), while a construction of the continuous extension is possible for every $m \in \mathbb{N}$, here we provide the details only for $m = 2$, which is the case of interest for the 2-bands models, as *e.g.* the celebrated Haldane model [15], and is such that an extension can be made completely explicit by elementary techniques. To obtain an extension for higher m's, one can reduce to the case $m = 2$ by recursively exploiting the fibrations $\mathcal{SU}(m-1) \longrightarrow \mathcal{SU}(m) \longrightarrow S^{2m-1}$.

Let $f^\flat : k \mapsto U^\flat(k) \in \mathcal{SU}(2)$ be a piecewise-smooth function. Then a piecewise-smooth extension $F^\flat : \mathbb{B}_{\text{eff}} \to \mathcal{SU}(2)$ is constructed as follows. First, we use the standard identification of $\mathcal{SU}(2)$ with the 3-sphere of unit norm vectors in $\mathbb{R}^4$ to look at $f^\flat$ as to a piecewise-smooth function $f^\flat : \partial\mathbb{B}_{\text{eff}} \to S^3$. Let $p \in S^3$ be a point not in the range[11] of $f^\flat$, and let $\psi_p : S^3 \setminus \{p\} \to \{p\}^\perp$ be the stereographic projection from p to the hyperplane through the origin of $\mathbb{R}^4$ orthogonal to the vector p. Explicitly, this map and its inverse read

$$\begin{aligned} \psi_p(v) &= p - \frac{1}{\langle v-p \,|\, p\rangle}\,(v-p) \\ \psi_p^{-1}(w) &= p + \frac{2}{\|w-p\|^2}\,(w-p). \end{aligned} \tag{4.22}$$

Second, we define a piecewise-smooth function $\varphi^\flat : [0,3] \to S^3$ by using the same formula as in (4.21), with f replaced by $f^\flat$.
Then, a piecewise-smooth extension of $f^\flat$ to a function $F^\flat : \mathbb{B}_{\text{eff}} \to S^3$ is given by

[11] Such a point does exists since the map $f^\flat$ is piecewise-smooth. Indeed, by an argument analogous to the Sard lemma, one can show that the range of $f^\flat$ is not dense in S^3. This is the only point in the construction where we need U piecewise-smooth, and hence a smooth input frame Ψ.

$$F^\flat(k_1,k_2) = \begin{cases} \psi_p^{-1}\left(-2k_2\,\psi_p(\varphi(\frac{k_2-2k_1+1/2}{4k_2}))\right) & \text{if } k_2 \le -|2k_1-1/2|, \\ \psi_p^{-1}\left((4k_1-1)\,\psi_p(\varphi(1+\frac{k_2}{4k_1-1}))\right) & \text{if } -|2k_1-1/2| \le k_2 \le |2k_1-1/2| \text{ and } k_1 \ge 1/4, \\ \psi_p^{-1}\left(2k_2\,\psi_p(\varphi(2-\frac{k_2+2k_1-1/2}{4k_2}))\right) & \text{if } k_2 \ge |2k_1-1/2|, \\ \psi_p^{-1}\left((-4k_1+1)\,\psi_p(\varphi(\frac{5}{2}-\frac{k_2}{-4k_1+1}))\right) & \text{if } -|2k_1-1/2| \le k_2 \le |2k_1-1/2| \text{ and } k_1 \le 1/4. \end{cases}$$

Notice that $F^\flat$ is continuous at $(1/4,0)$ with $F^\flat(1/4,0) = -p$, since $\psi_p \circ \varphi : [0,3] \to p^\perp \subseteq \mathbb{R}^4$ is continuous on $[0,3]$. This provides an explicit piecewise-smooth extension of $f^\flat$ for the case $m = 2$. ◊

4.5 Interlude: abstracting from the 1- and 2-dimensional case

Abstracting from the proofs in Subsections 4.3 and 4.4, we distillate two Lemmas which will become the "building bricks" of the higher dimensional construction. To streamline the statements, we denote by $\mathbb{B}^{(d)}$ (resp. $\mathbb{B}^{(d)}_{\text{eff}}$) the d-dimensional unit cell (resp. effective unit cell) and we adhere to the following convention:

$$\begin{aligned} &\mathbb{B}^{(0)} \simeq \{0\} \qquad\qquad \mathbb{B}^{(1)}_{\text{eff}} \simeq [0,1/2], \\ &\mathbb{B}^{(d+1)}_{\text{eff}} \simeq \mathbb{B}^{(1)}_{\text{eff}} \times \mathbb{B}^{(d)} = \{(k_1, \underbrace{k_2,\dots,k_{d+1}}_{k_\perp}) : k_1 \in [0,1/2],\ k_\perp \in \mathbb{B}^{(d)}\} \qquad \text{for } d \ge 1. \end{aligned} \tag{4.23}$$

We also refer to the following statement as the d-**dimensional problem**:
Given a continuous Bloch frame $\Psi : \mathbb{B}^{(d)}_{\text{eff}} \to \mathcal{H}^m$*, construct a continuous Bloch frame* $\Phi_{\text{eff}} : \mathbb{B}^{(d)}_{\text{eff}} \to \mathcal{H}^m$ *which, via* (3.1)*, continuously extends to a global continuous symmetric Bloch frame* $\Phi : \mathbb{R}^d \to \mathcal{H}^m$.
In other words, Φ_{eff} is defined only on the effective unit cell $\mathbb{B}^{(d)}_{\text{eff}}$, but satisfies all the relations on $\partial\mathbb{B}^{(d)}_{\text{eff}}$ (involving vertices, edges, faces, ...) which allow for a continuous symmetric extension to the whole $\mathbb{R}^d$. Hereafter, we will not further emphasize the fact that all the functions appearing in the construction are piecewise-smooth whenever Ψ is smooth, since this fact will be used only in Remark 4.3.

Notice that Subsection 4.2 already contains a solution to the 0-dimensional problem: indeed, in view of Corollary 4.1, for every $\lambda \in \Lambda$ there exists a Bloch frame, defined on the point k_λ, satisfying the vertex condition (4.6), thus providing a solution to the 0-dimensional problem in $\mathbb{B}^{(0)} \simeq \{k_\lambda\} \simeq \{0\}$.

A second look to Subsection 4.3 shows that it contains a solution to the 1-dimensional problem, given a solution to the 0-dimensional problem. Indeed, one extracts from the construction the following Lemma.

Lemma 4.3 (Macro 1). *Let* $\Phi_{\text{one}} : \mathbb{B}^{(0)} \simeq \{0\} \to \mathcal{H}^m$ *be a Bloch frame satisfying*

$$\Phi_{\mathrm{one}}(0) = \Theta\,\Phi_{\mathrm{one}}(0). \tag{4.24}$$

Then one constructs a continuous Bloch frame $\Phi_{\mathrm{two}} : \mathbb{B}^{(1)}_{\mathrm{eff}} \simeq [0,1/2] \to \mathcal{H}^m$ *such that*

$$\begin{cases} \Phi_{\mathrm{two}}(0) = \Phi_{\mathrm{one}}(0) \\ \Phi_{\mathrm{two}}(1/2) = \tau_{e_2}\Theta\,\Phi_{\mathrm{two}}(1/2). \end{cases} \tag{4.25}$$

In view of (4.25), Φ_{two} continuously extends, via (3.1), to a global continuous symmetric Bloch frame, thus providing a solution to the 1-dimensional problem.

Analogously, from the construction in Subsection 4.4 we distillate a general procedure. For convenience, we relabel the edges of $\mathbb{B}^{(2)}_{\mathrm{eff}}$ as follows:

$$E_{j,0} = \left\{ k = \sum_i k_i e_i \in \mathbb{B}^{(2)}_{\mathrm{eff}} : k_j = 0 \right\} \tag{4.26}$$

$$E_{j,\pm} = \left\{ k = \sum_i k_i e_i \in \mathbb{B}^{(2)}_{\mathrm{eff}} : k_j = \pm 1/2 \right\} \tag{4.27}$$

From the construction in Subsection 4.4, based on Lemma 4.2, one easily deduces the following result.

Lemma 4.4 (Macro 2). *Assume that* $\Phi_S : S \to \mathcal{H}^m$, *with* $S = E_{1,0} \cup E_{2,-} \cup E_{2,+} \subset \partial\mathbb{B}^{(2)}_{\mathrm{eff}}$, *is continuous and satisfies the following edge symmetries:*

$$\begin{cases} \Phi_S(t_{e_2}(k)) = \tau_{e_2}\Phi_S(k) & \text{for } k \in E_{2,-} \\ \Phi_S(t_{e_2}^{-1}(k)) = \tau_{e_2}^{-1}\Phi_S(k) & \text{for } k \in E_{2,+} \\ \Phi_S(c(k)) = \Theta\,\Phi_S(k) & \text{for } k \in E_{1,0}. \end{cases} \tag{4.28}$$

Then one constructs a continuous Bloch frame $\Phi_{\mathrm{eff}} : \mathbb{B}^{(2)}_{\mathrm{eff}} \to \mathrm{Fr}(m,\mathcal{H})$ *such that*

$$\begin{cases} \Phi_{\mathrm{eff}}(k) = \Phi_S(k) & \text{for } k \in S \\ \Phi_{\mathrm{eff}}(t_{e_1} c(k)) = \tau_{e_1}\Theta\,\Phi_{\mathrm{eff}}(k) & \text{for } k \in E_{1,+}. \end{cases} \tag{4.29}$$

To obtain (4.29) we implicitly used property (iii) in Lemma 4.2, which guarantees that it is possible to obtain the frame Φ_{eff} by acting only on the edge $E_{1,+} = E_3 \cup E_4$. Notice that, in view of (4.29), Φ_{eff} continuously extends, via (3.1), to a global continuous symmetric Bloch frame. Therefore, a solution to the 2-dimensional problem can always be constructed, whenever a continuous Bloch frame on the 1-dimensional set S, satisfying the edge symmetries (4.28), is provided.

The previous Lemmas 4.3 and 4.4 will yield a constructive and conceptually clear solution to the 3-dimensional problem, and a characterization of the obstruction to the solution to the 4-dimensional problem.

4.6 Construction in the 3*-dimensional case*

The faces of $\partial\mathbb{B}^{(3)}_{\mathrm{eff}}$ are labelled according to the following convention : for $j \in \{1,2,3\}$ we set

$$F_{j,0} = \left\{ k = \sum_{i=1}^{3} k_i e_i : k_j = 0 \right\} \tag{4.30}$$

$$F_{j,\pm} = \left\{ k = \sum_{i=1}^{3} k_i e_i : k_j = \pm 1/2 \right\} \tag{4.31}$$

Notice that two faces of $\partial\mathbb{B}^{(3)}_{\mathrm{eff}}$, namely $F_{1,0}$ and $F_{1,+}$ are identifiable with a 2-dimensional unit cell $\mathbb{B}^{(2)}$, while the remaining four faces, namely $F_{2,\pm}$ and $F_{3,\pm}$, are identifiable with a 2-dimensional effective unit cell $\mathbb{B}^{(2)}_{\mathrm{eff}}$.

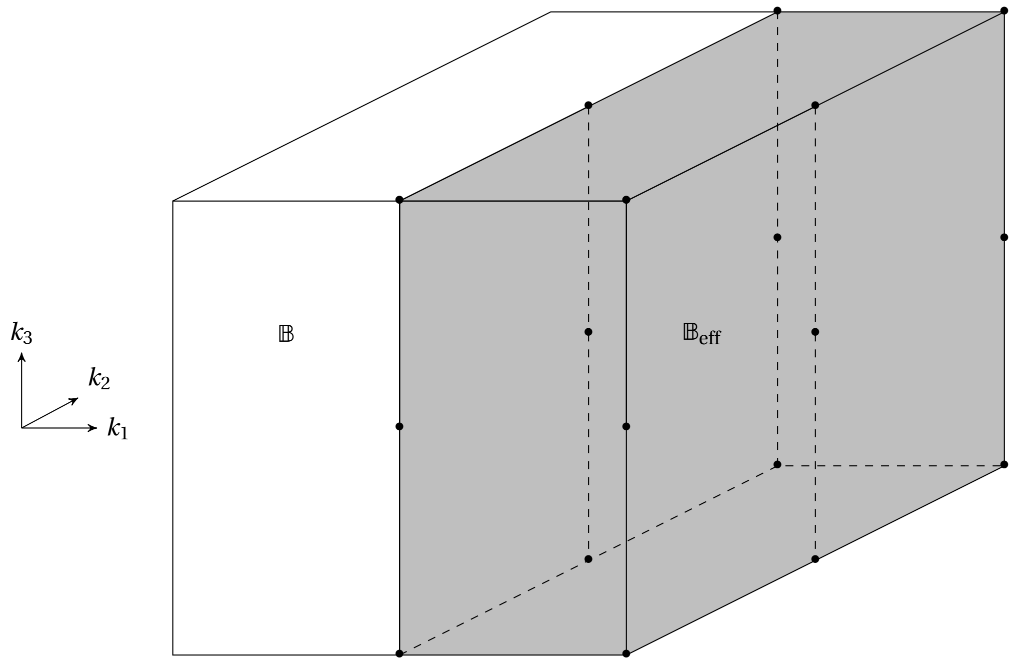


Fig. 2 The 3-dimensional (effective) unit cell.

We assume as given a continuous Bloch frame $\Psi : \mathbb{B}^{(3)}_{\mathrm{eff}} \to \mathcal{H}^m$ (the *input frame*) which does not satisfy any particular symmetry on the boundary $\partial\mathbb{B}^{(3)}_{\mathrm{eff}}$. Since $F_{1,0} \simeq \mathbb{B}^{(2)}$, in view of the construction in Subsection 4.4 we can assume that Ψ has been already modified to obtain a continuous Bloch frame $\Phi_{\mathrm{one}} : F_{1,0} \to \mathcal{H}^m$, $\Phi_{\mathrm{one}} = \Psi \triangleleft U_{\mathrm{one}}$, which satisfies the edge symmetries (4.13) on $F_{1,0}$.

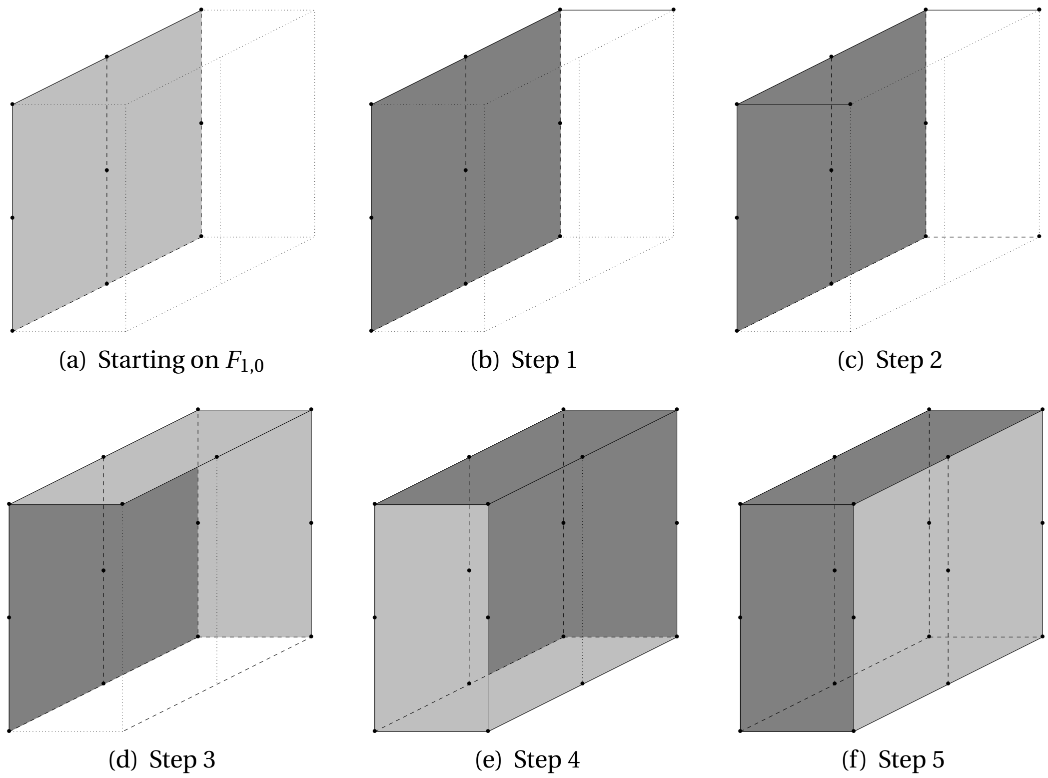
For convenience, we decompose the constructive algorithm into few steps:

• *Step 1. Extend to an edge by Macro 1.* Choose a vertex of $\partial\mathbb{B}^{(3)}_{\mathrm{eff}}$ contained in $F_{1,+}$, and let v_0 be the corresponding vertex on $F_{1,0}$. For the sake of concreteness, we choose $v_* = (1/2, 1/2, 1/2)$, so that $v_0 = (0, 1/2, 1/2)$. Then Lemma 4.3 (Macro 1) yields the existence of a continuous Bloch frame $\Phi_{\rm two} : [v_0, v_*] \simeq \mathbb{B}^{(1)}_{\rm eff} \to \mathcal{H}^m$ such that $\Phi_{\rm two}(v_0) = \Phi_{\rm one}(v_0)$ and $\Phi_{\rm two}(v_*)$ satisfies the vertex condition (4.6) at v_*.

• *Step 2. Extend by τ-equivariance.* By imposing property (F_2), $\Phi_{\rm two}$ naturally extends to the edges $t_{e_2}^{-1}([v_0, v_*])$ and $t_{e_3}^{-1}([v_0, v_*])$. Since $\Phi_{\rm one}$ is τ-equivariant on $F_{1,0} \simeq \mathbb{B}^{(2)}$, one has that $\Phi_{\rm two}(t_{e_j}^{-1}(v_0)) = \Phi_{\rm one}(t_{e_j}^{-1}(v_0))$ for $j \in \{2,3\}$. In view of that, we obtain a continuous Bloch frame by setting

$$\Phi_{\rm three}(k) := \begin{cases} \Phi_{\rm one}(k) & \text{for } k \in F_{1,0}, \\ \Phi_{\rm two}(k) & \text{for } k \in t_\lambda([v_0, v_*]) \text{ for } \lambda \in \{0, -e_2, -e_3\}. \end{cases} \tag{4.32}$$

• *Step 3. Extend to small faces by Macro 2.* Notice that $\Phi_{\rm three}$ restricted to $F_{3,+}$ (resp. $F_{2,+}$) is defined and continuous on a set $S_{3,+}$ (resp. $S_{2,+}$) which has the same structure as the set S appearing in Lemma 4.4 (Macro 2), and there satisfies the relations analogous to (4.28). Then $\Phi_{\rm three}$ continuously extends to the whole $F_{3,+}$ (resp. $F_{2,+}$) and the extension satisfies the relation analogous to (4.29) on the edge $\partial F_{j,+} \setminus S_{j,+}$ for $j = 3$ (resp. $j = 2$).



(a) Starting on $F_{1,0}$ (b) Step 1 (c) Step 2

(d) Step 3 (e) Step 4 (f) Step 5

Fig. 3 Steps in the construction.

• *Step 4. Extend by τ-equivariance.* By imposing τ-equivariance (property (F_2)), $\Phi_{\rm three}$ naturally extends to the faces $F_{3,-}$ and $F_{2,-}$, thus yielding a continuous Bloch frame $\Phi_{\rm four}$ defined on the set[12] $\partial\mathbb{B}^{(3)}_{\rm eff} \setminus F_{1,+} =: K_0$.

[12] According to a longstanding tradition in geometry, the choice of symbols is inspired by the German language: K_0 stands for *Kleiderschrank ohne Türen*. The reason for this name will be clear in few lines.

• *Step 5. Extend symmetrically to $F_{1,+}$ by Macro 2.* When considering the face $F_{1,+}$, we first notice that the two subsets[13]

$$T_{\pm} = \{k \in F_{1,+} : \pm k_2 \geq 0\} \tag{4.33}$$

are related by a non-trivial symmetry, since $t_{e_1} c(T_{\pm}) = T_{\mp}$. We construct a continuous extension of Φ_{four} which is compatible with the latter symmetry.

The restriction of Φ_{four}, defined on K_0, to the set $S_+ = \{k \in \partial F_{1,+} : k_2 \geq 0\}$ is continuous and satisfies symmetries analogous to (4.28). Then, in view of Lemma 4.4 (Macro 2), Φ_{four} continuously extends to the whole T_+ and the extension satisfies the relation analogous to (4.29) on the edge $\partial T_+ \setminus S_+$. We denote the extension by Φ_{five}.

To obtain a continuous symmetric Bloch frame $\widehat{\Phi} : \partial \mathbb{B}^{(3)}_{\text{eff}} \to \text{Fr}(m, \mathcal{H})$ we set

$$\widehat{\Phi}(k) := \begin{cases} \Phi_{\text{four}}(k) & \text{for } k \in K_0 \\ \Phi_{\text{five}}(k) & \text{for } k \in T_+ \\ \Phi_{\text{five}}(t_{e_1} c(k)) & \text{for } k \in T_-. \end{cases} \tag{4.34}$$

The function $\widehat{\Phi}$ is continuous in view of the edge and face symmetries which have been imposed in the construction.

• *Step 6. Extend to the interior of the effective cell.* The frame $\widehat{\Phi}$ and the input frame Ψ are related by the equation

$$\widehat{\Phi}(k) = \Psi(k) \triangleleft \widehat{U}(k) \qquad k \in \partial \mathbb{B}^{(3)}_{\text{eff}}, \tag{4.35}$$

which yields a continuous map $\widehat{U} : \partial \mathbb{B}^{(3)}_{\text{eff}} \to \mathcal{U}(\mathbb{C}^m)$.

We show that such a map extends to a continuous map $U_{\text{eff}} : \mathbb{B}^{(3)}_{\text{eff}} \to \mathcal{U}(\mathbb{C}^m)$. Indeed, a continuous function f from $\partial \mathbb{B}^{(3)}_{\text{eff}} \approx S^2$ to the topological space X can be continuously extended to $\mathbb{B}^{(3)}_{\text{eff}} \approx D^3$ if and only if its homotopy class $[f]$ is the trivial element of the group $\pi_2(X)$. In our case, since $\pi_2(\mathcal{U}(\mathbb{C}^m)) = \{0\}$ for every $m \in \mathbb{N}$, there is no obstruction to the continuous extension of the map $\widehat{U}$. Moreover, the extension can be explicitly constructed, as detailed in Remark 4.3.
Equipped with such a continuous extension, we obtain a continuous symmetric Bloch frame $\Phi_{\text{eff}} : \mathbb{B}^{(3)}_{\text{eff}} \to \mathcal{H}^m$ by setting

$$\Phi_{\text{eff}}(k) = \Psi(k) \triangleleft U_{\text{eff}}(k) \qquad k \in \mathbb{B}^{(3)}_{\text{eff}}. \tag{4.36}$$

• *Step 7. Use the smoothing procedure.* By using (3.1), Φ_{eff} extends to a global continuous symmetric Bloch frame. Then the symmetry-preserving smoothing procedure (Proposition 5.1) yields a global smooth symmetric Bloch frame.

This concludes the proof of Theorem 3.1 for $d = 3$.

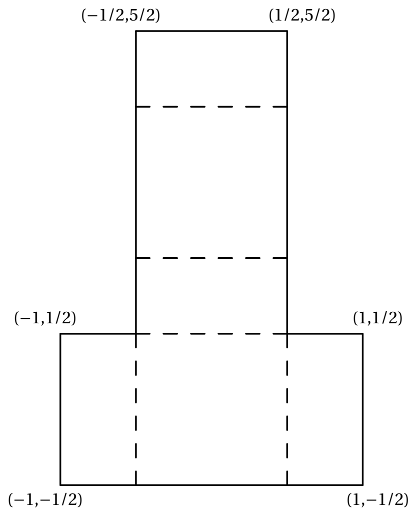
Remark 4.3 (Explicit extension to the whole effective cell, $d = 3$). As in the 2-dimensional case (Remark 4.2), we notice that the extension of the *piecewise-smooth*[14]

[13] Obviously, these subsets are *die Türen*, so they are denoted by $T_{\pm}$.
[14] The map $\widehat{U}$ is actually piecewise-smooth, whenever the input frame Ψ is smooth. Although this fact was not emphasized at every step of the 3-dimensional construction, as we did instead in Section 4.4, the reader can easily check it.

function $\widehat{U} : \partial\mathbb{B}^{(3)}_{\mathrm{eff}} \to \mathcal{U}(\mathbb{C}^m)$ to $\mathbb{B}^{(3)}_{\mathrm{eff}}$ is completely explicit. The problem is again reduced to the following two subproblems, namely to construct a continuos extension from $\partial\mathbb{B}^{(3)}_{\mathrm{eff}}$ to $\mathbb{B}^{(3)}_{\mathrm{eff}}$ of:

(a) a map $f : k \mapsto \det U(k) \in \mathcal{U}(1)$, and
(b) a map $f^\flat : k \mapsto U^\flat(k) \in \mathcal{SU}(m)$.

As for subproblem (a), given a degree-zero piecewise-smooth function $f : \partial\mathbb{B}^{(3)}_{\mathrm{eff}} \to \mathcal{U}(1)$, a piecewise-smooth extension $F : \mathbb{B}^{(3)}_{\mathrm{eff}} \to \mathcal{U}(1)$ is constructed as follows. Consider the region $\mathbb{D} \subseteq \mathbb{R}^2$ depicted below



and let $\varphi : \mathbb{D} \to \mathcal{U}(1)$ be the piecewise-smooth function defined by

$$\varphi(s,t) := \begin{cases} f(-s-\frac{1}{2}, -\frac{1}{2}, t) & \text{if } (s,t) \in [-1,-\frac{1}{2}] \times [-\frac{1}{2},\frac{1}{2}] \\ f(0,s,t) & \text{if } (s,t) \in [-\frac{1}{2},\frac{1}{2}] \times [-\frac{1}{2},\frac{1}{2}] \\ f(s-\frac{1}{2},\frac{1}{2},t) & \text{if } (s,t) \in [\frac{1}{2},1] \times [-\frac{1}{2},\frac{1}{2}] \\ f(t-\frac{1}{2},s,\frac{1}{2}) & \text{if } (s,t) \in [-\frac{1}{2},\frac{1}{2}] \times [\frac{1}{2},1] \\ f(\frac{1}{2},s,-t+\frac{3}{2}) & \text{if } (s,t) \in [-\frac{1}{2},\frac{1}{2}] \times [1,2] \\ f(-t+\frac{5}{2},s,-\frac{1}{2}) & \text{if } (s,t) \in [-\frac{1}{2},\frac{1}{2}] \times [2,\frac{5}{2}] \end{cases} \tag{4.37}$$

Choose $\theta_0 \in \mathbb{R}$ be such that $f(0,0,0) = \mathrm{e}^{2\pi \mathrm{i}\theta_0}$ and set

$$\theta(s,t) = \theta_0 + \frac{1}{2\pi i}\int_0^1 \varphi(\lambda s,\lambda t)^{-1}\left(s\varphi_s(\lambda s,\lambda t) + t\varphi_t(\lambda s,\lambda t)\right) d\lambda,$$

where φ_s and φ_t denote the partial derivatives of φ with respect to s and t, respectively. One has

$$\mathrm{e}^{2\pi\mathrm{i}\theta(s,t)} = \varphi(s,t)$$

for any $(s,t) \in \mathbb{D}$. Moreover,

$$\begin{cases} \theta(s,-\frac{1}{2}) = \theta(s,\frac{5}{2}) & \text{for } -\frac{1}{2} \le s \le \frac{1}{2} \\ \theta(s,-\frac{1}{2}) = \theta(-\frac{1}{2},3+s) & \text{for } -1 \le s \le -\frac{1}{2} \\ \theta(s,-\frac{1}{2}) = \theta(\frac{1}{2},3-s) & \text{for } \frac{1}{2} \le s \le 1 \\ \theta(s,\frac{1}{2}) = \theta(-\frac{1}{2},\frac{1}{2}-s) & \text{for } -1 \le s \le -\frac{1}{2} \\ \theta(s,\frac{1}{2}) = \theta(\frac{1}{2},\frac{1}{2}+s) & \text{for } \frac{1}{2} \le s \le 1 \\ \theta(-1,t) = \theta(-\frac{1}{2},\frac{3}{2}-t) & \text{for } -\frac{1}{2} \le t \le \frac{1}{2} \\ \theta(1,t) = \theta(\frac{1}{2},\frac{3}{2}-t) & \text{for } \frac{1}{2} \le t \le \frac{1}{2} \end{cases}$$

so that θ actually lifts f to a piecewise-smooth function $\theta : \partial\mathbb{B}^{(3)}_{\text{eff}} \to \mathbb{R}$. Then, one can choose $F(k_1,k_2,k_3) = \mathrm{e}^{2\pi \mathrm{i}\,\omega(k_1,k_2,k_3)}$, where

$$\omega(k_1,k_2,k_3) = \begin{cases} (-4k_1+1)\,\theta\left(-\frac{k_3}{4k_1-1}, -\frac{k_2}{4k_1-1}\right) & \text{if } 0 \le k_1 \le \min\{|\frac{1}{2}|k_2| - \frac{1}{4}|, |\frac{1}{2}|k_3| - \frac{1}{4}|\}, \\ 2k_3\,\theta\left(\frac{1}{2} + \frac{k_3+2k_1-1/2}{4k_3}, \frac{k_2}{2k_3}\right) & \text{if } \max\{|2k_1 - \frac{1}{2}|, |k_2|\} \le k_3 \le \frac{1}{2}, \\ 2k_2\,\theta\left(\frac{k_3}{2k_2}, \frac{1}{2} + \frac{k_2+2k_1-1/2}{4k_2}\right) & \text{if } \max\{|2k_1 - \frac{1}{2}|, |k_3|\} \le k_2 \le \frac{1}{2}, \\ (4k_1-1)\,\theta\left(\frac{k_3}{4k_1-1}, \frac{3}{2} - \frac{k_2}{4k_1-1}\right) & \text{if } \max\{|\frac{1}{2}|k_2| + \frac{1}{4}|, |\frac{1}{2}|k_3| + \frac{1}{4}|\} \le k_1 \le \frac{1}{2}, \\ -2k_3\,\theta\left(-\frac{1}{2} - \frac{k_3-2k_1+1/2}{4k_3}, -\frac{k_2}{2k_3}\right) & \text{if } -\frac{1}{2} \le k_3 \le \min\{-|2k_1 - \frac{1}{2}|, -|k_2|\}, \\ -2k_2\,\theta\left(-\frac{k_3}{2k_2}, \frac{5}{2} - \frac{k_2-2k_1+1/2}{4k_2}\right) & \text{if } -\frac{1}{2} \le k_2 \le \min\{-|2k_1 - \frac{1}{2}|, -|k_3|\}. \end{cases}$$

Note that ω is continuous at $(1/4,0,0)$ with $\omega(1/4,0,0) = 0$, since θ is continuous on the compact domain $\mathbb{D}$.

As mentioned in Remark 4.2, the solution to subproblem (b) can be obtained by recursive reduction of the rank m, up to $m = 2$. To construct the extension in the case $m = 2$, we identify $\mathcal{SU}(2)$ with S^3 and use the stereographic projection (4.22), with respect to a point $p \in S^3$ which is not included in the range[15] of the map $f^\flat$. By using Equation (4.37), with f replaced by $f^\flat$, one defines a piecewise-smooth function $\varphi : \mathbb{D} \to S^3$. Then, a piecewise-smooth extension of $f^\flat$ to a function $F^\flat : \mathbb{B}^{(3)}_{\text{eff}} \to S^3$ is explicitly given by

[15] This point does exist since the map $f^\flat$ is piecewise-smooth, as argued in footnote11.

$$F(k_1,k_2,k_3)=\begin{cases} \psi_p^{-1}\left((-4k_1+1)\psi_p\left(\varphi(-\frac{k_3}{4k_1-1},-\frac{k_2}{4k_1-1})\right)\right) & \text{if } 0\le k_1\le \min\{|\frac{1}{2}|k_2|-\frac{1}{4}|,|\frac{1}{2}|k_3|-\frac{1}{4}|\},\\ \psi_p^{-1}\left(2k_3\,\psi_p\left(\varphi(\frac{1}{2}+\frac{k_3+2k_1-1/2}{4k_3},\frac{k_2}{2k_3})\right)\right) & \text{if } \max\{|2k_1-\frac{1}{2}|,|k_2|\}\le k_3\le\frac{1}{2},\\ \psi_p^{-1}\left(2k_2\,\psi_p\left(\varphi(\frac{k_3}{2k_2},\frac{1}{2}+\frac{k_2+2k_1-1/2}{4k_2})\right)\right) & \text{if } \max\{|2k_1-\frac{1}{2}|,|k_3|\}\le k_2\le\frac{1}{2},\\ \psi_p^{-1}\left((4k_1-1)\psi_p\left(\varphi(\frac{k_3}{4k_1-1},\frac{3}{2}-\frac{k_2}{4k_1-1})\right)\right) & \text{if } \max\{|\frac{1}{2}|k_2|+\frac{1}{4}|,|\frac{1}{2}|k_3|+\frac{1}{4}|\}\le k_1\le\frac{1}{2},\\ \psi_p^{-1}\left(-2k_3\,\psi_p\left(\varphi(-\frac{1}{2}-\frac{k_3-2k_1+1/2}{4k_3},-\frac{k_2}{2k_3})\right)\right) & \text{if } -\frac{1}{2}\le k_3\le\min\{-|2k_1-\frac{1}{2}|,-|k_2|\},\\ \psi_p^{-1}\left(-2k_2,\psi_p\left(\varphi(-\frac{k_3}{2k_2},\frac{5}{2}-\frac{k_2-2k_1+1/2}{4k_2})\right)\right) & \text{if } -\frac{1}{2}\le k_2\le\min\{-|2k_1-\frac{1}{2}|,-|k_3|\}. \end{cases}$$

Note that F is continuous at $(1/4,0,0)$ with $F(1/4,0,0)=-p$, since $\psi_p\circ\varphi:\mathbb{D}\to p^\perp\subseteq\mathbb{R}^4$ is continuous on the compact domain $\mathbb{D}$. The map above provides an explicit continuous extension to $\mathbb{B}^{(3)}_{\text{eff}}$ for $m=2$. ◊

4.7 A glimpse to the higher-dimensional cases

The fundamental “building bricks” used to solve the 3-dimensional problem (Lemma 4.3 and 4.4) can be used to approach the higher-dimensional problems. However, additional topological obstruction might appear, related to the fact that the k-th homotopy group $\pi_k(\mathcal{U}(\mathbb{C}^m))$, for $k\ge 3$, might be non-trivial if $m>1$.

We illustrate this phenomenon in the case $d=4$. An iterative procedure analogous to the construction in Subsection 4.6, based again only on Lemma 4.3 and 4.4, yields a continuous Bloch frame $\widehat{\Phi}:\partial\mathbb{B}^{(4)}_{\text{eff}}\to\mathcal{H}^m$ satisfying all the relevant symmetries (on vertices, edges, faces and 3-dimensional hyperfaces). By comparison with the input frame $\Psi:\mathbb{B}^{(4)}_{\text{eff}}\to\mathcal{H}^m$, one obtains a continuos map $\widehat{U}:\partial\mathbb{B}^{(4)}_{\text{eff}}\to\mathcal{U}(\mathbb{C}^m)$ such that $\widehat{\Phi}(k)=\Psi(k)\triangleleft\widehat{U}(k)$ for all $k\in\partial\mathbb{B}^{(4)}_{\text{eff}}$. Arguing as in Subsection 4.6, one concludes that the existence of a continuos extension $U_{\text{eff}}:\mathbb{B}^{(4)}_{\text{eff}}\to\mathcal{U}(\mathbb{C}^m)$ of $\widehat{U}$ is equivalent to the fact that the homotopy class $[\widehat{U}]$ is the trivial element of $\pi_3(\mathcal{U}(\mathbb{C}^m))$. Since the latter group is not trivial (for $m>1$), there might be *a priori* topological obstruction to the existence of a continuous extension. This possible obstruction corresponds, in the abstract approach used in [37, 31], to the appearance for $d\ge 4$ of the second Chern class of the Bloch bundle, which always vanishes for $d\le 3$ or $m=1$.

On the other hand, our constructive algorithm works without obstruction in the case $m=1$, since $\pi_k\left(\mathcal{U}(\mathbb{C}^1)\right)=0$ for all $k\ge 2$, yielding an explicit construction of a global smooth symmetric Bloch frame. However, since a constructive proof in the case $m=1$ is already known for every $d\in\mathbb{N}$ [18], we do not provide the details of the construction.

5 A symmetry-preserving smoothing procedure

In this Section we develop a smoothing procedure which, given a global continuous symmetric Bloch frame, yields a global *smooth symmetric* Bloch frame arbitrarily close to the given one. The following Proposition, which holds true in any dimension, might be of independent interest.

Proposition 5.1 (Symmetry-preserving smoothing procedure). *For $d \in \mathbb{N}$, let $\mathcal{P} = \{P(k)\}_{k\in\mathbb{R}^d}$ be a family of orthogonal projectors satisfying Assumption 3.1. Assume that $\Phi : \mathbb{R}^d \to \mathcal{H}^m$ is a global* continuous symmetric *Bloch frame, i. e. it satisfies properties* (F_0), (F_2) *and* (F_3).
Choose $\varepsilon > 0$. Then one constructs a global smooth symmetric *Bloch frame Φ_{sm} such that*

$$\sup_{k\in\mathbb{R}^d} \operatorname{dist}(\Phi(k), \Phi_{sm}(k)) < \varepsilon \tag{5.1}$$

where $\operatorname{dist}(\Phi, \Psi) = \left(\sum_a \|\phi_a - \psi_a\|^2_{\mathcal{H}}\right)^{1/2}$ *is the distance in* $\operatorname{Fr}(m, \mathcal{H})$.

Notice that, for any $\Phi \in \operatorname{Fr}(m, \mathcal{H})$ and $U, W \in \mathcal{U}(m)$, one has

$$\operatorname{dist}(\Phi \triangleleft U, \Phi \triangleleft W) = \|U - W\|_{HS} \tag{5.2}$$

where $\|U\|^2_{HS} = \sum_{a,b=1}^m |U_{ab}|^2$ is the Hilbert-Schmidt norm. Thus, the distance between the frames $\Phi \triangleleft U$ and $\Phi \triangleleft W$ is the length of the chord between U and W in the ambient space $\mathbb{C}^{m^2} \simeq M_m(\mathbb{C}) \supset \mathcal{U}(m)$. On the other hand, each frame space $F_k := \operatorname{Fr}\operatorname{Ran} P(k) \simeq \mathcal{U}(m)$ inherits from $\mathcal{U}(m)$ a Riemannian structure[16], and the corresponding geodesic distance $\mathrm{d}(U, W)$ can be compared to the chord distance (5.2). In a neighborhood of the identity, the geodesic distance and the ambient distance are locally Lipschitz equivalent, namely

$$1/2\, \mathrm{d}(\mathbb{I}, U) \le \|\mathbb{I} - U\|_{HS} \le \mathrm{d}(\mathbb{I}, U) \qquad \forall U \in \mathcal{U}(M) : \ \|\mathbb{I} - U\|_{HS} < 1/2\tau_m, \tag{5.3}$$

where τ_m is defined as the largest number having the following property: The open normal bundle over $\mathcal{U}(m)$ of radius r is embedded in $\mathbb{R}^{2m^2} \simeq M_m(\mathbb{C})$ for every $r < \tau_m$. The first inequality in (5.3) is a straightforward consequence of [36, Prop. 6.3], where also the relation between τ_m and the principal curvature of $\mathcal{U}(m)$ is discussed.

Proof. Following [37], we recall that, to a family of projectors $\mathcal{P}$ satisfying properties (P_1) and (P_2), one can canonically associate a smooth Hermitian vector bundle $\mathcal{E}_{\mathcal{P}} = (E_{\mathcal{P}} \to \mathbb{T}^d_*)$, where $\mathbb{T}^d_* = \mathbb{R}^d/\Lambda$. In particular, $\mathcal{E}_{\mathcal{P}}$ is defined by using an equivalence relation $\sim_\tau$ on $\mathbb{R}^d \times \mathcal{H}$, namely

$$(k, \phi) \sim_\tau (k', \phi') \qquad \text{if and only if} \qquad \exists \lambda \in \Lambda : k' = k + \lambda,\ \phi' = \tau_\lambda \phi.$$

An equivalence class is denoted by $[k, \phi]_\tau$. Then, the total space is defined by

[16] Recall that $\mathcal{U}(m)$ is a Riemannian manifold with respect to the bi-invariant metric defined, for A, B in the Lie algebra $\mathfrak{u}(m) = \{A \in M_m(\mathbb{C}) : A^* = -A\}$, by $\langle A, B\rangle_{HS} = \operatorname{Tr}(A^* B)$.

$$E_{\mathcal{P}} = \left\{ [k,\phi]_\tau \in \left(\mathbb{R}^d \times \mathcal{H} \right) / \sim_\tau : \phi \in \operatorname{Ran} P(k) \right\},$$

and the projection $\pi : E_{\mathcal{P}} \to \mathbb{T}^d_*$ by $\pi([k,\phi]_\tau) = k \pmod \Lambda$. The fact that $\mathcal{E}_{\mathcal{P}}$ is a smooth vector bundle follows from (P_1) and the Kato-Nagy formula, see [37, 38] for the proof. Moreover, a natural Hermitian structure is induced by the inner product in $\mathcal{H}$.

Equipped with the above definition, we observe that a continuous τ-equivariant global Bloch frame $\Phi : \mathbb{R}^d \to \mathcal{H}^m$ is identified with a continuous global section σ_Φ of the (principal) bundle of the orthonormal frames of the bundle $\mathcal{E}_{\mathcal{P}}$, denoted by $\operatorname{Fr} \mathcal{E}_{\mathcal{P}}$. The identification is given by

$$\sigma_\Phi(x) = \left([k,\phi_1(k)]_\tau, \dots, [k,\phi_m(k)]_\tau \right) \in (\operatorname{Fr} E_{\mathcal{P}})_x \qquad \text{for } x = k \bmod \Lambda.$$

According to a classical result, the Steenrod's Approximation Theorem ([52]; see [54] for recent generalizations), there exists a smooth global section $\sigma'_\Phi : \mathbb{T}^d_* \to \operatorname{Fr} E_{\mathcal{P}}$ such that

$$\sup_{x \in \mathbb{T}^d_*} \operatorname{dist}\left(\sigma_\Phi(x), \sigma'_\Phi(x) \right) < 1/2\,\varepsilon.$$

Going back to the language of Bloch frames, one concludes the existence of a global smooth τ-equivariant Bloch frame $\Phi'_{\mathrm{sm}} : \mathbb{R}^d \to \mathcal{H}^m$, such that

$$\sup_{k \in \mathbb{R}^d} \operatorname{dist}\left(\Phi(k), \Phi'_{\mathrm{sm}}(k) \right) < 1/2\,\varepsilon. \tag{5.4}$$

In general, the Bloch frame Φ'_{sm} does not satisfy property (F_3). In order to recover time-reversal symmetry, we use the following symmetrization procedure.

First, we recall that there exists $\delta > 0$ such that the exponential map $\exp : \mathfrak{u}(m) \to \mathcal{U}(m)$ is a diffeomorphism from the ball $B_\delta(0) \subset \mathfrak{u}(m)$ to the geodesic ball $B_\delta(\mathbb{1}) \subset \mathcal{U}(m)$, see *e.g.* [19, Chapter II] or [48, Chapter VII]. In particular, for any $U \in B_\delta(\mathbb{1})$, there exists a unique $A_U \in B_\delta(0)$ such that

$$U = \exp(A_U), \qquad U \in B_\delta(\mathbb{1}), \tag{5.5}$$

and, moreover, the map $U \mapsto A_U$ is C^∞-smooth on $B_\delta(\mathbb{1})$. Since the exponential map is normalized so that $\mathrm{d}(\mathbb{1}, U) = \| A_U \|_{\mathrm{HS}}$, then $\mathrm{d}(\mathbb{1}, \overline{U}) = \mathrm{d}(\mathbb{1}, U) = \mathrm{d}(\mathbb{1}, U^{-1})$. In particular, both $\overline{U}$ and U^{-1} are in the geodesic ball $B_\delta(\mathbb{1})$, whenever $U \in B_\delta(\mathbb{1})$.
For $U \in B_\delta(\mathbb{1})$, the midpoint $M(\mathbb{1}, U)$ between $\mathbb{1}$ and U is defined by[17]

$$M(\mathbb{1}, U) := \exp(1/2\,A_U) \qquad \in B_\delta(\mathbb{1}) \subset \mathcal{U}(m). \tag{5.6}$$

One immediately checks that, for $U \in B_\delta(\mathbb{1})$,

$$M(\mathbb{1}, \overline{U}) = \exp\left(1/2\,\overline{A_U} \right) = \overline{M(\mathbb{1}, U)} \tag{5.7}$$

$$M(\mathbb{1}, U^{-1}) = \exp\left(-1/2\,A_U \right) = U^{-1} M(\mathbb{1}, U). \tag{5.8}$$

Moreover,

[17] Definition (5.6) agrees with the geodesic midpoint between $\mathbb{1}$ and U in the Riemannian manifold $\mathcal{U}(m)$, since the exponential map is normalized so that $\mathrm{d}(\mathbb{1}, \exp(sN)) = s$, for $s < \delta$ and $\|N\|_{\mathrm{HS}} = 1$.

$$\mathrm{d}(\mathbb{1}, M(\mathbb{1},U)) = 1/2\,\mathrm{d}(\mathbb{1},U). \tag{5.9}$$

Consider now two orthonormal frames $\Phi, \Psi \in \mathrm{Fr}\,\mathrm{Ran}\,P(k)$, such that $\mathrm{dist}(\Phi,\Psi) < \varepsilon$. For ε sufficiently small, we define the **midpoint** $\widehat{M}(\Phi,\Psi) \in \mathrm{Fr}\,\mathrm{Ran}\,P(k)$ in the following way.
Let $U_{\Phi,\Psi} \in \mathcal{U}(m)$ be the unique unitary such that $\Psi = \Phi \triangleleft U_{\Phi,\Psi}$, namely $\left(U_{\Phi,\Psi}\right)_{ab} = \left\langle \phi_a, \psi_b \right\rangle$. Taking (5.2) and (5.3) into account, one has

$$\varepsilon > \mathrm{dist}(\Phi,\Psi) = \mathrm{dist}(\Phi, \Phi \triangleleft U_{\Phi,\Psi}) = \left\| \mathbb{1} - U_{\Phi,\Psi} \right\|_{\mathrm{HS}} \geq 1/2\ \mathrm{d}(\mathbb{1}, U_{\Phi,\Psi}).$$

Choose ε sufficiently small, namely $\varepsilon < \delta/2$. Then $U_{\Phi,\Psi}$ is in the geodesic ball $B_\delta(\mathbb{1}) \subset \mathcal{U}(m)$. By using (5.6), we define

$$\widehat{M}(\Phi,\Psi) := \Phi \triangleleft M(\mathbb{1}, U_{\Phi,\Psi}) \qquad \in \mathrm{Fr}\,\mathrm{Ran}\,P(k). \tag{5.10}$$

We show that

$$\widehat{M}(\Theta\Phi,\Theta\Psi) = \Theta\,\widehat{M}(\Phi,\Psi) \tag{5.11}$$

$$\widehat{M}(\tau_\lambda\Phi,\tau_\lambda\Psi) = \tau_\lambda\,\widehat{M}(\Phi,\Psi). \tag{5.12}$$

Notice preliminarily that, since both Θ and τ_λ are isometries of $\mathcal{H}$, one has

$$\mathrm{dist}(\Theta\Phi,\Theta\Psi) = \mathrm{dist}(\Phi,\Psi) = \mathrm{dist}(\tau_\lambda\Phi,\tau_\lambda\Psi) \tag{5.13}$$

for all $\Phi,\Psi \in \mathrm{Fr}(m,\mathcal{H})$. Thus, the midpoints appearing on the left-hand sides of (5.11) and (5.12) are well-defined, whenever $\mathrm{dist}(\Phi,\Psi) < 1/2\delta$.
Equation (5.11) follows from (5.7) and from the fact that $\Theta\left(\Phi \triangleleft U_{\Phi,\Psi}\right) = (\Theta\Phi) \triangleleft \overline{U_{\Phi,\Psi}}$. Indeed, one has

$$\begin{aligned}
\widehat{M}(\Theta\Phi,\Theta\Psi) &= \widehat{M}\left(\Theta\Phi, \Theta\left(\Phi \triangleleft U_{\Phi,\Psi}\right)\right) = \widehat{M}\left(\Theta\Phi, (\Theta\Phi) \triangleleft \overline{U_{\Phi,\Psi}}\right) \\
&= (\Theta\Phi) \triangleleft M(\mathbb{1}, \overline{U_{\Phi,\Psi}}) = (\Theta\Phi) \triangleleft \overline{M(\mathbb{1}, U_{\Phi,\Psi})} \\
&= \Theta\left(\Phi \triangleleft M(\mathbb{1}, U_{\Phi,\Psi})\right) = \Theta\,\widehat{M}(\Phi,\Psi).
\end{aligned}$$

Analogously, equation (5.12) follows from the fact that $\tau_\lambda\left(\Phi \triangleleft U_{\Phi,\Psi}\right) = (\tau_\lambda\Phi) \triangleleft U_{\Phi,\Psi}$.

We focus now on the smooth τ-equivariant Bloch frame $\Phi'_{\mathrm{sm}} : \mathbb{R}^d \to \mathcal{H}^m$ obtained, via Steenrod's theorem, from the continuous symmetric frame Φ. Since $\mathrm{Ran}\,P(k) = \Theta\,\mathrm{Ran}\,P(-k)$, one has that $\Theta\Phi'_{\mathrm{sm}}(-k)$ is in $F_k = \mathrm{Fr}\,\mathrm{Ran}\,P(k)$. Thus, we set

$$\Phi_{\mathrm{sm}}(k) := \widehat{M}\left(\Phi'_{\mathrm{sm}}(k), \Theta\Phi'_{\mathrm{sm}}(-k)\right) \qquad \in F_k. \tag{5.14}$$

The definition (5.14) is well-posed. Indeed, taking (5.4) and (5.13) into account, one has

$$\begin{aligned}
&\mathrm{dist}(\Phi'_{\mathrm{sm}}(k), \Theta\Phi'_{\mathrm{sm}}(-k)) \\
&\leq \mathrm{dist}(\Phi'_{\mathrm{sm}}(k), \Phi(k)) + \mathrm{dist}(\Phi(k), \Theta\Phi(-k)) + \mathrm{dist}(\Theta\Phi(-k), \Theta\Phi'_{\mathrm{sm}}(-k)) \\
&= \mathrm{dist}(\Phi'_{\mathrm{sm}}(k), \Phi(k)) + \mathrm{dist}(\Phi(-k), \Phi'_{\mathrm{sm}}(-k)) < \varepsilon < 1/2\delta,
\end{aligned} \tag{5.15}$$

where we used the fact that the central addendum (in the second line) vanishes since Φ satisfies (F_3).

We claim that (5.14) defines a smooth symmetric global Bloch frame satisfying (5.1). We explicitly check that:

1. the map $k \mapsto \Phi_{\rm sm}(k)$ is smooth. Indeed, since Θ is an isometry of $\mathcal{H}$, the map $k \mapsto \Theta \Phi'_{\rm sm}(-k) =: \Psi'_{\rm sm}(k)$ is smooth. Hence $k \mapsto U_{\Phi'_{\rm sm}(k),\Psi'_{\rm sm}(k)} \in \mathcal{U}(m)$ is smooth, since $\left(U_{\Phi,\Psi}\right)_{ab} = \langle \phi_a , \psi_b \rangle$. In view of (5.15) and (5.3), $U_{\Phi'_{\rm sm}(k),\Psi'_{\rm sm}(k)}$ is, for every $k \in \mathbb{R}^d$, in the geodesic ball $B_\delta(\mathbb{1})$ where the exponential map defines a diffeomorphism. As a consequence,

$$k \mapsto \Phi'_{\rm sm}(k) \triangleleft M(\mathbb{1}, U_{\Phi'_{\rm sm}(k),\Psi'_{\rm sm}(k)}) = \Phi_{\rm sm}(k)$$

is smooth from $\mathbb{R}^d$ to $\mathcal{H}^m$.

2. the Bloch frame $\Phi_{\rm sm}$ satisfies (F_2). Indeed, by using (P_4) and (5.12), one obtains

$$\begin{aligned}
\Phi_{\rm sm}(k+\lambda) &= \widehat{M}\big(\Phi'_{\rm sm}(k+\lambda), \Theta\Phi'_{\rm sm}(-k-\lambda)\big) \\
&= \widehat{M}\big(\tau_\lambda \Phi'_{\rm sm}(k), \Theta\tau_{-\lambda}\Phi'_{\rm sm}(-k)\big) \\
&= \widehat{M}\big(\tau_\lambda \Phi'_{\rm sm}(k), \tau_\lambda\Theta\Phi'_{\rm sm}(-k)\big) \\
&= \tau_\lambda \widehat{M}\big(\Phi'_{\rm sm}(k), \Theta\Phi'_{\rm sm}(-k)\big) = \tau_\lambda \Phi_{\rm sm}(k).
\end{aligned}$$

3. the Bloch frame $\Phi_{\rm sm}$ satisfies (F_3). Indeed, by using $\Theta^2 = \mathbb{1}$ and (5.11), one has

$$\begin{aligned}
\Phi_{\rm sm}(-k) &= \widehat{M}\big(\Theta^2\Phi'_{\rm sm}(-k), \Theta\Phi'_{\rm sm}(k)\big) \\
&= \Theta\widehat{M}\big(\Theta\Phi'_{\rm sm}(-k), \Phi'_{\rm sm}(k)\big) \\
&= \Theta\widehat{M}\big(\Phi'_{\rm sm}(k), \Theta\Phi'_{\rm sm}(-k)\big) = \Theta\Phi_{\rm sm}(k),
\end{aligned}$$

where we used the fact that $\widehat{M}(\Phi,\Psi) = \widehat{M}(\Psi,\Phi)$, whenever $\mathrm{dist}(\Phi,\Psi) < \delta/2$. The latter fact is a direct consequence of (5.8), since

$$\begin{aligned}
\widehat{M}(\Phi,\Psi) &= \Phi \triangleleft M(\mathbb{1}, U_{\Phi,\Psi}) = \big(\Psi \triangleleft U_{\Phi,\Psi}^{-1}\big) \triangleleft M(\mathbb{1}, U_{\Phi,\Psi}) \\
&= \Psi \triangleleft \big(U_{\Phi,\Psi}^{-1} M(\mathbb{1}, U_{\Phi,\Psi})\big) = \Psi \triangleleft M(\mathbb{1}, U_{\Phi,\Psi}^{-1}) \\
&= \Psi \triangleleft M(\mathbb{1}, U_{\Psi,\Phi}) = \widehat{M}(\Psi,\Phi).
\end{aligned}$$

4. equation (5.1) is satisfied in view of (5.15). Indeed, setting $U_{\Phi'_{\rm sm}(k),\Psi'_{\rm sm}(k)} \equiv U(k)$ for notational convenience and using (5.2), (5.3) and (5.9), one obtains

$$\begin{aligned}
\mathrm{dist}(\Phi'_{\rm sm}(k), \Phi_{\rm sm}(k)) &= \mathrm{dist}\big(\Phi'_{\rm sm}(k), \Phi'_{\rm sm}(k) \triangleleft M(\mathbb{1}, U(k))\big) \\
&= \|\mathbb{1} - M(\mathbb{1}, U(k))\|_{\rm HS} \le \mathrm{d}\,(\mathbb{1}, M(\mathbb{1}, U(k))) = 1/2\,\mathrm{d}(\mathbb{1}, U(k)) \\
&\le \|\mathbb{1} - U(k)\|_{\rm HS} = \mathrm{dist}\big(\Phi'_{\rm sm}(k), \Theta\Phi'_{\rm sm}(-k)\big) < \varepsilon.
\end{aligned}$$

This concludes the proof of the Proposition. □

References

1. BLOUNT, E. I. : Formalism of Band Theory. In : Seitz, F., Turnbull, D. (eds.), *Solid State Physics* **13**, pages 305–373, Academic Press, 1962.
2. BROUDER CH.; PANATI G.; CALANDRA M.; MOUROUGANE CH.; MARZARI N.: Exponential localization of Wannier functions in insulators. *Phys. Rev. Lett.* **98** (2007), 046402.
3. CANCÈS, E.; LEWIN, M. : The dielectric permittivity of crystals in the reduced Hartree-Fock approximation. *Arch. Ration. Mech. Anal.* **197** (2010), 139–177.
4. CERULLI IRELLI, G. ; FIORENZA, D.; MONACO, D.; PANATI, G. : Geometry of Bloch bundles: a unifying quiver-theoretic approach, in preparation (2015).
5. DES CLOIZEAUX, J. : Energy bands and projection operators in a crystal: Analytic and asymptotic properties. *Phys. Rev.* **135** (1964), A685–A697.
6. DES CLOIZEAUX, J. : Analytical properties of n-dimensional energy bands and Wannier functions. *Phys. Rev.* **135** (1964), A698–A707.
7. CORNEAN, H.D.; HERBST, I.; NENCIU, G. : in preparation (2015).
8. CORNEAN, H.D.; NENCIU A.; NENCIU, G. : Optimally localized Wannier functions for quasi one-dimensional nonperiodic insulators. *J. Phys. A: Math. Theor.* **41** (2008), 125202.
9. E, W.; LU, J. : The electronic structure of smoothly deformed crystals: Wannier functions and the Cauchy-Born rule. *Arch. Ration. Mech. Anal.* **199** (2011), 407–433.
10. FIORENZA, D.; MONACO, D.; PANATI, G. : $\mathbb{Z}_2$ invariants of topological insulators as geometric obstructions, (2014).
11. FU, L.; KANE, C.L. : Time reversal polarization and a $\mathbb{Z}_2$ adiabatic spin pump. *Phys. Rev. B* **74** (2006), 195312.
12. FU, L.; KANE, C.L.; MELE, E.J. : Topological insulators in three dimensions. *Phys. Rev. Lett.* **98** (2007), 106803.
13. GOEDECKER, S. : Linear scaling electronic structure methods, *Rev. Mod. Phys.* **71** (1999), 1085–1111.
14. GRAF, G.M.; PORTA, M. : Bulk-edge correspondence for two-dimensional topological insulators, *Commun. Math. Phys.* **324** (2013), 851–895.
15. HALDANE, F.D.M. : Model for a Quantum Hall effect without Landau levels: condensed-matter realization of the "parity anomaly". *Phys. Rev. Lett.* **61** (1988), 2017.
16. HASAN, M.Z.; KANE, C.L. : Colloquium: Topological Insulators. *Rev. Mod. Phys.* **82** (2010), 3045–3067.
17. HASTINGS, M. B.: Topology and phases in fermionic systems. *J. Stat. Mech. Theory Exp.* (2008), L01001.
18. HELFFER, B.; SJÖSTRAND, J. : Équation de Schrödinger avec champ magnétique et équation de Harper. In: Schrödinger operators, Lecture Notes in Physics 345, Springer, Berlin, 1989, 118–197.
19. HELGASON, S. : *Differential Geometry, Lie Groups, and Symmetric Spaces*, Academic Press, New York, 1978.
20. IBAÑEZ-AZPIROZ, J.; EIGUREN, A.; BERGARA, A.; PETTINI, G.; MODUGNO, M. : Tight-binding models for ultracold atoms in honeycomb optical lattices. *Phys. Rev. A* **87** (2013), 011602.
21. IBAÑEZ-AZPIROZ, J.; EIGUREN, A.; BERGARA, A.; PETTINI, G.; MODUGNO, M. : Self-consistent tight-binding description of Dirac points moving and merging in two-dimensional optical lattices. *Phys. Rev. A* **88** (2013), 033631.
22. KANE, C.L.; MELE, E.J. : $\mathbb{Z}_2$ Topological Order and the Quantum Spin Hall Effect. *Phys. Rev. Lett.* **95** (2005), 146802.
23. KANE, C.L.; MELE, E.J. : Quantum Spin Hall Effect in graphene. *Phys. Rev. Lett.* **95** (2005), 226801.
24. KATO, T. : *Perturbation theory for linear operators*, Springer, Berlin, 1966.
25. KIEVELSEN, S. : Wannier functions in one-dimensional disordered systems: application to fractionally charged solitons. *Phys. Rev. B* **26** (1982), 4269–4274.
26. KING-SMITH, R. D. ; VANDERBILT, D. : Theory of polarization of crystalline solids. *Phys. Rev. B* **47** (1993), 1651–1654.
27. KOHN, W. : Analytic Properties of Bloch Waves and Wannier Functions. *Phys. Rev.* **115** (1959), 809.
28. LEWIN, M.; SÉRÉ, É. : Spectral pollution and how to avoid it (with applications to Dirac and periodic Schrödinger operators). *Proc. Lond. Math. Soc.* **100** (2010), 864–900.
29. MARZARI, N. ; VANDERBILT, D. : Maximally localized generalized Wannier functions for composite energy bands. *Phys. Rev. B* **56** (1997), 12847–12865.

30. Marzari, N.; Mostofi A.A.; Yates J.R.; Souza I.; Vanderbilt D. : Maximally localized Wannier functions: Theory and applications. *Rev. Mod. Phys.* **84** (2012), 1419.
31. Monaco, D.; Panati, G. : Symmetry and localization in periodic crystals: triviality of Bloch bundles with a fermionic time-reversal symmetry, to appear in the proceedings of the conference *"SPT2014 – Symmetry and Perturbation Theory"*, Cala Gonone, Italy (2014).
32. Nenciu, G. : Existence of the exponentially localised Wannier functions. *Commun. Math. Phys.* **91** (1983), 81–85.
33. Nenciu, G. : Dynamics of band electrons in electric and magnetic fields: Rigorous justification of the effective Hamiltonians. *Rev. Mod. Phys.* **63** (1991), 91–127.
34. Nenciu, A.; Nenciu, G. : Dynamics of Bloch electrons in external electric fields. II. The existence of Stark-Wannier ladder resonances. *J. Phys. A***15** (1982), 3313–3328.
35. Nenciu, A.; Nenciu, G. : The existence of generalized Wannier functions for one-dimensional systems. *Commun. Math. Phys.* **190** (1988), 541–548.
36. Niyogi, P.; Smale, S.; Weinberger, S. : Finding the homology of submanifolds with high confidence from random samples, *Discrete Comput. Geom.* **39** (2008), 419–441.
37. Panati, G.: Triviality of Bloch and Bloch-Dirac bundles. *Ann. Henri Poincaré* **8** (2007), 995–1011.
38. Panati, G.; Pisante, A.: Bloch bundles, Marzari-Vanderbilt functional and maximally localized Wannier functions. *Commun. Math. Phys.* **322** (2013), 835–875.
39. Panati, G.; Sparber, C.; Teufel, S. : Geometric currents in piezoelectricity. *Arch. Rat. Mech. Anal.* **91** (2009), 387–422.
40. Panati, G.; Spohn, H.; Teufel, S. : Effective dynamics for Bloch electrons: Peierls substitution and beyond. *Commun. Math. Phys.* **242** (2003), 547–578.
41. Pelinovsky, D.; Schneider, G.; MacKay, R. S. : Justification of the lattice equation for a nonlinear elliptic problem with a periodic potential. *Commun. Math. Phys.* **284** (2008), 803–831.
42. Pelinovsky, D. ; Schneider, G. : Bounds on the tight-binding approximation for the Gross-Pitaevskii equation with a periodic potential. *J. Differ. Equations* **248** (2010), 837–849.
43. Prodan, E. : Robustness of the spin-Chern number. *Phys. Rev. B* **80** (2009), 125327.
44. Prodan, E. : Disordered topological insulators: A non-commutative geometry perspective. *J. Phys. A* **44** (2011), 113001.
45. Reed M., Simon, B. : Methods of Modern Mathematical Physics. Volume IV: Analysis of Operators. Academic Press, New York, 1978.
46. Resta, R. : Theory of the electric polarization in crystals. *Ferroelectrics* **136** (1992), 51–75.
47. Ryu, S.; Schnyder, A. P.; Furusaki, A.; Ludwig, A. W. W. : Topological insulators and superconductors: Tenfold way and dimensional hierarchy. *New J. Phys.* **12** (2010), 065010.
48. Simon, B. : *Representations of Finite and Compact Groups*, Graduate studies in mathematics, vol. 10, American Mathematical Society, 1996.
49. Soluyanov, A.; Vanderbilt, D. : Wannier representation of $\mathbb{Z}_2$ topological insulators. *Phys. Rev. B* **83** (2011), 035108.
50. Soluyanov, A.A.; Vanderbilt, D. : Computing topological invariants without inversion symmetry, *Phys. Rev. B* **83** (2011), 235401.
51. Soluyanov, A.; Vanderbilt, D. : Smooth gauge for topological insulators. *Phys. Rev. B* (2012), 115415.
52. Steenrod, N. : *The Topology of Fibre Bundles*, Princeton Mathematical Series vol.14, Princeton University Press, Princeton, 1951.
53. Walters, R.; Cotugno, G.; Johnson, T. H.; Clark, S. R.; Jaksch, D. : Ab initio derivation of Hubbard models for cold atoms in optical lattices. *Phys. Rev. A* **87** (2013), 043613.
54. Wockel, Ch. : A generalization of Steenrod's Approximation Theorem. *Arch. Math. (Brno)* **45** (2009), 95–104.

$\mathbb{Z}_2$ invariants of topological insulators as geometric obstructions

Domenico Fiorenza, Domenico Monaco, and Gianluca Panati

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 $-\mathbb{1}$. 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 $\mathbb{Z}_2$-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 $\mathbb{Z}_2$ 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.

Key words: Topological insulators, time-reversal symmetry, Kane-Mele model, $\mathbb{Z}_2$ invariants, Bloch frames.

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 [40], in the context of the Integer Quantum Hall Effect. The first topological invariants to make their appearance in the condensed matter lit-

Domenico Fiorenza
Dipartimento di Matematica, “La Sapienza” Università di Roma, Piazzale Aldo Moro 2, 00185 Rome, Italy
e-mail: fiorenza@mat.uniroma1.it

Domenico Monaco
SISSA, Via Bonomea 265, 34136 Trieste, Italy
e-mail: dmonaco@sissa.it

Gianluca Panati
Dipartimento di Matematica, “La Sapienza” Università di Roma, Piazzale Aldo Moro 2, 00185 Rome, Italy
e-mail: panati@mat.uniroma1.it

erature 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 [14] and references therein). These topological invariants are related to an observable quantity, namely to the transverse (Hall) conductivity of the system under consideration [40, 14]; 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 [16]. Since this pioneering observation, the field of *Chern insulators* flourished [36, 7, 11].

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 [2, 17] 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 [20, 21]. 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 Θ is such that $\Theta^2 = -\mathbb{1}$.

In a milestone paper [20], 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 [16], 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 [12], 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 [13].

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 [39], and to study the localization of Wannier functions in TRS topological insulators [37, 38]. 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 [28]), 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 [1, 27, 24, 32, 23], C^*-algebraic and functional-analytic approaches [29, 30, 33, 34], the bulk-edge correspondence [3, 15], monodromy arguments [31], or gauge-theoretic methods [10, 4, 5]. However, we believe that a clear and simple topological explanation of how they arise from the symmetries of the system is still in a initiatory stage.

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 [12] on mathematical grounds. We consider a gapped periodic quantum system in presence of fermionic time-reversal symmetry (compare Assumption 2.1), and we investigate whether there exists a global continuous Bloch frame which is both periodic and time-reversal symmetric. While in $1d$ this always exists, a topological obstruction may arise in $2d$. We show in Section 3 that such obstruction is encoded in a $\mathbb{Z}_2$ index δ, 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 $\Delta \in \mathbb{Z}_2$ [12], 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 $3d$, 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 [13]. 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).

A similar obstruction-theoretic approach to the invariants of 2-dimensional topological insulators was adopted in [15]. In particular, aiming at a proof of the bulk-edge correspondence, there the authors associate a $\mathbb{Z}_2$ index to the *time-reversal invariant bundle* associated to the bulk Hamiltonian for a semi-infinite crystal, enjoying a time-reversal symmetry of fermionic type.

Even though our starting assumptions on the family of projectors, to which we associate $\mathbb{Z}_2$-valued topological invariants, are modeled on the properties of the spectral projectors of a time-reversal symmetric Hamiltonian retaining *full* periodicity in dimension $d \le 3$ (compare Assumption 2.1), the setting of [15] is also covered by our method: our results can be applied to the family of projectors associated to the bulk time-reversal invariant bundle, up to an identification of the coordinates on the basis torus.

Indeed, the main advantage of our method is that, being geometric in nature, it is based only on the *fundamental symmetries* of the system, namely invariance by (lattice) translations (*i. e.* periodicity) and fermionic time-reversal symmetry. This makes our approach *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 insultators. The method proposed here encompasses all models studied by the community, in particular the Fu-Kane-Mele models in $2d$ and $3d$ [20, 12, 13], as well as more general tight-binding models in 2 dimensions like the ones considered *e. g.* in [3] and, as already mentioned, in [15].

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.

Acknowledgments. We thank H. Schulz-Baldes, G.M. Graf and M. Porta for interesting discussions. We are grateful to the *Institut Henri Poincaré* for the kind hospitality in the framework of the trimester "Variational and Spectral Methods in Quantum Mechanics", organized by M. J. Esteban and M. Lewin, and to the *Erwin Schrödinger Institute* for the kind hospitality in the framework of the thematic programme "Topological Phases of Quantum Matter", organized by N. Read, J. Yngvason, and M. Zirnbauer.
The project was supported by INdAM-GNFM (Progetto Giovane Ricercatore) and by MIUR (Progetto PRIN 2012).

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

$$P(k) = \sum_{n \in \mathcal{I}_{\mathrm{occ}}} |u_n(k)\rangle \langle u_n(k)|, \quad k \in \mathbb{R}^d, \tag{2.1}$$

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 $\Lambda = \mathrm{Span}_{\mathbb{Z}} \{e_1, \ldots, e_d\} \simeq \mathbb{Z}^d \subset \mathbb{R}^d$: in applications, Λ is the dual lattice to the periodicity Bravais lattice Γ in position space. The object of our study will be a family of orthogonal projectors $\{P(k)\}_{k \in \mathbb{R}^d} \subset \mathcal{B}(\mathcal{H})$, satisfying the following

Assumption 2.1. The family of orthogonal projectors $\{P(k)\}_{k \in \mathbb{R}^d}$ enjoys the following properties:

- (P_1) *smoothness*: the map $\mathbb{R}^d \ni k \mapsto P(k) \in \mathcal{B}(\mathcal{H})$ is C^∞-smooth;
- (P_2) *τ-covariance*: the map $k \mapsto P(k)$ is covariant with respect to a unitary representation[1] $\tau \colon \Lambda \to \mathcal{U}(\mathcal{H})$ of the lattice Λ on the Hilbert space $\mathcal{H}$, *i. e.*

$$P(k+\lambda) = \tau(\lambda) P(k) \tau(\lambda)^{-1}, \quad \text{for all } k \in \mathbb{R}^d, \text{ for all } \lambda \in \Lambda;$$

- ($P_{3,-}$) *time-reversal symmetry*: the map $k \mapsto P(k)$ is time-reversal symmetric, *i. e.* there exists an antiunitary operator[2] $\Theta \colon \mathcal{H} \to \mathcal{H}$, called the *time-reversal operator*, such that

$$\Theta^2 = -\mathbb{1}_{\mathcal{H}} \quad \text{and} \quad P(-k) = \Theta P(k) \Theta^{-1}.$$

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

$$\Theta \tau(\lambda) = \tau(\lambda)^{-1} \Theta \quad \text{for all } \lambda \in \Lambda. \tag{P_4}$$ ◊

Assumption 2.1 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 $k \mapsto P(k)$ defined in (2.1) will be smooth (compare (P_1)), while τ-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

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

[2] Recall that a surjective antilinear operator $\Theta \colon \mathcal{H} \to \mathcal{H}$ is called *antiunitary* if $\langle \Theta\psi_1, \Theta\psi_2 \rangle = \langle \psi_2, \psi_1 \rangle$ for all $\psi_1, \psi_2 \in \mathcal{H}$.

models satisfy the previous Assumption, including the eigenprojectors for the tight-binding Hamiltonians proposed by Fu, Kane and Mele in [20, 12, 13], as well as in many *continuous* models. Finally, Assumption 2.1 is satisfied also in the tight-binding models studied in [15]: 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[3] (k_1, k_2) with the variables (k, z) appearing in [15].

For a family of projectors satisfying Assumption 2.1, 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

$$(\phi, \psi) := \langle \Theta\phi, \psi \rangle \quad \text{for} \quad \phi, \psi \in \mathcal{H}$$

defines a bilinear, skew-symmetric, non-degenerate form on $\mathcal{H}$; its restriction to $\operatorname{Ran} P(0) \subset \mathcal{H}$ (which is an invariant subspace for the action of Θ 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 2.1 ((Symmetric) Bloch frame). Let $\{P(k)\}_{k \in \mathbb{R}^d}$ be a family of projectors satisfying Assumption 2.1, and let also Ω be a region in $\mathbb{R}^d$. A **Bloch frame** for $\{P(k)\}_{k \in \mathbb{R}^d}$ on Ω is a collection of maps $\Omega \ni k \mapsto \phi_a(k) \in \mathcal{H}$, $a \in \{1, \dots, m\}$, such that for all $k \in \Omega$ the set $\Phi(k) := \{\phi_1(k), \dots, \phi_m(k)\}$ is an orthonormal basis spanning $\operatorname{Ran} P(k)$. When $\Omega = \mathbb{R}^d$, the Bloch frame is said to be *global*. A Bloch frame is called

(F_0) *continuous* if all functions $\phi_a \colon \Omega \to \mathcal{H}$, $a \in \{1, \dots, m\}$, are continous;
(F_1) *smooth* if all functions $\phi_a \colon \Omega \to \mathcal{H}$, $a \in \{1, \dots, m\}$, are C^∞-smooth.

We also say that a global Bloch frame is

(F_2) τ*-equivariant* if

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

(F_3) *time-reversal invariant* if

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

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

A global Bloch frame which is both τ-equivariant and time-reversal invariant is called **symmetric**. ◊

We are now in position to state our goal: we seek the answer to the following

Question $(\mathbf{Q}_d)$. *Let $d \le 3$. Given a family of projectors $\{P(k)\}_{k \in \mathbb{R}^d}$ satisfying Assumption 2.1 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)*?*

[3] The coordinates $(k_1, \dots, k_d)$ are expressed in terms of a basis $\{e_1, \dots, e_d\} \subset \mathbb{R}^d$ generating the lattice Λ as $\Lambda = \operatorname{Span}_{\mathbb{Z}} \{e_1, \dots, e_d\}$.

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 *topologically obstructed*. Explicitly, the main results of this paper are the following.

Theorem 2.1 (Answer to (Q_1)). *Let $d = 1$, and let $\{P(k)\}_{k\in\mathbb{R}}$ be a family of projectors satisfying Assumption 2.1. Then there exists a global continuous symmetric Bloch frame for $\{P(k)\}_{k\in\mathbb{R}}$. Moreover, such Bloch frame can be explicitly constructed.*

The proof of Theorem 2.1 is contained in Section 3.3 (see Remark 3.1).

Theorem 2.2 (Answer to (Q_2)). *Let $d = 2$, and let $\{P(k)\}_{k\in\mathbb{R}^2}$ be a family of projectors satisfying Assumption 2.1. Then there exists a global continuous symmetric Bloch frame for $\{P(k)\}_{k\in\mathbb{R}^2}$ if and only if*

$$\delta(P) = 0 \in \mathbb{Z}_2, \tag{2.2}$$

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 2.2, 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 *topological invariant* of the family of projectors (Proposition 3.4), which agrees with the Fu-Kane index (Theorem 4.1).

Theorem 2.3 (Answer to (Q_3)). *Let $d = 3$, and let $\{P(k)\}_{k\in\mathbb{R}^3}$ be a family of projectors satisfying Assumption 2.1. Then there exists a global continuous symmetric Bloch frame for $\{P(k)\}_{k\in\mathbb{R}^3}$ if and only if*

$$\delta_{1,0}(P) = \delta_{1,+}(P) = \delta_{2,+}(P) = \delta_{3,+}(P) = 0 \in \mathbb{Z}_2, \tag{2.3}$$

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 2.3, 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.

Remark 2.1 (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 *smooth* symmetric Bloch frames exist for $\{P(k)\}_{k\in\mathbb{R}^d}$, *i. e.* global Bloch frames satisfying (F_1), (F_2) and (F_3). We show in Appendix A that, whenever a global *continuous* symmetric Bloch frame exists, then one can also find an arbitrarily close symmetric Bloch frame which is also *smooth*. ◊

2.2 Properties of the reshuffling matrix ε

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

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

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

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 $\Theta\colon \mathcal{H} \to \mathcal{H}$ to m-frames, by setting

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

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

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

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

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

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

$$(F_3') \qquad \Phi(k+\lambda) = \tau_\lambda \Phi(k), \quad \text{for all } k \in \mathbb{R}^d$$

and

$$(F_4') \qquad \Phi(-k) = \Theta\Phi(k) \triangleleft \varepsilon, \quad \text{for all } k \in \mathbb{R}^d.$$

Remark 2.2 (Compatibility conditions on ε). Observe that, by antiunitarity of Θ, we have that for all $\phi \in \mathcal{H}$

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

and hence $\langle \Theta\phi, \phi \rangle = 0$; the vectors ϕ and $\Theta\phi$ are always orthogonal. This motivates the presence of the "reshuffling" unitary matrix ε 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 $\{\phi_a(k)\}_{a=1,\dots,m}$ form a basis for $\operatorname{Ran} P(k)$ for example at $k = 0$. Notice, however, that if property ($P_{3,-}$) is replaced by

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

then (2.4) does not hold anymore, and one can indeed impose the compatibility of a Bloch frame Φ with the time-reversal operator by requiring that $\Phi(-k) = \Theta\Phi(k)$. Indeed, one can show [9] 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 ε in condition (F_3) is necessary. The further assumption of skew-symmetry on ε 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 ε^{-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, one gets

$$\Phi(k) \triangleleft \varepsilon^{-1} = \left(\Theta^2 \Phi(k)\right) \triangleleft \overline{\varepsilon} = \Phi(k) \triangleleft (-\overline{\varepsilon})$$

and hence we deduce that $\varepsilon^{-1} = -\overline{\varepsilon}$. On the other hand, by unitarity $\varepsilon^{-1} = \overline{\varepsilon}^{\mathsf{T}}$ and hence $\varepsilon^{\mathsf{T}} = -\varepsilon$. So ε must be not only unitary, but also skew-symmetric. In particular $\varepsilon\overline{\varepsilon} = -\mathbb{1}$.

Notice that, according to [18, Theorem 7], the matrix ε, being unitary and skew-symmetric, can be put in the form

$$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \oplus \cdots \oplus \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \tag{2.5}$$

in a suitable orthonormal basis. Hence, up to a reordering of such basis, there is no loss of generality in assuming that ε is in the *standard symplectic form*[4]

$$\varepsilon = \begin{pmatrix} 0 & \mathbb{1}_n \\ -\mathbb{1}_n & 0 \end{pmatrix} \tag{2.6}$$

where $n = m/2$ (remember that m is even). We will make use of this fact later on. ◊

Remark 2.3 (Geometric reinterpretation). Let us recast the above definitions in a more geometric language. Given a smooth and τ-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 $\operatorname{Ran} P(k)$ (see [28, Section 2.1] for details). The main result in [28] (see also [26]) is that, if $d \le 3$ 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^∞-smooth vector bundles. This is equivalent to the existence of a global τ-equivariant Bloch frame: this can be seen as a section of the *frame bundle* $\operatorname{Fr}(\mathcal{P}) \to \mathbb{T}^d$, 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 $\operatorname{Ran} P(k)$.

The time-reversal operator Θ induces by restriction a (non-vertical) automorphism of $\mathcal{P}$, *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 $\theta\colon \mathbb{T}^d \to \mathbb{T}^d$ denotes the involution $\theta(k) = -k$. This means that a vector in the fibre $\operatorname{Ran} P(k)$ is mapped via $\widehat{\Theta}$ into a vector in the fibre $\operatorname{Ran} P(-k)$. The morphism $\widehat{\Theta}\colon \mathcal{P} \to \mathcal{P}$ still satisfies $\widehat{\Theta}^2 = -\mathbb{1}$, *i. e.* it squares to the vertical automorphism of $\mathcal{P}$ 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 $d = 2$.

[4] 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 appearence of the standard symplectic matrix [6].

3.1 Effective unit cell, vertices and edges

Consider the unit cell

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

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 $\theta t_\lambda = t_{-\lambda}\theta$. Consequently, they form a subgroup of the affine group $\mathrm{Aut}(\mathbb{R}^2)$, consisting of the set $\{t_\lambda, \theta t_\lambda\}_{\lambda\in\Lambda}$. Periodicity (or rather, τ-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*

$$\mathbb{B}_{\mathrm{eff}} := \{k = (k_1, k_2) \in \mathbb{B} : k_1 \ge 0\}.$$

A more precise statement is contained in Proposition 3.1. Let us first introduce some further terminology. We define the *vertices* of the effective unit cell to be the points $k_\lambda \in \mathbb{B}_{\mathrm{eff}}$ 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, namely

$$\begin{gathered} v_1 = (0,0), \quad v_2 = \left(0, -\frac{1}{2}\right), \quad v_3 = \left(\frac{1}{2}, -\frac{1}{2}\right), \\ v_4 = \left(\frac{1}{2}, 0\right), \quad v_5 = \left(\frac{1}{2}, \frac{1}{2}\right), \quad v_6 = \left(0, \frac{1}{2}\right). \end{gathered} \tag{3.1}$$

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).

We start with an auxiliary *extension* result, which reduces 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 $\mathbb{B}_{\mathrm{eff}}$, satisfying further conditions on its boundary.

Proposition 3.1. *Let $\{P(k)\}_{k\in\mathbb{R}^2}$ be a family of orthogonal projectors satisfying Assumption 2.1. 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 Φ satisfies the* vertex conditions

$$\Phi(k_\lambda) = \tau_\lambda \Theta\Phi(k_\lambda) \triangleleft \varepsilon, \quad k_\lambda \in \{v_1, \dots, v_6\} \tag{V}$$

and the edge symmetries

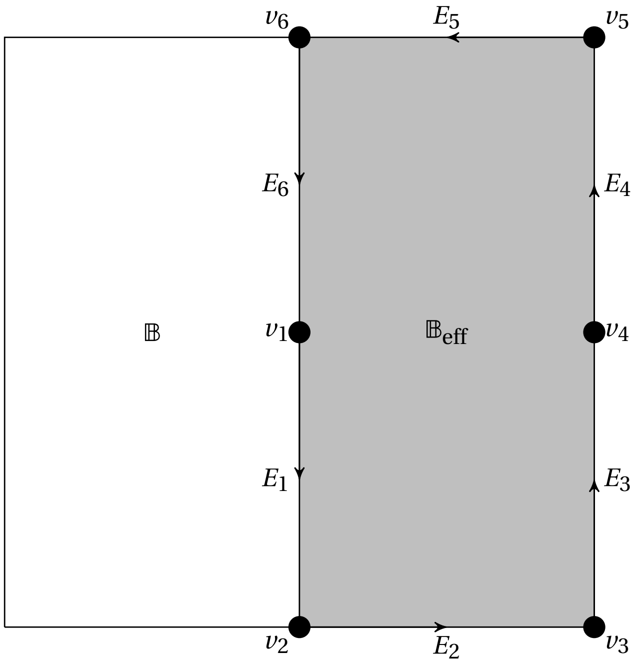


Fig. 1 The effective unit cell (shaded area), its vertices and its edges. We use adapted coordinates (k_1, k_2) such that $k = k_1 e_1 + k_2 e_2$.

$$\text{(E)} \qquad \begin{array}{ll} \Phi(\theta(k)) = \Theta\Phi(k) \triangleleft \varepsilon & \textit{for } k \in E_1 \cup E_6, \\ \Phi(t_{e_2}(k)) = \tau_{e_2}\Phi(k) & \textit{for } k \in E_2, \\ \Phi(\theta\, t_{-e_1}(k)) = \tau_{e_1}\Theta\Phi(k) \triangleleft \varepsilon & \textit{for } k \in E_3 \cup E_4, \\ \Phi(t_{-e_2}(k)) = \tau_{-e_2}\Phi(k) & \textit{for } k \in E_5. \end{array}$$

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

Proof. Let Φ be a global Bloch frame as in the statement of the Proposition. Then conditions (F_3') and (F_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 (V). The edge symmetries (E) can be checked similarly, again by making use of (F_3') and (F_4').

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

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

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

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

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 2.1. □

In view of Proposition 3.1, our strategy to examine Question (Q_2) will be to consider a continuous Bloch frame Ψ defined over the effective unit cell $\mathbb{B}_{\mathrm{eff}}$ (whose existence is guaranteed by the fact that $\mathbb{B}_{\mathrm{eff}}$ is contractible and no further symmetry is required), and try to modify it in order to obtain a new continuous Bloch frame Φ, which is defined on the effective unit cell and satisfies also the vertex conditions and the edge symmetries; by the above extension procedure one obtains a global continuous *symmetric* Bloch frame. Notice that, since both are orthonormal frames in $\operatorname{Ran} P(k)$, the given Bloch frame $\Psi(k)$ and the unknown symmetric Bloch frame $\Phi(k)$ differ by the action of a unitary matrix $U(k)$:

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

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

3.2 Solving the vertex conditions

Let k_λ be one of the six vertices in (3.1). If Φ is a symmetric Bloch frame, then, by Proposition 3.1, $\Phi(k_\lambda)$ satisfies the vertex condition (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 Ψ, 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 $\operatorname{Ran} P(k_\lambda)$, so there exists a unique unitary matrix $U_{\mathrm{obs}}(k_\lambda) \in \mathcal{U}(\mathbb{C}^m)$ such that

$$\Psi(k_\lambda) \triangleleft U_{\mathrm{obs}}(k_\lambda) = \tau_\lambda \Theta \Psi(k_\lambda) \triangleleft \varepsilon. \tag{3.3}$$

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

$$\begin{aligned} \tau_\lambda \Theta \left(\Psi(k_\lambda) \triangleleft U_{\mathrm{obs}}(k_\lambda) \right) &= \tau_\lambda \Theta \left(\tau_\lambda \Theta \Psi(k_\lambda) \triangleleft \varepsilon \right) = \\ &= \tau_\lambda \Theta \tau_\lambda \Theta \Psi(k_\lambda) \triangleleft \overline{\varepsilon} = \\ &= \tau_\lambda \tau_{-\lambda} \Theta^2 \Psi(k_\lambda) \triangleleft \overline{\varepsilon} = \\ &= \Psi(k_\lambda) \triangleleft (-\overline{\varepsilon}) \end{aligned}$$

where in the second-to-last equality we used the commutation relation (P_4). On the other hand, the left-hand side of this equality is also given by

$$\begin{aligned} \tau_\lambda \Theta \left(\Psi(k_\lambda) \triangleleft U_{\mathrm{obs}}(k_\lambda) \right) &= \tau_\lambda \Theta \Psi(k_\lambda) \triangleleft \overline{U_{\mathrm{obs}}}(k_\lambda) = \\ &= \left(\Psi(k_\lambda) \triangleleft \left(U_{\mathrm{obs}}(k_\lambda) \varepsilon^{-1} \right) \right) \triangleleft \overline{U_{\mathrm{obs}}}(k_\lambda) = \\ &= \Psi(k_\lambda) \triangleleft \left(U_{\mathrm{obs}}(k_\lambda) \varepsilon^{-1} \overline{U_{\mathrm{obs}}}(k_\lambda) \right). \end{aligned}$$

By the freeness of the action of $\mathcal{U}(\mathbb{C}^m)$ on frames and the fact that $\varepsilon^{-1} = -\overline{\varepsilon}$ by Remark 2.2, we deduce that

$$U_{\mathrm{obs}}(k_\lambda)\,\overline{\varepsilon}\,\overline{U_{\mathrm{obs}}}(k_\lambda) = \overline{\varepsilon}, \quad \textit{i.e.} \quad U_{\mathrm{obs}}(k_\lambda)^{\mathsf{T}}\varepsilon = \varepsilon\, U_{\mathrm{obs}}(k_\lambda). \tag{3.4}$$

Now, notice that the given Bloch frame $\Psi(k)$ and the unknown symmetric Bloch frame $\Phi(k)$, satisfying the vertex condition (V), differ by the action of a unitary matrix $U(k)$, as in (3.2). We want to relate the obstruction unitary $U_{\mathrm{obs}}(k_\lambda)$ to the unknown $U(k_\lambda)$. In order to do so, we rewrite (V) as

$$\begin{aligned}
\Psi(k_\lambda) \triangleleft U(k_\lambda) = \Phi(k_\lambda) &= \tau_\lambda \Theta \Phi(k_\lambda) \triangleleft \varepsilon = \\
&= \tau_\lambda \Theta \left(\Psi(k_\lambda) \triangleleft U(k_\lambda)\right) \triangleleft \varepsilon = \\
&= \tau_\lambda \Theta \Psi(k_\lambda) \triangleleft \left(\overline{U}(k_\lambda)\varepsilon\right) = \\
&= \left(\Psi(k_\lambda) \triangleleft \left(U_{\mathrm{obs}}(k_\lambda)\varepsilon^{-1}\right)\right) \triangleleft \left(\overline{U}(k_\lambda)\varepsilon\right) = \\
&= \Psi(k_\lambda) \triangleleft \left(U_{\mathrm{obs}}(k_\lambda)\varepsilon^{-1}\overline{U}(k_\lambda)\varepsilon\right).
\end{aligned}$$

Again by the freeness of the $\mathcal{U}(\mathbb{C}^m)$-action, we conclude that

$$U(k_\lambda) = U_{\mathrm{obs}}(k_\lambda)\varepsilon^{-1}\overline{U}(k_\lambda)\varepsilon, \quad \textit{i.e.} \quad U_{\mathrm{obs}}(k_\lambda) = U(k_\lambda)\varepsilon^{-1}U(k_\lambda)^{\mathsf{T}}\varepsilon. \tag{3.5}$$

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

Lemma 3.1. *Let $\varepsilon \in \mathcal{U}(\mathbb{C}^m) \cap \bigwedge^2\mathbb{C}^m$ 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 $V^{\mathsf{T}}\varepsilon = \varepsilon V$;*
(*b*) *there exists a matrix $U \in \mathcal{U}(\mathbb{C}^m)$ such that $V = U\varepsilon^{-1}U^{\mathsf{T}}\varepsilon$.*

Proof. The implication (*b*) ⇒ (*a*) is obvious. We prove the implication (*a*) ⇒ (*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 $\Lambda = \mathrm{diag}(\lambda_1, \ldots, \lambda_m)$ such that

$$V = W \mathrm{e}^{\mathrm{i}\Lambda} W^*$$

where the collection $\left\{\mathrm{e}^{\mathrm{i}\lambda_1}, \ldots, \mathrm{e}^{\mathrm{i}\lambda_m}\right\}$ forms the spectrum of V. The condition $V^{\mathsf{T}}\varepsilon = \varepsilon V$ is then equivalent to

$$\overline{W}\mathrm{e}^{\mathrm{i}\Lambda}W^{\mathsf{T}}\varepsilon = \varepsilon W \mathrm{e}^{\mathrm{i}\Lambda}W^* \quad \Longleftrightarrow \quad \mathrm{e}^{\mathrm{i}\Lambda}W^{\mathsf{T}}\varepsilon W = W^{\mathsf{T}}\varepsilon W \mathrm{e}^{\mathrm{i}\Lambda},$$

i. e. the matrix $A := W^{\mathsf{T}}\varepsilon W$ commutes with the diagonal matrix $\mathrm{e}^{\mathrm{i}\Lambda}$.

According to [18, 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 $Z = \mathrm{e}^{\mathrm{i}\Lambda}$ is diagonal, and give an explicit form of Y: Normalize the arguments λ_i of the eigenvalues of V so that $\lambda_i \in [0, 2\pi)$, and define $Y := \mathrm{e}^{\mathrm{i}\Lambda/2} = \mathrm{diag}\left(\mathrm{e}^{\mathrm{i}\lambda_1/2}, \ldots, \mathrm{e}^{\mathrm{i}\lambda_m/2}\right)$.

We claim now that the matrix

$$U := W\mathrm{e}^{\mathrm{i}\Lambda/2}W^*,$$

which is clearly unitary, satisfies condition (b) in the statement. Indeed, upon multiplying by $WW^* = \mathbb{1}$, we get that

$$U\varepsilon^{-1}U^{\mathsf{T}}\varepsilon = W\mathrm{e}^{\mathrm{i}\Lambda/2}W^*\varepsilon^{-1}\overline{W}\mathrm{e}^{\mathrm{i}\Lambda/2}W^{\mathsf{T}}\varepsilon WW^* = W\mathrm{e}^{\mathrm{i}\Lambda/2}A^{-1}\mathrm{e}^{\mathrm{i}\Lambda/2}AW^* = W\mathrm{e}^{\mathrm{i}\Lambda}W^* = V.$$

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 3.1 to $V = U_{\mathrm{obs}}(k_\lambda)$ 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 $\partial\mathbb{B}_{\mathrm{eff}}$, we use the path-connectedness of the group $\mathcal{U}(\mathbb{C}^m)$. Indeed, we can choose a continuous path [5] $W_i\colon [0,1/2] \to \mathcal{U}(\mathbb{C}^m)$ 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

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

In this way we obtain a continuous map $\widetilde{U}\colon E_1 \cup E_2 \cup E_3 \to \mathcal{U}(\mathbb{C}^m)$. Let $\widetilde{\Phi}(k) := \Psi(k) \triangleleft \widetilde{U}(k)$ for $k \in E_1 \cup E_2 \cup E_3$; we extend this frame to a τ-equivariant, time-reversal invariant frame on $\partial\mathbb{B}_{\mathrm{eff}}$ by setting

$$\widehat{\Phi}(k) := \begin{cases} \widetilde{\Phi}(k) & \text{if } k \in E_1 \cup E_2 \cup E_3, \\ \tau_{e_1}\Theta\widetilde{\Phi}(\theta t_{-e_1}(k)) \triangleleft \varepsilon & \text{if } k \in E_4, \\ \tau_{e_2}\widetilde{\Phi}(t_{-e_2}(k)) & \text{if } k \in E_5, \\ \Theta\widetilde{\Phi}(\theta(k)) \triangleleft \varepsilon & \text{if } k \in E_6. \end{cases} \tag{3.6}$$

By construction, $\widehat{\Phi}(k)$ satisfies all the edge symmetries for a symmetric Bloch frame Φ listed in (E), as one can immediately check.

Remark 3.1 (Proof of Theorem 2.1). 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 2.1 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 (F_2) and (F_3). Thus, by forcing τ-equivariance, one can extend the definition of the frame continuously on the whole $\mathbb{R}$, as in the proof of Proposition 3.1. Hence, this proves Theorem 2.1. ◊

[5] Explicitly, a continuous path of unitaries $W\colon [0,1/2] \to \mathcal{U}(\mathbb{C}^m)$ connecting two unitary matrices U_1 and U_2 can be constructed as follows. Diagonalize $U_1^{-1}U_2 = PDP^*$, where $D = \mathrm{diag}\left(\mathrm{e}^{\mathrm{i}\mu_1}, \dots, \mathrm{e}^{\mathrm{i}\mu_m}\right)$ and $P \in \mathcal{U}(\mathbb{C}^m)$. For $t \in [0,1/2]$ set

$$W(t) = U_1PD_tP^*, \quad \text{where} \quad D_t := \mathrm{diag}\left(\mathrm{e}^{\mathrm{i}2t\mu_1}, \dots, \mathrm{e}^{\mathrm{i}2t\mu_m}\right).$$

One easily realizes that $W(0) = U_1$, $W(1/2) = U_2$ and $W(t)$ depends continuously on t, as required.

3.4 Extending to the face: a $\mathbb{Z}_2$ obstruction

In order to see whether it is possible to extend the frame $\widehat{\Phi}$ to a continuous symmetric Bloch frame Φ defined on the whole effective unit cell $\mathbb{B}_{\text{eff}}$, we first introduce the unitary map $\widehat{U}(k)$ which maps the input frame $\Psi(k)$ to the frame $\widehat{\Phi}(k)$, *i. e.* such that

$$\widehat{\Phi}(k) = \Psi(k) \triangleleft \widehat{U}(k), \quad k \in \partial\mathbb{B}_{\text{eff}} \tag{3.7}$$

(compare (3.2)). This defines a continuous map $\widehat{U}\colon \partial\mathbb{B}_{\text{eff}} \to \mathcal{U}(\mathbb{C}^m)$; we are interested in finding a continuous extension $U\colon \mathbb{B}_{\text{eff}} \to \mathcal{U}(\mathbb{C}^m)$ of $\widehat{U}$ 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 [8, Thm. 17.3.1] that, if X is a topological space, then a continuous map $f\colon S^1 \to X$ defines an element in the fundamental group $\pi_1(X)$ by taking its homotopy class $[f]$. Moreover, f extends to a continuous map $F\colon D^2 \to X$, 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 $\mathcal{U}(\mathbb{C}^m)$, and it is also well-known [19, Ch. 8, Sec. 12] that the exact sequence of groups

$$1 \longrightarrow \mathcal{SU}(\mathbb{C}^m) \longrightarrow \mathcal{U}(\mathbb{C}^m) \xrightarrow{\det} U(1) \longrightarrow 1$$

induces an isomorphism $\pi_1(\mathcal{U}(\mathbb{C}^m)) \simeq \pi_1(U(1))$. On the other hand, the degree homomorphism [8, §13.4(b)]

$$\deg\colon \pi_1(U(1)) \xrightarrow{\sim} \mathbb{Z}, \quad [\varphi\colon S^1 \to U(1)] \mapsto \frac{1}{2\pi \mathrm{i}} \oint_{S^1} \mathrm{d}z\, \partial_z \log\varphi(z) \tag{3.8}$$

establishes an isomorphism of groups $\pi_1(U(1)) \simeq \mathbb{Z}$. We conclude that a continuous map $f\colon \partial\mathbb{B}_{\text{eff}} \to \mathcal{U}(\mathbb{C}^m)$ can be continuously extended to $F\colon \mathbb{B}_{\text{eff}} \to \mathcal{U}(\mathbb{C}^m)$ if and only if $\deg([\det f]) \in \mathbb{Z}$ is zero.

In our case, we want to extend the continuous map $\widehat{U}\colon \partial\mathbb{B}_{\text{eff}} \to \mathcal{U}(\mathbb{C}^m)$ to the whole effective unit cell $\mathbb{B}_{\text{eff}}$. However, rather than checking whether $\deg([\det \widehat{U}])$ vanishes, it is sufficient to find a unitary-matrix-valued map that "unwinds" the determinant of $\widehat{U}(k)$, while preserving the relevant symmetries on Bloch frames. More precisely, the following result holds.

Proposition 3.2. *Let $\widehat{\Phi}$ be the Bloch frame defined on $\partial\mathbb{B}_{\text{eff}}$ that appears in* (3.7), *satisfying the vertex conditions* (V) *and the edge symmetries* (E). *Assume that there exists a continuous map $X\colon \partial\mathbb{B}_{\text{eff}} \to \mathcal{U}(\mathbb{C}^m)$ such that*

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

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

Conversely, if Φ is a global continuous symmetric Bloch frame, then its restriction to $\partial\mathbb{B}_{\text{eff}}$ differs from $\widehat{\Phi}$ 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 $U := \widehat{U}X\colon \partial\mathbb{B}_{\text{eff}} \to \mathcal{U}(\mathbb{C}^m)$ satisfies $\deg([\det U]) = 0$ (because deg is a group homomorphism), and hence extends continuously to $U_{\text{eff}}\colon \mathbb{B}_{\text{eff}} \to \mathcal{U}(\mathbb{C}^m)$. 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 $\mathbb{B}_{\text{eff}}$, and by Proposition 3.1 such definition can be then extended continuously to $\mathbb{R}^2$ to obtain the desired global continuous symmetric Bloch frame Φ.

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

Proposition 3.2 reduces the question of existence of a global continuous symmetric Bloch frame to that of existence of a continuous map $X \colon \partial\mathbb{B}_{\text{eff}} \to \mathcal{U}(\mathbb{C}^m)$ 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 $\widehat{\Phi} \triangleleft X$ to satisfy the edge symmetries (E), provided that $\widehat{\Phi}$ satisfies them. For $k = (0, k_2) \in E_1 \cup E_6$, we obtain that

$$\widehat{\Phi}(0,-k_2) \triangleleft X(0,-k_2) = \Theta\left(\widehat{\Phi}(0,k_2) \triangleleft X(0,k_2)\right) \triangleleft \varepsilon$$
$$\Updownarrow$$
$$\Theta\widehat{\Phi}(0,k_2) \triangleleft (\varepsilon X(0,-k_2)) = \Theta\widehat{\Phi}(0,k_2) \triangleleft \left(\overline{X}(0,k_2)\varepsilon\right),$$

by which we deduce that

$$\varepsilon X(0,-k_2) = \overline{X}(0,k_2)\,\varepsilon, \quad k_2 \in [-1/2, 1/2]. \tag{3.9}$$

Similarly, for $k = (1/2, k_2) \in E_3 \cup E_4$, we obtain

$$\varepsilon X(1/2,-k_2) = \overline{X}(1/2,k_2)\,\varepsilon, \quad k_2 \in [-1/2, 1/2]. \tag{3.10}$$

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

$$X(k_1,-1/2) = X(k_1,1/2), \quad k_1 \in [0, 1/2]. \tag{3.11}$$

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 $\widehat{\Phi} \triangleleft X$ satifies the vertex conditions (V) whenever $\widehat{\Phi}$ does. Explicitly, these relations on $X(k_\lambda)$ read

$$\varepsilon X(k_\lambda) = \overline{X}(k_\lambda)\,\varepsilon, \quad \textit{i. e.} \quad X(k_\lambda)^{\mathsf{T}} \varepsilon\, X(k_\lambda) = \varepsilon. \tag{3.12}$$

This relation has interesting consequences. Indeed, in view of Remark 2.2, we may assume that ε is in the standard symplectic form (2.6). Then (3.12) implies that the matrices $X(k_\lambda)$ belong to the *symplectic group* $\mathrm{Sp}(2n,\mathbb{C})$. As such, they must be unimodular [25], *i. e.*

$$\det X(k_\lambda) = 1. \tag{3.13}$$

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 $\xi := \det X \colon \partial\mathbb{B}_{\text{eff}} \to U(1)$ can attain. The integral on the boundary $\partial\mathbb{B}_{\text{eff}}$ of the effective unit cell splits as the sum of the integrals over the oriented edges $E_1, \dots, E_6$:

$$\deg([\xi]) = \frac{1}{2\pi\mathrm{i}} \oint_{\partial\mathbb{B}_{\text{eff}}} \mathrm{d}z\, \partial_z \log\det X(z) = \sum_{i=1}^{6} \frac{1}{2\pi\mathrm{i}} \int_{E_i} \mathrm{d}z\, \partial_z \log\det X(z).$$

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 $\xi_i := \det X\big|_{E_i} \colon E_i \to U(1)$, $i = 1, \dots, 6$, 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

$$\deg([\xi]) = \sum_{i=1}^{6} \frac{1}{2\pi\mathrm{i}} \oint_{S^1_i} \mathrm{d}z\, \partial_z \log\det X(z) = \sum_{i=1}^{6} \deg([\xi_i]). \tag{3.14}$$

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_1 and S^1_6 (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

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

which implies in particular that

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

Thus, calling $z = -k_2$ the coordinate on S^1_1 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

$$\begin{aligned} \deg([\xi_6]) &= -\deg([\overline{\xi_1}]) && \text{(because evaluation at } (-z) \text{ changes the orientation of } S^1_1) \\ &= \deg([\xi_1]) && \text{(because if } \varphi \colon S^1 \to U(1) \text{ then } \deg([\overline{\varphi}]) = -\deg([\varphi])). \end{aligned}$$

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

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

We have thus proved the following

Proposition 3.3. *Let $X\colon \partial\mathbb{B}_{\mathrm{eff}} \to \mathcal{U}(\mathbb{C}^m)$ satisfy condition* (X_2), *as in the statement of Proposition 3.2. 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 3.1. *Let $\{P(k)\}_{k\in\mathbb{R}^2}$ be a family of orthogonal projectors satisfying Assumption 2.1. Let $\widehat{U}\colon \partial\mathbb{B}_{\mathrm{eff}} \to \mathcal{U}(\mathbb{C}^m)$ be defined as in* (3.7). *Then there exists a global continuous symmetric Bloch frame Φ for $\{P(k)\}_{k\in\mathbb{R}^2}$ if and only if*

$$\deg([\det \widehat{U}]) \equiv 0 \bmod 2.$$

Proof. By Proposition 3.2, we know that the existence of a global continuous symmetric Bloch frame is equivalent to that of a continuous map $X\colon \partial\mathbb{B}_{\mathrm{eff}} \to \mathcal{U}(\mathbb{C}^m)$ satisfying conditions (X_1) and (X_2), so that in particular it should have $\deg([\det X]) = -\deg([\det \widehat{U}])$. In view of Proposition 3.3, condition (X_2) cannot hold in the case where $\deg([\det \widehat{U}])$ is odd.

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

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

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

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

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 $X\colon \partial\mathbb{B}_{\mathrm{eff}} \to \mathcal{U}(\mathbb{C}^m)$. Since X is constant on E_1, formula (3.15) for the degree of the determinant of $X(k)$ simplifies to

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

One immediately computes $\deg([\det X]) = -2s$, as wanted. □

The index

$$\delta(P) := \deg([\det \widehat{U}]) \bmod 2 \tag{3.16}$$

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 2.1, which encodes the obstruction to the existence of a global continuous symmetric Bloch frame. One of our main results, Theorem 2.2, is then reduced to Theorem 3.1.

3.5 Well-posedness of the definition of δ

In the construction of the previous Subsection, leading to the definition (3.16) of the $\mathbb{Z}_2$ index δ, a number of choices has to be performed, namely the input frame Ψ and the interpolation $\widetilde{U}$ on $E_1 \cup E_2 \cup E_3$. 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 δ is also independent of the choice of a basis $\{e_1, e_2\}$ for the lattice Λ, as will be manifest from the equivalent formulation (5.2) of the invariant we will provide in Section 5.

Gauge independence of δ

As a first step, we will prove that the $\mathbb{Z}_2$ index δ is independent of the choice of the input Bloch frame Ψ.

Indeed, assume that another input Bloch frame Ψ_{new} is chosen: the two frames will be related by a continuous unitary gauge transformation, say

$$\Psi_{\text{new}}(k) = \Psi(k) \triangleleft G(k), \quad G(k) \in \mathcal{U}(\mathbb{C}^m), \quad k \in \mathbb{B}_{\text{eff}}. \tag{3.17}$$

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

$$\widehat{\Phi}(k) = \Psi(k) \triangleleft \widehat{U}(k) \quad \text{and} \quad \widehat{\Phi}_{\text{new}}(k) = \Psi_{\text{new}}(k) \triangleleft \widehat{U}_{\text{new}}(k), \qquad k \in \partial\mathbb{B}_{\text{eff}}.$$

From (3.17) we can rewrite the second equality as

$$\widehat{\Phi}_{\text{new}}(k) = \Psi(k) \triangleleft \left(G(k)\widehat{U}_{\text{new}}(k)\right), \quad k \in \partial\mathbb{B}_{\text{eff}}.$$

The two frames $\widehat{\Phi}$ and $\widehat{\Phi}_{\text{new}}$ both satisfy the vertex conditions (V) and the edge symmetries (E), hence the matrix $X(k) := \left(G(k)\widehat{U}_{\text{new}}(k)\right)^{-1}\widehat{U}(k)$, which transforms $\widehat{\Phi}_{\text{new}}$ into $\widehat{\Phi}$, enjoys condition (X_2) from Proposition 3.2. Applying Proposition 3.3 we deduce that

$$\deg([\det \widehat{U}]) \equiv \deg\left(\left[\det\left(G\widehat{U}_{\text{new}}\right)\right]\right) \mod 2. \tag{3.18}$$

Observe that, since the degree is a group homomorphism,

$$\deg\left(\left[\det\left(G\widehat{U}_{\text{new}}\right)\right]\right) = \deg([\det \widehat{U}_{\text{new}}]) + \deg([\det G]).$$

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 $\deg([\det(G\widehat{U}_{\text{new}})]) = \deg([\det \widehat{U}_{\text{new}}])$; plugging this in (3.18) we conclude that

$$\delta = \deg([\det \widehat{U}]) \equiv \deg([\det \widehat{U}_{\text{new}}]) = \delta_{\text{new}} \mod 2,$$

as we wanted.

Invariance under edge extension

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

Assume that a different interpolation $\widetilde{U}_{\text{new}}(k)$ has been chosen on $E_1 \cup E_2 \cup E_3$, leading to a different unitary-matrix-valued map $\widehat{U}_{\text{new}} \colon \partial\mathbb{B}_{\text{eff}} \to \mathcal{U}(\mathbb{C}^m)$. Starting from the input frame Ψ, we thus obtain two different Bloch frames:

$$\widehat{\Phi}(k) = \Psi(k) \triangleleft \widehat{U}(k) \quad \text{and} \quad \widehat{\Phi}_{\text{new}}(k) = \Psi(k) \triangleleft \widehat{U}_{\text{new}}(k), \qquad k \in \partial\mathbb{B}_{\text{eff}}.$$

From the above equalities, we deduce at once that $\widehat{\Phi}(k) = \widehat{\Phi}_{\text{new}}(k) \triangleleft X(k)$, where $X(k) := \widehat{U}_{\text{new}}(k)^{-1}\widehat{U}(k)$. We now follow the same line of argument as in the previous Subsection. Since both $\widehat{\Phi}$ and $\widehat{\Phi}_{\text{new}}$ satisfy the vertex conditions (V) and the edge symmetries (E) by construction, the matrix-valued map $X \colon \partial\mathbb{B}_{\text{eff}} \to \mathcal{U}(\mathbb{C}^m)$ just defined enjoys condition (X_2), as in the statement of Proposition 3.2. It follows now by Proposition 3.3 that the degree $\deg([\det X])$ is even. Since the degree defines a group homomorphism, this means that

$$\deg([\det X]) = \deg([\det \widehat{U}]) - \deg([\det \widehat{U}_{\text{new}}]) \equiv 0 \bmod 2$$

or equivalently

$$\delta = \deg([\det \widehat{U}]) \equiv \deg([\det \widehat{U}_{\text{new}}]) = \delta_{\text{new}} \bmod 2,$$

as claimed.

3.6 Topological invariance of δ

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 2.1. More formally, the following result holds.

Proposition 3.4. *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 2.1. 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 2.1 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 $[0,1] \times \mathbb{B}_{\text{eff}}$, and hence is uniformly continuous. Thus, there exists $\mu > 0$ such that

$$\left\| P_t(k) - P_{\tilde{t}}(\tilde{k}) \right\|_{\mathcal{B}(\mathcal{H})} < 1 \quad \text{if } \max\left\{ \left|k - \tilde{k}\right|, \left|t - \tilde{t}\right| \right\} < \mu.$$

In particular, choosing $t_0 < \mu$, we have that

(3.19) $$\|P_t(k) - P_0(k)\|_{\mathcal{B}(\mathcal{H})} < 1 \quad \text{if } t \in [0, t_0], \text{ uniformly in } k \in \mathbb{B}_{\text{eff}}.$$

We will show that $\delta(P_0) = \delta(P_{t_0})$. Iterating this construction a finite number of times will prove that $\delta(P_0) = \delta(P_1)$.

In view of (3.19), the Kato-Nagy unitary [22, Sec. I.6.8]

$$W(k) := \left(\mathbb{1} - (P_0(k) - P_{t_0}(k))^2\right)^{-1/2} \left(P_{t_0}(k)P_0(k) + (\mathbb{1} - P_{t_0}(k))(\mathbb{1} - P_0(k))\right) \in \mathcal{U}(\mathcal{H})$$

is well-defined and provides an intertwiner between $\operatorname{Ran} P_0(k)$ and $\operatorname{Ran} P_{t_0}(k)$, 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:

(W_1) the map $\mathbb{B}_{\text{eff}} \ni k \mapsto W(k) \in \mathcal{U}(\mathcal{H})$ is C^∞-smooth;

(W_2) the map $k \mapsto W(k)$ is τ-covariant, in the sense that whenever k and $k + \lambda$ are both in $\mathbb{B}_{\text{eff}}$ for $\lambda \in \Lambda$, then
$$W(k + \lambda) = \tau(\lambda)W(k)\tau(\lambda)^{-1};$$

(W_3) the map $k \mapsto W(k)$ is time-reversal symmetric, in the sense that whenever k and $-k$ are both in $\mathbb{B}_{\text{eff}}$, then
$$W(-k) = \Theta W(k)\Theta^{-1}.$$

Let now $\{\Psi_0(k)\}_{k\in\mathbb{B}_{\text{eff}}}$ 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 $k \in \mathbb{B}_{\text{eff}}$, and obtain a continuous Bloch frame $\left\{\Psi_{t_0}(k)\right\}_{k\in\mathbb{B}_{\text{eff}}}$ for $\left\{P_{t_0}(k)\right\}_{k\in\mathbb{R}^2}$. 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 $\left\{P_{t_0}(k)\right\}_{k\in\mathbb{R}^2}$, namely

$$\widehat{\Phi}_0(k) = \Psi_0(k) \triangleleft \widehat{U}_0(k) \quad \text{and} \quad \widehat{\Phi}_{t_0}(k) = \Psi_{t_0}(k) \triangleleft \widehat{U}_{t_0}(k), \quad k \in \partial\mathbb{B}_{\text{eff}}.$$

From the above equalities, we deduce that

$$\begin{aligned}\widehat{\Phi}_{t_0}(k) &= \Psi_{t_0}(k) \triangleleft \widehat{U}_{t_0}(k) = (W(k)\Psi_0(k)) \triangleleft \widehat{U}_{t_0}(k) = \\ &= W(k)\left(\Psi_0(k) \triangleleft \widehat{U}_{t_0}(k)\right) = W(k)\left(\widehat{\Phi}_0(k) \triangleleft \left(\widehat{U}_0(k)^{-1}\widehat{U}_{t_0}(k)\right)\right) = \\ &= \left(W(k)\widehat{\Phi}_0(k)\right) \triangleleft \left(\widehat{U}_0(k)^{-1}\widehat{U}_{t_0}(k)\right)\end{aligned}$$

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 (W_1), (W_2) and (W_3), the frame $\left\{W(k)\widehat{\Phi}_0(k)\right\}_{k\in\partial\mathbb{B}_{\text{eff}}}$ gives a continuous Bloch frame for $\left\{P_{t_0}(k)\right\}_{k\in\mathbb{R}^2}$ which still satisfies the vertex conditions (V) and the edge symmetries (E), since $\widehat{\Phi}_0$ does. Hence the matrix $X(k) := \widehat{U}_0(k)^{-1}\widehat{U}_{t_0}(k)$ satisfies hypothesis (X_2), and in view of Proposition 3.3 its determinant has even degree. We conclude that

$$\delta(P_0) = \deg([\det \widehat{U}_0]) \equiv \deg([\det \widehat{U}_{t_0}]) = \delta(P_{t_0}) \bmod 2. \qquad \square$$

4 Comparison with the Fu-Kane index

In this Section, we will compare our $\mathbb{Z}_2$ invariant δ with the $\mathbb{Z}_2$ invariant Δ proposed by Fu and Kane [12], and show that they are equal. For the reader's convenience, we recall the definition of Δ, rephrasing it in our terminology.

Let $\Psi(k) = \{\psi_1(k), \dots, \psi_m(k)\}$ be a global τ-*equivariant*[6] Bloch frame. Define the unitary matrix $w(k) \in \mathcal{U}(\mathbb{C}^m)$ by

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

In terms of the right action of matrices on frames, one can equivalently say that $w(k)$ is the matrix such that [7]

$$\Theta\Psi(k) = \Psi(-k) \triangleleft w(k). \tag{4.1}$$

Comparing (4.1) with (F_4'), we see that if Ψ were already symmetric then $w(k) = \varepsilon^{-1}$ for all $k \in \mathbb{R}^d$.

One immediately checks how $w(k)$ changes when the inversion or translation symmetries are applied to k. One has that

$$\begin{aligned} w(\theta(k))_{ab} &= \langle \psi_a(k), \Theta\psi_b(-k) \rangle = \langle \Theta^2\psi_b(-k), \Theta\psi_a(k) \rangle = \\ &= -\langle \psi_b(-k), \Theta\psi_a(k) \rangle = -w(k)_{ba} \end{aligned}$$

or in matrix form $w(\theta(k)) = -w(k)^{\mathsf{T}}$. Moreover, by using the τ-equivariance of the frame Ψ one obtains

$$\begin{aligned} w(t_\lambda(k))_{ab} &= \langle \psi_a(\theta t_\lambda(k)), \Theta\psi_b(t_\lambda(k)) \rangle = \langle \psi_a(t_{-\lambda}\theta(k)), \Theta\tau(\lambda)\psi_b(k) \rangle = \\ &= \langle \tau(-\lambda)\psi_a(-k), \tau(-\lambda)\Theta\psi_b(k) \rangle = \langle \psi_a(-k), \Theta\psi_b(k) \rangle = w(k)_{ab} \end{aligned}$$

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_λ of the effective unit cell we get

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

[6] This assumption is crucial in the definition of the Fu-Kane index, whereas the definition of our $\mathbb{Z}_2$ invariant does not need Ψ to be already τ-equivariant. Nonetheless, the existence of a global τ-equivariant Bloch frame is guaranteed by a straightforward modification of the proof in [28], as detailed in [26].

[7] 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 $\{\psi_a(-k)\}_{a=1,\dots,m}$ is an *orthonormal* frame in $\operatorname{Ran} P(-k)$.

In other words, the matrix $w(k_\lambda)$ is skew-symmetric, and hence it has a well-defined Pfaffian, satisfying $(\mathrm{Pf}\, w(k_\lambda))^2 = \det w(k_\lambda)$. The Fu-Kane index Δ is then defined as [12, Equations (3.22) and (3.25)]

$$\Delta := P_\theta(1/2) - P_\theta(0) \bmod 2, \tag{4.2}$$

where for $k_* \in \{0, 1/2\}$

$$P_\theta(k_*) := \frac{1}{2\pi \mathrm{i}} \left(\int_0^{1/2} \mathrm{d}k_2 \, \mathrm{Tr}\left(w(k_*, k_2)^* \partial_{k_2} w(k_*, k_2) \right) - 2 \log \frac{\mathrm{Pf}\, w(k_*, 1/2)}{\mathrm{Pf}\, w(k_*, 0)} \right). \tag{4.3}$$

We are now in position to prove the above-mentioned equality between our $\mathbb{Z}_2$ invariant δ and the Fu-Kane index Δ.

Theorem 4.1. *Let $\{P(k)\}_{k \in \mathbb{R}^2}$ be a family of projectors satisfying Assumption 2.1, and let $\delta = \delta(P) \in \mathbb{Z}_2$ be as in* (3.16). *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 δ, in order to make the comparison with Δ more accessible. Recall that δ is defined as the degree of the determinant of the matrix $\widehat{U}(k)$, for $k \in \partial \mathbb{B}_{\mathrm{eff}}$, satisfying $\widehat{\Phi}(k) = \Psi(k) \triangleleft \widehat{U}(k)$, where $\widehat{\Phi}(k)$ is as in (3.6). The unitary $\widehat{U}(k)$ coincides with the unitary $\widetilde{U}(k)$ for $k \in E_1 \cup E_2 \cup E_3$, where $\widetilde{U}(k)$ 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 $\widehat{\Phi}(k)$, as in Section 3.3.

We 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

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

This means that

$$\widehat{U}(k) = w(-k) \overline{\widetilde{U}}(1/2, -k_2) \varepsilon, \quad k = (1/2, k_2) \in E_4. \tag{4.4}$$

Analogously, for $k \in E_5$, say $k = (k_1, 1/2)$, we obtain

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

Finally, for $k \in E_6$, say $k = (0, k_2)$ with $k_2 \geq 0$, we obtain in analogy with (4.4)

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

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 (4.4) and (4.6) as

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

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

$$w(k_*,k_2) = \widehat{U}(k_*,-k_2)\varepsilon^{-1}\widehat{U}(k_*,k_2)^{\mathsf{T}}, \quad (k_*,k_2) \in S^1_*, \tag{4.7}$$

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 $w(t_\lambda(k)) = w(k)$.

We are now able to compute the degree of the determinant of $\widehat{U}$. Firstly, an easy computation [8] shows that

[8] If $\widehat{U}(z) \in \mathcal{U}(\mathbb{C}^m)$ has spectrum $\{e^{i\lambda_j(z)}\}_{j=1,\ldots,m}$, then

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

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

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

one immediately deduces that

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

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

$$P_j(z)\partial_z P_j(z) = \left(\partial_z P_j(z)\right)\left(\mathbb{1} - P_j(z)\right)$$

so that

$$\partial_z P_j(z) = P_j(z)\left(\partial_z P_j(z)\right)\left(\mathbb{1} - P_j(z)\right) + \left(\mathbb{1} - P_j(z)\right)\left(\partial_z P_j(z)\right)P_j(z).$$

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

$$\begin{aligned}\mathrm{Tr}\left(P_\ell(z)\left(\partial_z P_j(z)\right)\right) = &\,\mathrm{Tr}\left(P_j(z)P_\ell(z)\left(\partial_z P_j(z)\right)\left(\mathbb{1} - P_j(z)\right)\right) + \\ &+ \mathrm{Tr}\left(\left(\mathbb{1} - P_j(z)\right)P_\ell(z)\left(\partial_z P_j(z)\right)P_j(z)\right) = 0.\end{aligned}$$

We are now able to compute

$$\begin{aligned}\mathrm{Tr}\left(\widehat{U}(z)^*\partial_z\widehat{U}(z)\right) = &\sum_{j,\ell=1}^m \mathrm{Tr}\left(e^{-i\lambda_\ell(z)}P_\ell(z)\left(\partial_z e^{i\lambda_j(z)}\right)P_j(z)\right) + \\ &+ e^{-i\left(\lambda_\ell(z)-\lambda_j(z)\right)}\mathrm{Tr}\left(P_\ell(z)\left(\partial_j P(z)\right)\right) = \\ = &\sum_{j,\ell=1}^m e^{-i\lambda_\ell(z)}\left(\partial_z e^{i\lambda_j(z)}\right)\delta_{j,\ell}\,\mathrm{Tr}\left(P_j(z)\right) = \sum_{j=1}^m e^{-i\lambda_j(z)}\partial_z e^{i\lambda_j(z)}.\end{aligned}$$

$$\deg([\det \widehat{U}]) = \frac{1}{2\pi \mathrm{i}} \oint_{\partial \mathbb{B}_{\mathrm{eff}}} \mathrm{d}z\, \partial_z \log \det \widehat{U}(z) = \\ = \frac{1}{2\pi \mathrm{i}} \oint_{\partial \mathbb{B}_{\mathrm{eff}}} \mathrm{d}z\, \mathrm{Tr}\left(\widehat{U}(z)^* \partial_z \widehat{U}(z)\right) = \sum_{i=1}^{6} \frac{1}{2\pi \mathrm{i}} \int_{E_i} \mathrm{d}z\, \mathrm{Tr}\left(\widehat{U}(z)^* \partial_z \widehat{U}(z)\right).$$

Clearly we have

$$\int_{E_i} \mathrm{d}z\, \mathrm{Tr}\left(\widehat{U}(z)^* \partial_z \widehat{U}(z)\right) = \int_{E_i} \mathrm{d}z\, \mathrm{Tr}\left(\widetilde{U}(z)^* \partial_z \widetilde{U}(z)\right) \quad \text{for } i = 1,2,3, \tag{4.8}$$

because $\widehat{U}$ and $\widetilde{U}$ coincide on $E_1 \cup E_2 \cup E_3$. Using now Equation (4.5) we compute

$$\int_{E_5} \mathrm{d}z\, \mathrm{Tr}\left(\widehat{U}(z)^* \partial_z \widehat{U}(z)\right) = \int_{1/2}^{0} \mathrm{d}k_1\, \mathrm{Tr}\left(\widehat{U}(k_1, 1/2)^* \partial_{k_1} \widehat{U}(k_1, 1/2)\right) = \\ = -\int_{0}^{1/2} \mathrm{d}k_1\, \mathrm{Tr}\left(\widetilde{U}(k_1, -1/2)^* \partial_{k_1} \widetilde{U}(k_1, -1/2)\right) = \\ = -\int_{E_2} \mathrm{d}z\, \mathrm{Tr}\left(\widetilde{U}(z)^* \partial_z \widetilde{U}(z)\right)$$

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

$$\int_{E_2 + E_5} \mathrm{d}z\, \mathrm{Tr}\left(\widehat{U}(z)^* \partial_z \widehat{U}(z)\right) = 0. \tag{4.9}$$

Making use of (4.7), we proceed now to evaluate the integrals on E_1, E_3, E_4 and E_6, which give the non-trivial contributions to $\deg([\det \widehat{U}])$. Indeed, Equation (4.7) implies

$$w(k_*, k_2)^* = \overline{\widehat{U}}(k_*, k_2)\, \varepsilon\, \widehat{U}(k_*, -k_2)^*, \\ \partial_{k_2} w(k_*, k_2) = -\partial_{k_2} \widehat{U}(k_*, -k_2) \varepsilon^{-1} \widehat{U}(k_*, k_2)^{\mathsf{T}} + \widehat{U}(k_*, -k_2) \varepsilon^{-1} \partial_{k_2} \widehat{U}(k_*, k_2)^{\mathsf{T}},$$

from which one computes

$$\mathrm{Tr}(w(k_*, k_2)^* \partial_{k_2} w(k_*, k_2)) = -\mathrm{Tr}\left(\widehat{U}(k_*, -k_2)^* \partial_{k_2} \widehat{U}(k_*, -k_2)\right) + \\ + \mathrm{Tr}\left(\widehat{U}(k_*, k_2)^* \partial_{k_2} \widehat{U}(k_*, k_2)\right).$$

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

$$\int_{0}^{1/2} \mathrm{d}k_2\, \mathrm{Tr}(w(k_*, k_2)^* \partial_{k_2} w(k_*, k_2)) = -\int_{-1/2}^{0} \mathrm{d}k_2\, \mathrm{Tr}\left(\widehat{U}(k_*, k_2)^* \partial_{k_2} \widehat{U}(k_*, k_2)\right) + \\ + \int_{0}^{1/2} \mathrm{d}k_2\, \mathrm{Tr}\left(\widehat{U}(k_*, k_2)^* \partial_{k_2} \widehat{U}(k_*, k_2)\right) = \\ = (-1)^{1+2k_*} \oint_{S^1_*} \mathrm{d}z\, \mathrm{Tr}\left(\widehat{U}(z)^* \partial_z \widehat{U}(z)\right) + \\ + 2 \int_{0}^{1/2} \mathrm{d}k_2\, \mathrm{Tr}\left(\widehat{U}(k_*, k_2)^* \partial_{k_2} \widehat{U}(k_*, k_2)\right). \tag{4.10}$$

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

Now, notice that

$$\begin{aligned}\int_0^{1/2} \mathrm{d}k_2 \operatorname{Tr}\left(\widehat{U}(k_*,k_2)^* \partial_{k_2} \widehat{U}(k_*,k_2)\right) &= \int_0^{1/2} \mathrm{d}k_2 \, \partial_{k_2} \log\det \widehat{U}(k_*,k_2) \\ &\equiv \log \frac{\det \widehat{U}(k_*,1/2)}{\det \widehat{U}(k_*,0)} \mod 2\pi \mathrm{i}.\end{aligned} \tag{4.11}$$

Furthermore, evaluating Equation (4.7) at the six vertices k_λ, we obtain

$$w(k_\lambda) = \widehat{U}(k_\lambda) \varepsilon^{-1} \widehat{U}(k_\lambda)^{\mathsf{T}}$$

which implies that

$$\operatorname{Pf} w(k_\lambda) = \det \widehat{U}(k_\lambda) \operatorname{Pf} \varepsilon^{-1} \tag{4.12}$$

by the well known property $\operatorname{Pf}(CAC^{\mathsf{T}}) = \det(C)\operatorname{Pf}(A)$, for a skew-symmetric matrix A and a matrix $C \in M_m(\mathbb{C})$ [25].

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

$$\begin{aligned}\frac{1}{2\pi \mathrm{i}} \left(\int_0^{1/2} \mathrm{d}k_2 \operatorname{Tr}(w(k_*,k_2)^* \partial_{k_2} w(k_*,k_2)) - 2 \log \frac{\operatorname{Pf} w(k_*,1/2)}{\operatorname{Pf} w(k_*,0)} \right) \equiv \\ \equiv \frac{s_*}{2\pi \mathrm{i}} \int_{S^1_*} \mathrm{d}z \operatorname{Tr}\left(\widehat{U}(z)^* \partial_z \widehat{U}(z)\right) \mod 2.\end{aligned}$$

On the left-hand side of this equality, we recognize $P_\theta(k_*)$, as defined in (4.3). Taking care of the orientation of S^1_*, we conclude, also in view of (4.9), that

$$\begin{aligned}\Delta &\equiv P_\theta(1/2) - P_\theta(0) \mod 2 \\ &\equiv \frac{1}{2\pi \mathrm{i}} \int_{E_1+E_3+E_4+E_6} \mathrm{d}z \operatorname{Tr}\left(\widehat{U}(z)^* \partial_z \widehat{U}(z)\right) \mod 2 \\ &\equiv \deg([\det \widehat{U}]) \equiv \delta \mod 2.\end{aligned}$$

This concludes the proof. □

Remark 4.1 (On the rôle of Pfaffians). Equation (4.7) is the crucial point in the above argument. Indeed, since $\det \varepsilon = 1$ (compare Remark 2.2), from (4.7) it follows that

$$\det w(k_*,k_2) = \det \widehat{U}(k_*,-k_2) \det \widehat{U}(k_*,k_2), \quad (k_*,k_2) \in S^1_*. \tag{4.13}$$

If we evaluate this equality at the six vertices k_λ, we obtain

$$\det w(k_\lambda) = \left(\det \widehat{U}(k_\lambda)\right)^2 = (\operatorname{Pf} w(k_\lambda))^2. \tag{4.14}$$

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

In view of the equality $\Delta = \delta \in \mathbb{Z}_2$, we have a clear intepretation of the Fu-Kane index as the obstruction to the existence of a global continuous symmetric Bloch frame, as claimed in [12, App. A].

5 A simpler formula for the $\mathbb{Z}_2$ invariant

The fact that the $\mathbb{Z}_2$ invariant δ, 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) shows that its value depends only on the value of $\widehat{U}$ at the vertices. 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 should be compared with [12, Equation (3.26)].

In the previous Section, we have rewritten our invariant as $\delta = \widehat{P}_\theta(1/2) - \widehat{P}_\theta(0) \bmod 2$, with

$$\begin{aligned} -\widehat{P}_\theta(k_*) :=& \frac{1}{2\pi \mathrm{i}} \left(\int_{-1/2}^{0} \mathrm{d}k_2 \operatorname{Tr}\left(w(k_*, k_2)^* \partial_{k_2} w(k_*, k_2) \right) + \right. \\ & \left. - 2 \int_{-1/2}^{0} \mathrm{d}k_2 \operatorname{Tr}\left(\widehat{U}(k_*, k_2)^* \partial_{k_2} \widehat{U}(k_*, k_2) \right) \right) = \\ =& \frac{1}{2\pi \mathrm{i}} \left(\log \frac{\det w(k_*, 0)}{\det w(k_*, -1/2)} - 2 \log \frac{\det \widehat{U}(k_*, 0)}{\det \widehat{U}(k_*, -1/2)} \right). \end{aligned}$$

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

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

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

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

and each $(-1)^{\widehat{\eta}_{v_i}}$ 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,

$$(5.1)\qquad (-1)^{(\log\alpha)/(2\pi \mathrm{i})} = (\mathrm{e}^{\mathrm{i}\pi})^{(\log\alpha)/(2\pi \mathrm{i})} = \mathrm{e}^{(\log\alpha)/2} = \sqrt{\alpha},$$

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

$$(5.2)\qquad (-1)^\delta = \prod_{i=1}^{4} \frac{\sqrt{\left(\det \widehat{U}(v_i)\right)^2}}{\det \widehat{U}(v_i)}$$

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 [12, Equation (3.26)] for the Fu-Kane index Δ, namely

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

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

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

so that (5.2) may be rewritten as

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

This reformulation shows that our $\mathbb{Z}_2$ invariant can be computed starting just from the "input" Bloch frame Ψ (provided it is *continuous* on $\mathbb{B}_{\mathrm{eff}}$), and more specifically from its values at the vertices k_λ. Indeed, the obstruction $U_{\mathrm{obs}}(k_\lambda)$ at the vertices is defined by (3.3) solely in terms of $\Psi(k_\lambda)$; moreover, $U(k_\lambda)$ is determined by $U_{\mathrm{obs}}(k_\lambda)$ as explained in the proof of Lemma 3.1.

We have thus the following **algorithmic recipe** to compute δ:

- given a continuous Bloch frame $\Psi(k) = \{\psi_a(k)\}_{a=1,\dots,m}$, $k \in \mathbb{B}_{\mathrm{eff}}$, compute the unitary matrix
$$U_{\mathrm{obs}}(k_\lambda)_{a,b} = \sum_{c=1}^{m} \left\langle \psi_a(k_\lambda), \tau(\lambda)\Theta\psi_c(k_\lambda)\right\rangle \varepsilon_{cb},$$
defined as in (3.3), at the four inequivalent time-reversal invariant momenta $k_\lambda = v_1, \dots, v_4$;
- compute the spectrum $\left\{\mathrm{e}^{\mathrm{i}\lambda_1^{(i)}}, \dots, \mathrm{e}^{\mathrm{i}\lambda_m^{(i)}}\right\} \subset U(1)$ of $U_{\mathrm{obs}}(v_i)$, so that in particular
$$\det U_{\mathrm{obs}}(v_i) = \exp\left(\mathrm{i}\left(\lambda_1^{(i)} + \cdots + \lambda_m^{(i)}\right)\right);$$
normalize the arguments of such phases so that $\lambda_j^{(i)} \in [0, 2\pi)$ for all $j \in \{1, \dots, m\}$;
- compute $U(v_i)$ as in the proof of Lemma 3.1: in particular we obtain that

$$\det U(v_i) = \exp\left(\mathrm{i}\left(\frac{\lambda_1^{(i)}}{2} + \dots + \frac{\lambda_m^{(i)}}{2}\right)\right);$$

- finally, compute δ from the formula (5.4), *i. e.*

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

6 Construction of a symmetric Bloch frame in 3*d*

In this Section, we investigate the existence of a global continuous symmetric Bloch frame in the 3-dimensional setting. In particular, we will recover the four $\mathbb{Z}_2$ indices proposed by Fu, Kane and Mele [13]. We will first focus on the topological obstructions that arise, and then provide the construction of a symmetric Bloch frame in 3*d* 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

$$\mathbb{B}^{(3)} := \left\{ k = \sum_{j=1}^{3} k_j e_j \in \mathbb{R}^3 : -\frac{1}{2} \le k_j \le \frac{1}{2},\ j = 1,2,3 \right\}$$

(the superscript $^{(3)}$ stands for "3-dimensional"), where $\{e_1, e_2, e_3\}$ is a basis in $\mathbb{R}^3$ such that $\Lambda = \mathrm{Span}_{\mathbb{Z}}\{e_1, e_2, e_3\}$. If a continuous Bloch frame is given on $\mathbb{B}^{(3)}$, then it can be extended to a continuous τ-equivariant Bloch frame on $\mathbb{R}^3$ by considering its τ-translates, provided it satisfies the obvious compatibility conditions of τ-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 (see Figure 2)

$$\mathbb{B}^{(3)}_{\mathrm{eff}} := \left\{ k = (k_1, k_2, k_3) \in \mathbb{B}^{(3)} : k_1 \ge 0 \right\}.$$

Vertices of the (effective) unit cell are defined again as those points k_λ 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 3.1. 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 $\mathbb{B}^{(3)}_{\mathrm{eff}}$ by using the path-connectedness of the group $\mathcal{U}(\mathbb{C}^m)$, 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

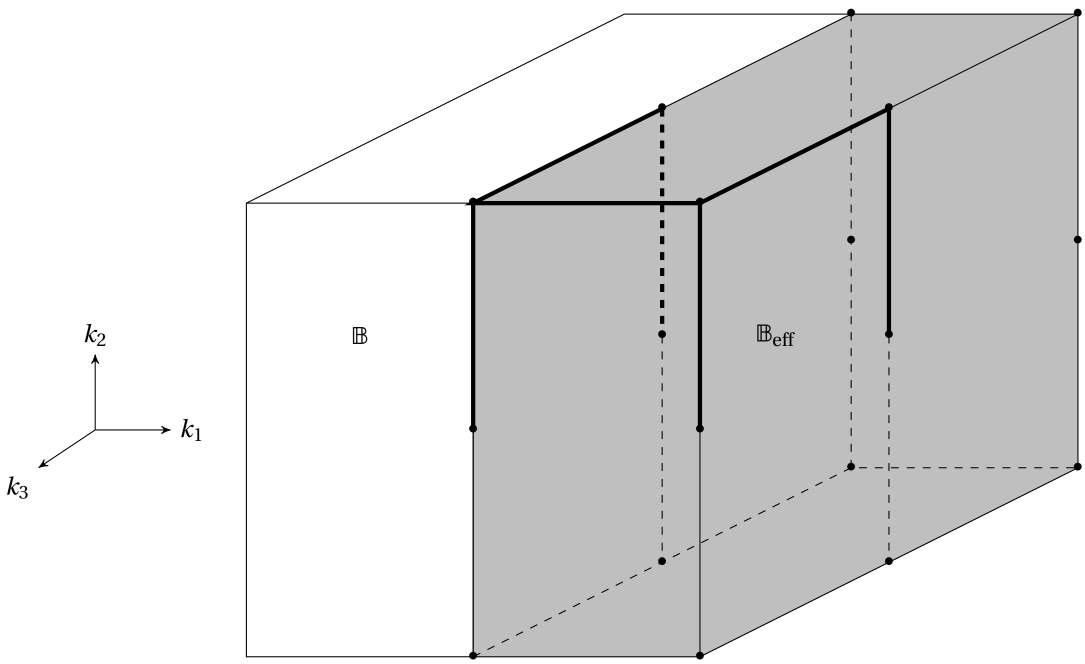


Fig. 2 The 3-dimensional effective unit cell (shaded area).

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 an input 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 Φ 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 Φ 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 Φ: 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 $\mathbb{B}^{(2)}_{\mathrm{eff}}$, then we can extend it to the whole face by using the time reversal operator Θ 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 to the continuous extension of the symmetric Bloch frame from the edges of $\mathbb{B}^{(3)}_{\mathrm{eff}}$ to the boundary $\partial\mathbb{B}^{(3)}_{\mathrm{eff}}$.

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

Topologically, the boundary of the effective unit cell in 3 dimensions is equivalent to a sphere: $\partial\mathbb{B}^{(3)}_{\mathrm{eff}} \simeq S^2$. Moreover, it is known that, if X is any topological space, then a continuous map $f\colon S^2 \to X$ extends to a continuous map $F\colon D^3 \to X$, 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. In our case, where $X = \mathcal{U}(\mathbb{C}^m)$, it is a well-known fact that $\pi_2(\mathcal{U}(\mathbb{C}^m)) = 0$ [19, 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 $\mathbb{B}^{(3)}_{\mathrm{eff}}$. In other words, there is no topological obstruction to the continuous extension of a symmetric frame from $\partial\mathbb{B}^{(3)}_{\mathrm{eff}}$ to $\mathbb{B}^{(3)}_{\mathrm{eff}}$, and hence to $\mathbb{R}^3$: indeed, one can argue, as in Proposition 3.1, that a symmetric Bloch frame on $\mathbb{B}^{(3)}_{\mathrm{eff}}$ can always be extended to all of $\mathbb{R}^3$, by imposing τ-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

$$\delta_*(P) := \delta\left(P\big|_{F_*}\right), \quad F_* \in \left\{F_{1,0}, F_{1,+}, F_{2,+}, F_{3,+}\right\}. \tag{6.1}$$

6.3 Proof of Theorem 2.3

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 $\Phi(k) = \Psi(k) \triangleleft U(k)$ on the effective unit cell $\mathbb{B}^{(3)}_{\text{eff}}$ (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 $\mathbb{B}^{(3)}_{\text{eff}}$.

The two main "tools" in this algorithm are provided by the following Lemmas, which are "distilled" from the procedure elaborated in Section 3.

Lemma 6.1 (From 0d to 1d). *Let $\{P(k)\}_{k\in\mathbb{R}}$ be a family of projectors satisfying Assumption 2.1. Denote $\mathbb{B}^{(1)}_{\text{eff}} = \{k = k_1 e_1 : -1/2 \le k_1 \le 0\} \simeq [-1/2, 0]$. Let $\Phi(-1/2)$ be a frame in* $\operatorname{Ran} P(-1/2)$ *such that*

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

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

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

Proof. Solve the vertex condition at $k_\lambda = 0 \in \mathbb{B}^{(1)}_{\text{eff}}$ using Lemma 3.1, and then extend the frame to $\mathbb{B}^{(1)}_{\text{eff}}$ as in Section 3.3. □

Lemma 6.2 (From 1d to 2d). *Let $\{P(k)\}_{k\in\mathbb{R}^2}$ be a family of projectors satisfying Assumption 2.1. Let v_i and E_i denote the edges of the effective unit cell $\mathbb{B}^{(2)}_{\text{eff}}$, as defined in Section 3.1. 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* (V) *at v_1, v_2, v_3 and v_4. Assume that*

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

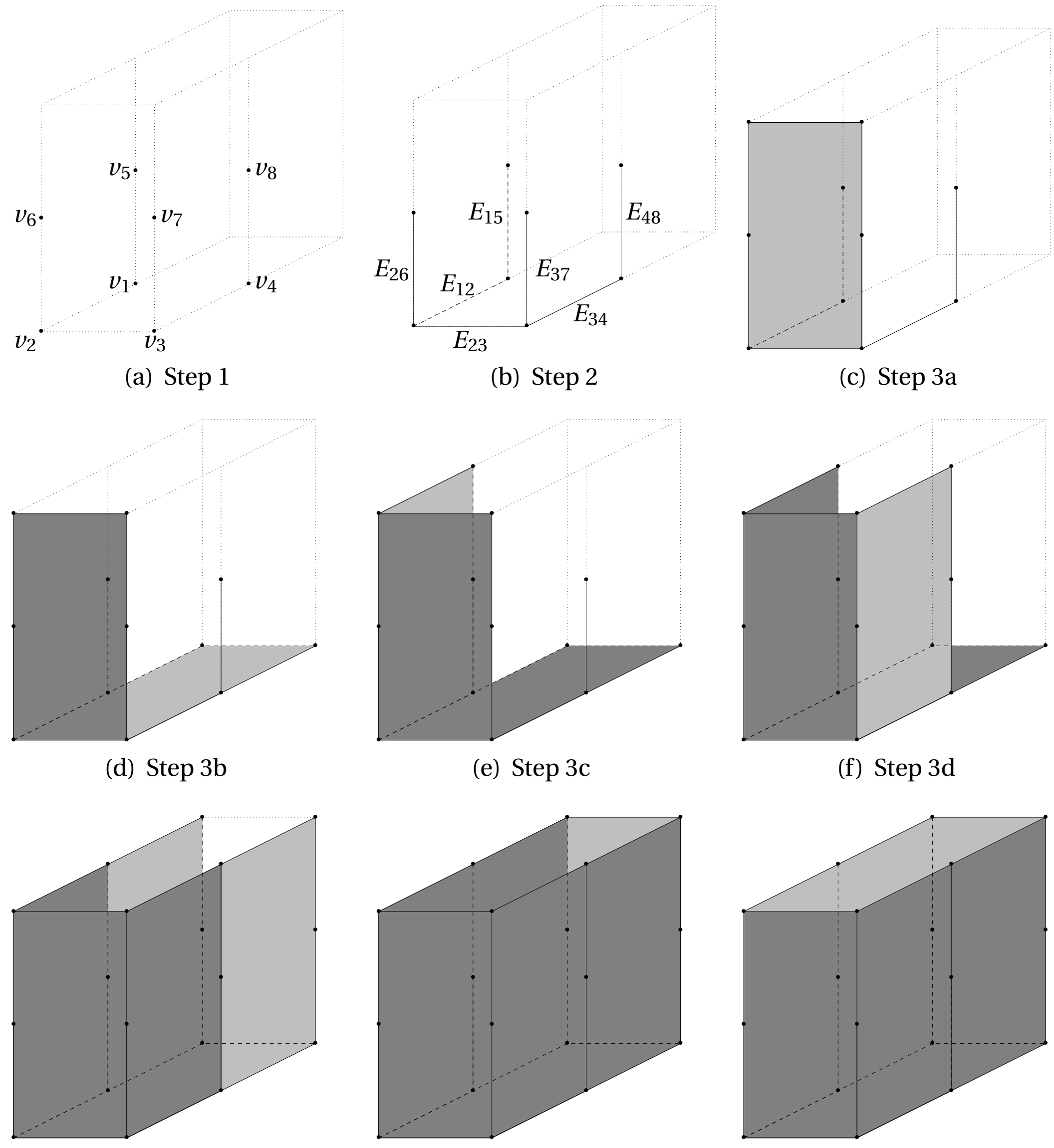
Then one constructs a continuous Bloch frame $\{\Phi_{\text{eff}}(k)\}_{k\in\mathbb{B}^{(2)}_{\text{eff}}}$, satisfying the vertex conditions (V) *and the edge symmetries* (E)*, and moreover such that*

$$\Phi_{\text{eff}}(k) = \Phi(k) \quad \textit{for } k \in E_1 \cup E_2. \tag{6.2}$$

Proof. This is just a different formulation of what was proved in Section 3.4. From the datum of $\Phi(k)$ on the edges $E_1 \cup E_2 \cup E_3$ one can construct the unitary matrix $\widehat{U} : \partial\mathbb{B}^{(2)}_{\text{eff}} \to \mathcal{U}(\mathbb{C}^m)$, such that $\Phi(k) \triangleleft \widehat{U}(k)$ is a symmetric Bloch frame, for $k \in \partial\mathbb{B}^{(2)}_{\text{eff}}$. The hypothesis $\delta(P) = 0 \in \mathbb{Z}_2$ ensures that $\deg([\det \widehat{U}]) = 2s$, $s \in \mathbb{Z}$. The proof of Theorem 3.1 then gives an explicit family of unitary matrices $X : \partial\mathbb{B}^{(2)}_{\text{eff}} \to \mathcal{U}(\mathbb{C}^m)$ such that $\deg([\det X]) = -2s$ and that $\Phi_{\text{eff}}(k) := \Phi(k) \triangleleft \big(\widehat{U}(k)\, X(k)\big)$ is still symmetric, so it extends to the whole $\mathbb{B}^{(2)}_{\text{eff}}$. 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. □

We are now ready to prove Theorem 2.3.

Proof of Theorem 2.3. Consider the region $Q = \mathbb{B}^{(3)}_{\text{eff}} \cap \{k_2 \leq 0, k_3 \geq 0\}$. 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 counter-clockwise) and $v_5 = (0,0,0)$, $v_6, v_7, v_8 \in Q \cap \{k_2 = 0\}$ (again counted counter-clockwise). We also let E_{ij} denote the edge joining v_i and v_j. The labels are depicted in Figure 3.



(a) Step 1 (b) Step 2 (c) Step 3a

(d) Step 3b (e) Step 3c (f) Step 3d

(g) Step 4 (h) Step 5 (i) Step 6

Fig. 3 Steps in the proof of Theorem 2.3.

Step 1. Choose a continuous Bloch frame $\{\Psi(k)\}_{k \in \mathbb{B}^{(3)}_{\text{eff}}}$ for $\{P(k)\}_{k \in \mathbb{R}^3}$. Solve the vertex conditions at all v_i's, using Lemma 3.1 to obtain frames $\Phi_{\text{ver}}(v_i)$, $i = 1, \dots, 8$.

Step 2. Using repeatedly Lemma 6.1, extend the definition of Φ_{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 6.2 to extend further the definition of Φ_{edg} as follows.

3a. Extend the definition of Φ_{edg} on $F_{3,+}$: this can be done since $\delta_{3,+}$ vanishes. This will change the original definition of Φ_{edg} only on E_{37}.
3b. Extend the definition of Φ_{edg} on $F_{2,-}$: this can be done since $\delta_{2,-} = \delta_{2,+}$ vanishes. This will change the original definition of Φ_{edg} only on E_{34}.
3c. Extend the definition of Φ_{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 Φ_{edg} only on E_{15}. (Here we give $F_{1,0}$ the *opposite* orientation to the one inherited from $\partial\mathbb{B}^{(3)}_{\text{eff}}$, but this is inessential.)
3d. Extend the definition of Φ_{edg} on $F_{1,+} \cap \{k_3 \geq 0\}$. Although we have already changed the definition of Φ_{edg} on $E_{37} \cup E_{34}$, this extension can still be performed since we have proved in Section 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 Φ_{edg} only on E_{48}.

We end up with a Bloch frame Φ_S defined on

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

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

$$\begin{aligned} \Phi_{S'}(k) &:= \Phi_S(k) && \text{for } k \in S, \\ \Phi_{S'}(\theta(k)) &:= \Theta\Phi_S(k) \triangleleft \varepsilon && \text{for } k \in F_{1,0} \cap \{k_3 \geq 0\}, \quad \text{and} \\ \Phi_{S'}(t_{e_1}\theta(k)) &:= \tau_{e_1}\Theta\Phi_S(k) \triangleleft \varepsilon && \text{for } k \in F_{1,+} \cap \{k_3 \geq 0\}. \end{aligned}$$

This extension is continuous. Indeed, continuity along $E_{15} \cup \theta(E_{15}) = F_{1,0} \cap \{k_3 = 0\}$ (respectively $E_{48} \cup t_{e_1}\theta(E_{48}) = F_{1,+} \cap \{k_3 = 0\}$) is a consequence of the edge symmetries that we have imposed on Φ_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 $t_{-e_2}\theta(E_{12}) = (F_{1,0} \cap \{k_3 \leq 0\}) \cap F_{2,-}$ and $t_{e_1-e_2}\theta(E_{34}) = (F_{1,+} \cap \{k_3 \leq 0\}) \cap F_{2,-}$ agrees with the definition of Φ_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

$$\begin{aligned} \Phi_S(t_{-e_2}\theta(k)) &= \tau_{-e_2}\Theta\Phi_S(k) \triangleleft \varepsilon = \tau_{-e_2}\Theta\Phi_{S'}(k) \triangleleft \varepsilon = \\ &= \tau_{-e_2}\Theta\tau_{-e_2}\Phi_{S'}(t_{e_2}(k)) \triangleleft \varepsilon \end{aligned}$$

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 ($P_4$) and of the definition of $\Phi_{S'}$ on $F_{1,0} \cap \{k_3 \leq 0\}$, we conclude that

$$\Phi_S(t_{-e_2}\theta(k)) = \Theta\Phi_{S'}(t_{e_2}(k)) \triangleleft \varepsilon = \Phi_{S'}(\theta\, t_{e_2}(k)) = \Phi_{S'}(t_{-e_2}\theta(k))$$

as wanted. This shows that $\Phi_{S'}$ is continuous on

$$S' := S \cup \left(F_{1,0} \cap \{k_3 \leq 0\}\right) \cup \left(F_{1,+} \cap \{k_3 \leq 0\}\right).$$

Step 5. Extend the definition of $\Phi_{S'}$ to $F_{3,-}$ by setting

$$\begin{aligned} \Phi_{S''}(k) &:= \Phi_{S'}(k) && \text{for } k \in S', \quad \text{and} \\ \Phi_{S''}(t_{-e_3}(k)) &:= \tau_{-e_3}\Phi_{S'}(k) && \text{for } k \in F_{3,+}. \end{aligned}$$

This extension is continuous on $t_{-e_3}(E_{23}) = F_{2,-} \cap F_{3,-}$ because in Step 3b we have imposed on Φ_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 $t_{-e_3}(E_{37}) \cup t_{e_1}\theta(E_{37}) = F_{1,+} \cap F_{3,-}$, because by construction $\Phi_{S'}$ is τ-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

$$\begin{aligned} \widehat{\Phi}(k) &:= \Phi_{S''}(k) && \text{for } k \in S'', \quad \text{and} \\ \widehat{\Phi}(t_{e_2}(k)) &:= \tau_{e_2}\Phi_{S''}(k) && \text{for } k \in F_{2,-}. \end{aligned}$$

Similarly to what was argued in Step 5, the edge symmetries (*i. e.* τ-equivariance) on $\partial F_{2,-}$ and $\partial F_{2,+}$ imply that this extension is continuous. The Bloch frame $\widehat{\Phi}$ is now defined and continuous on $\partial\mathbb{B}^{(3)}_{\text{eff}}$.
Step 7. Finally, extend the definition of $\widehat{\Phi}$ on the interior of $\mathbb{B}^{(3)}_{\text{eff}}$. As was argued before at the end of Section 6.2, this step is topologically unobstructed. Thus, we end up with a continuous symmetric Bloch frame Φ_{eff} on $\mathbb{B}^{(3)}_{\text{eff}}$. Set now

$$\Phi_{\text{uc}}(k) := \begin{cases} \Phi_{\text{eff}}(k) & \text{if } k \in \mathbb{B}^{(3)}_{\text{eff}}, \\ \Theta\Phi_{\text{eff}}(\theta(k)) \triangleleft \varepsilon & \text{if } k \in \mathbb{B}^{(3)} \setminus \mathbb{B}^{(3)}_{\text{eff}}. \end{cases}$$

The symmetries satisfied by Φ_{eff} on $F_{1,0}$ (imposed in Step 4) imply that the Bloch frame Φ_{uc} is still continuous. We extend now the definition of Φ_{uc} to the whole $\mathbb{R}^3$ by setting

$$\Phi(k) := \tau_\lambda \Phi_{\text{uc}}(k'), \quad \text{if } k = k' + \lambda \text{ with } k' \in \mathbb{B}^{(3)},\ \lambda \in \Lambda.$$

Again, the symmetries imposed on Φ_{uc} in the previous Steps of the proof ensure that Φ is continuous, and by construction it is also symmetric. This concludes the proof of Theorem 2.3. □

6.4 Comparison with the Fu-Kane-Mele indices

In their work [13], Fu, Kane and Mele generalized the definition of $\mathbb{Z}_2$ indices for $2d$ topological insulators, appearing in [12], 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_λ, 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_λ 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 Ψ is a continuous and τ-equivariant Bloch frame (whose existence is guaranteed again by the generalization of the results of [28] given in [26]). Set

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

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 [13, 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 $(-1)^{\nu_i}$ 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_λ.

Since our invariants $\delta_{1,0}$ 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

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

where (compare (5.2))

$$\widehat{\eta}_{n_1,n_2,n_3} := \left.\frac{\sqrt{(\det U(k_\lambda))^2}}{\det U(k_\lambda)}\right|_{\lambda=(n_1/2,n_2/2,n_3/2)}.$$

As we have also shown in Section 4 that our 2-dimensional invariant δ agrees with the Fu-Kane index Δ, from the previous considerations it follows at once that

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

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 ν_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 Λ, while the index ν_0 is *independent* of such a choice. This substantiates the terminology of [13], where ν_0 is called "strong" invariant, while ν_1, ν_2 and ν_3 are referred to as "weak" invariants.

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 2.1. 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

$$\mathrm{dist}(\Phi,\Psi) := \sup_{k\in\mathbb{R}^d}\left(\sum_{a=1}^{m}\left\|\phi_a(k)-\psi_a(k)\right\|^2_{\mathcal{H}}\right)^{1/2}$$

for two global Bloch frames $\Phi = \left\{\phi_a(k)\right\}_{a=1,\dots,m,\,k\in\mathbb{R}^d}$ and $\Psi = \left\{\psi_a(k)\right\}_{a=1,\dots,m,\,k\in\mathbb{R}^d}$. The following result holds in any dimension $d \geq 0$.

Proposition A.1. *Let $\{P(k)\}_{k\in\mathbb{R}^d}$ be a family of orthogonal projectors satisfying Assumption 2.1. Assume that a* continuous *global symmetric Bloch frame Φ exists for $\{P(k)\}_{k\in\mathbb{R}^d}$. Then for any $\mu > 0$ there exists a* smooth *global symmetric Bloch frame Φ_{sm} such that*

$$\mathrm{dist}(\Phi,\Phi_{\mathrm{sm}}) < \mu.$$

Proof. We use the same strategy used to prove Proposition 5.1 in [9], to which we refer for most details.

A global Bloch frame gives a section of the principal $\mathcal{U}(\mathbb{C}^m)$-bundle $\mathrm{Fr}(\mathcal{P}) \to \mathbb{T}^d$, the *frame bundle* associated with the Bloch bundle $\mathcal{P} \to \mathbb{T}^d$, whose fibre $\mathrm{Fr}(\mathcal{P})_k =: F_k$ over the point $k \in \mathbb{T}^d$ consists of all orthonormal bases in $\operatorname{Ran} P(k)$. The existence of a continuous global Bloch frame Φ is thus equivalent to the existence of a continous global section of the frame bundle $\mathrm{Fr}(\mathcal{P})$. By Steenrod's ironing principle [35, 41], 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 $\widetilde{\Phi}_{\mathrm{sm}}$ such that

$$\mathrm{dist}(\Phi,\widetilde{\Phi}_{\mathrm{sm}}) < \frac{1}{2}\mu.$$

The Bloch frame $\widetilde{\Phi}_{\mathrm{sm}}$ will not in general be also symmetric, so we apply a symmetrization procedure to $\widetilde{\Phi}_{\mathrm{sm}}$ to obtain the desired smooth symmetric Bloch frame Φ_{sm}. In order to do so, we define the *midpoint* between two sufficiently close frames Φ and Ψ in F_k as follows. Write $\Psi = \Phi \triangleleft U_{\Phi,\Psi}$, with $U_{\Phi,\Psi}$ a unitary matrix. If Ψ is sufficiently close to Φ, then $U_{\Phi,\Psi}$ is sufficiently close to the identity matrix $\mathbb{1}_m$ in the standard Riemannian metric of $\mathcal{U}(\mathbb{C}^m)$ (see [9, Section 5] for details). As such, we have that $U_{\Phi,\Psi} = \exp\left(A_{\Phi,\Psi}\right)$, for $A_{\Phi,\Psi} \in \mathfrak{u}(\mathbb{C}^m)$ a skew-Hermitian matrix, and $\exp\colon \mathfrak{u}(\mathbb{C}^m) \to \mathcal{U}(\mathbb{C}^m)$ the exponential map[1]. We define then the *midpoint* between Φ and Ψ to be the frame

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

[1] It is known that the exponential map $\exp\colon \mathfrak{u}(\mathbb{C}^m) \to \mathcal{U}(\mathbb{C}^m)$ defines a diffeomorphism between a ball $B_\delta(0) \subset \mathfrak{u}(\mathbb{C}^m)$ and a Riemannian ball $B_\delta(\mathbb{1}_m) \subset \mathcal{U}(\mathbb{C}^m)$, for some $\delta > 0$. When we say that the two frames Φ and Ψ should be "sufficiently close", we mean (here and in the following) that the unitary matrix $U_{\Phi,\Psi}$ lies in the ball $B_\delta(\mathbb{1}_m)$.

Set

$$\Phi_{\mathrm{sm}}(k) := \widehat{M}\left(\widetilde{\Phi}_{\mathrm{sm}}(k), \Theta\widetilde{\Phi}_{\mathrm{sm}}(-k) \triangleleft \varepsilon\right). \tag{A.1}$$

The proof that Φ_{sm} defines a *smooth* global Bloch frame, which satisfies the τ-equivariance property (F'_3), and that moreover its distance from the frame Φ is less than μ goes exactly as the proof of [9, Prop. 5.1]. A slightly different argument is needed, instead, to prove that Φ_{sm} is also time-reversal symmetric, *i. e.* that it satisfies also (F'_4). To show this, we need a preliminary result.

Lemma A.1. *Let $\Phi, \Psi \in F_k$ be two frames, and assume that Φ and $\Psi \triangleleft \varepsilon$ are sufficiently close. Then*

$$\widehat{M}(\Phi, \Psi \triangleleft \varepsilon) = \widehat{M}(\Phi \triangleleft \varepsilon^{-1}, \Psi) \triangleleft \varepsilon. \tag{A.2}$$

Proof. Notice first that

$$\Psi = \Phi \triangleleft U_{\Phi,\Psi} \quad \Longrightarrow \quad \Psi \triangleleft \varepsilon = \Phi \triangleleft \left(U_{\Phi,\Psi}\varepsilon\right) \text{ and } \Psi = (\Phi \triangleleft \varepsilon^{-1}) \triangleleft \left(\varepsilon U_{\Phi,\Psi}\right),$$

which means that

$$U_{\Phi,\Psi\triangleleft\varepsilon} = U_{\Phi,\Psi}\varepsilon \quad \text{and} \quad U_{\Phi\triangleleft\varepsilon^{-1},\Psi} = \varepsilon U_{\Phi,\Psi}.$$

Write

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

for $A, B \in B_\delta(0) \subset \mathfrak{u}(\mathbb{C}^m)$, where $\delta > 0$ is such that $\exp\colon B_\delta(0) \subset \mathfrak{u}(\mathbb{C}^m) \to B_\delta(\mathbb{1}_m) \subset \mathcal{U}(\mathbb{C}^m)$ is a diffeomorphism. Since the Hilbert-Schmidt norm $\|A\|^2_{\mathrm{HS}} := \mathrm{Tr}(A^* A)$ is invariant under unitary conjugation, also $\varepsilon^{-1} A \varepsilon \in B_\delta(0)$. Then we have that

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

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

$$\begin{aligned}\widehat{M}(\Phi \triangleleft \varepsilon^{-1}, \Psi) \triangleleft \varepsilon = (\Phi \triangleleft \varepsilon^{-1}) \triangleleft \left(\exp\left(\frac{1}{2}A\right)\varepsilon\right) &= \\ = \Phi \triangleleft \exp\left(\frac{1}{2}\varepsilon^{-1} A \varepsilon\right) = \Phi \triangleleft \exp\left(\frac{1}{2}B\right) &= \\ = \widehat{M}(\Phi, \Psi \triangleleft \varepsilon)&\end{aligned}$$

which is exactly (A.2). □

We are now in position to prove that Φ_{sm}, defined in (A.1), satisfies (F'_4). Indeed, we compute

$$\begin{aligned}
\Theta\Phi_{\mathrm{sm}}(k) \triangleleft \varepsilon &= \Theta\widehat{M}\left(\widetilde{\Phi}_{\mathrm{sm}}(k), \Theta\widetilde{\Phi}_{\mathrm{sm}}(-k) \triangleleft \varepsilon\right) \triangleleft \varepsilon = \\
&= \widehat{M}\left(\Theta\widetilde{\Phi}_{\mathrm{sm}}(k), \Theta^2\widetilde{\Phi}_{\mathrm{sm}}(-k) \triangleleft \overline{\varepsilon}\right) \triangleleft \varepsilon = && \text{(by [9, Eqn. (5.11)])} \\
&= \widehat{M}\left(\Theta\widetilde{\Phi}_{\mathrm{sm}}(k), \widetilde{\Phi}_{\mathrm{sm}}(-k) \triangleleft \varepsilon^{-1}\right) \triangleleft \varepsilon = && \text{(because } -\overline{\varepsilon} = \varepsilon^{-1} \text{ by Remark 2.2)} \\
&= \widehat{M}\left(\widetilde{\Phi}_{\mathrm{sm}}(-k) \triangleleft \varepsilon^{-1}, \Theta\widetilde{\Phi}_{\mathrm{sm}}(k)\right) \triangleleft \varepsilon = && \text{(because } \widehat{M}(\Phi,\Psi) = \widehat{M}(\Psi,\Phi)\text{)} \\
&= \widehat{M}\left(\widetilde{\Phi}_{\mathrm{sm}}(-k), \Theta\widetilde{\Phi}_{\mathrm{sm}}(k) \triangleleft \varepsilon\right) = \Phi_{\mathrm{sm}}(-k) && \text{(by (A.2))}.
\end{aligned}$$

This concludes the proof of the Proposition. □

References

1. ALTLAND, A.; ZIRNBAUER, M. : Non-standard symmetry classes in mesoscopic normal-superconducting hybrid structures, *Phys. Rev. B* **55** (1997), 1142–1161.
2. ANDO, Y. : Topological insulator materials, *J. Phys. Soc. Jpn.* **82** (2013), 102001.
3. AVILA, J.C.; SCHULZ-BALDES, H.; VILLEGAS-BLAS, C. : Topological invariants of edge states for periodic two-dimensional models, *Mathematical Physics, Analysis and Geometry* **16** (2013), 136–170.
4. CARPENTIER, D.; DELPLACE, P.; FRUCHART, M.; GAWEDZKI, K. : Topological index for periodically driven time-reversal invariant 2D systems, *Phys. Rev. Lett.* **114** (2015), 106806.
5. CARPENTIER, D.; DELPLACE, P.; FRUCHART, M.; GAWEDZKI, K.; TAUBER, C. : Construction and properties of a topological index for periodically driven time-reversal invariant 2D crystals, preprint available at `arXiv:1503.04157`.
6. CERULLI IRELLI, G. ; FIORENZA, D.; MONACO, D.; PANATI, G. : Geometry of Bloch bundles: a unifying quiver-theoretic approach, in preparation (2015).
7. CHANG, C.-Z. *et al.* : Experimental Observation of the Quantum Anomalous Hall Effect in a Magnetic Topological Insulator, *Science* **340** (2013), 167–170.
8. DUBROVIN, B.A.; NOVIKOV, S.P.; FOMENKO, A.T. : Modern Geometry – Methods and Applications. Part II: The Geometry and Topology of Manifolds. No. 93 in Graduate Texts in Mathematics. Springer-Verlag, New York, 1985.
9. FIORENZA, D.; MONACO, D.; PANATI, G. : Construction of real-valued localized composite Wannier functions for insulators, to appear in *Ann. Henri Poincaré*. Preprint available at `arXiv:1408.0527`.
10. FRÖHLICH, J. ; WERNER, PH. : Gauge theory of topological phases of matter, *EPL* **101** (2013), 47007.
11. FRUCHART, M. ; CARPENTIER, D. : An introduction to topological insulators, *Comptes Rendus Phys.* **14** (2013), 779–815.
12. FU, L.; KANE, C.L. : Time reversal polarization and a $\mathbb{Z}_2$ adiabatic spin pump, *Phys. Rev. B* **74** (2006), 195312.
13. FU, L.; KANE, C.L.; MELE, E.J. : Topological insulators in three dimensions, *Phys. Rev. Lett.* **98** (2007), 106803.
14. GRAF, G.M. : Aspects of the Integer Quantum Hall Effect, *Proceedings of Symposia in Pure Mathematics* **76** (2007), 429–442.
15. GRAF, G.M.; PORTA, M. : Bulk-edge correspondence for two-dimensional topological insulators, *Commun. Math. Phys.* **324** (2013), 851–895.
16. HALDANE, F.D.M. : Model for a Quantum Hall Effect without Landau levels: condensed-matter realization of the "parity anomaly", *Phys. Rev. Lett.* **61** (1988), 2017.
17. HASAN, M.Z.; KANE, C.L. : Colloquium: Topological Insulators, *Rev. Mod. Phys.* **82** (2010), 3045–3067.
18. HUA, L.-K.: On the theory of automorphic functions of a matrix variable I – Geometrical basis, *Am. J. Math.* **66** (1944), 470–488.
19. HUSEMOLLER, D.: *Fibre bundles*, 3rd edition. No. 20 in Graduate Texts in Mathematics. Springer-Verlag, New York, 1994.
20. KANE, C.L.; MELE, E.J. : $\mathbb{Z}_2$ Topological Order and the Quantum Spin Hall Effect, *Phys. Rev. Lett.* **95** (2005), 146802.

21. KANE, C.L.; MELE, E.J. : Quantum Spin Hall Effect in graphene, *Phys. Rev. Lett.* **95** (2005), 226801.
22. KATO, T. : Perturbation theory for linear operators. Springer, Berlin, 1966.
23. KENNEDY, R.; GUGGENHEIM, C. : Homotopy theory of strong and weak topological insulators, preprint available at `arXiv:1409.2529`.
24. KITAEV, A. : Periodic table for topological insulators and superconductors, *AIP Conf. Proc.* **1134** (2009), 22.
25. MACKEY, D.S.; MACKEY, N. : On the Determinant of Symplectic Matrices. *Numerical Analysis Report* **422** (2003), Manchester Centre for Computational Mathematics, Manchester, England.
26. MONACO, D.; PANATI, G. : Symmetry and localization in periodic crystals: triviality of Bloch bundles with a fermionic time-reversal symmetry. Proceedings of the conference *"SPT2014 – Symmetry and Perturbation Theory", Cala Gonone, Italy*, to appear in *Acta App. Math.* (2015).
27. MOORE, J.E.; BALENTS, L. : Topological invariants of time-reversal-invariant band structures, *Phys. Rev. B* **75** (2007), 121306(R).
28. PANATI, G.: Triviality of Bloch and Bloch-Dirac bundles, *Ann. Henri Poincaré* **8** (2007), 995–1011.
29. PRODAN, E. : Robustness of the Spin-Chern number, *Phys. Rev. B* **80** (2009), 125327.
30. PRODAN, E. : Disordered topological insulators: A non-commutative geometry perspective, *J. Phys. A* **44** (2011), 113001.
31. PRODAN, E. : Manifestly gauge-independent formulations of the $\mathbb{Z}_2$ invariants, *Phys. Rev. B* **83** (2011), 235115.
32. RYU, S.; SCHNYDER, A.P.; FURUSAKI, A.; LUDWIG, A.W.W. : Topological insulators and superconductors: Tenfold way and dimensional hierarchy, *New J. Phys.* **12** (2010), 065010.
33. SCHULZ-BALDES, H. : Persistence of spin edge currents in disordered Quantum Spin Hall systems, *Commun. Math. Phys.* **324** (2013), 589–600.
34. SCHULZ-BALDES, H. : $\mathbb{Z}_2$ indices of odd symmetric Fredholm operators, preprint available at `arXiv:1311.0379`.
35. STEENROD, N. : *The Topology of Fibre Bundles.* No. 14 in Princeton Mathematical Series. Princeton University Press, Princeton, 1951.
36. STICLET, D. ; PÉCHON, F.; FUCHS, J.-N.; KALUGIN, P.; SIMON P. : Geometrical engineering of a two-band Chern insulator in two dimensions with arbitrary topological index, *Phys. Rev. B* **85** (2012), 165456.
37. SOLUYANOV, A.A.; VANDERBILT, D. : Wannier representation of $\mathbb{Z}_2$ topological insulators, *Phys. Rev. B* **83** (2011), 035108.
38. SOLUYANOV, A.A.; VANDERBILT, D. : Computing topological invariants without inversion symmetry, *Phys. Rev. B* **83** (2011), 235401.
39. SOLUYANOV, A.A.; VANDERBILT, D. : Smooth gauge for topological insulators, *Phys. Rev. B* **85** (2012), 115415.
40. THOULESS D.J.; KOHMOTO, M.; NIGHTINGALE, M.P.; DE NIJS, M. : Quantized Hall conductance in a two-dimensional periodic potential, *Phys. Rev. Lett.* **49** (1982), 405–408.
41. WOCKEL, CH. : A generalization of Steenrod's Approximation Theorem, *Arch. Math. (Brno)* **45** (2009), 95–104.

Conclusions

Open problems and perspectives

The line of research in which this dissertation fits, namely that of geometric phases of quantum matter, is very active, and of course several questions remain to be answered. Here we would like to illustrate some possible further developments of the analysis initiated in the works presented in this dissertation.

1 Disordered topological insulators

The $\mathbb{Z}_2$ invariants introduced in [5], which was reproduced in Part II of this thesis, provide a geometric origin for the indices proposed by Fu, Kane and Mele to distinguish different geometric phases in time-reversal symmetric topological insulators, when the time-reversal operator is of fermionic nature. It is costumary, in the physics literature, to dub a phase "topological" if it is stable under (small) perturbations of the system: usually these perturbations include *disorder* and *impurities*. Our current formulation cannot encompass also this more general framework, since the introduction of a random potential usually breaks the periodicity of the system at a microscopic level; the mathematical consequence of this is that we cannot employ the Bloch-Floquet-Zak transform and pass to the crystal momentum description of the system. It should be noticed however that $\mathbb{Z}_2$ invariants for disordered quantum spin Hall systems have been already proposed [15, 16], at least under the assumption of quasi-conservation of spin.

In the context of the quantum Hall effect, it has been suggested by Bellissard and collaborators (see [1] and references therein) to replace the notion of periodicity with that of *homogeneity*. Roughly speaking, this notion requires to consider the Hamiltonian of the system not as a single operator, but rather as a *family* of operators $\{H_\omega\}_{\omega\in\Omega}$, labelled by the disorder configurations $\omega \in \Omega$. Such a family is called *homogeneous* if the periodicity of the system is restored at a *macroscopic* level, namely if the Hamiltonian at disorder configuration ω and the one at the "translated disorder configuration" $\mathrm{T}_\lambda\omega$ are unitarily equivalent:

$$H_{\mathrm{T}_\lambda\omega} = \tau_\lambda \, H_\omega \, \tau_\lambda^{-1}, \quad \lambda \in \Lambda, \, \omega \in \Omega, \quad \tau_\lambda^{-1} = \tau_\lambda^*.$$

Here $\mathrm{T}\colon \Lambda \times \Omega \to \Omega$, $(\lambda, \omega) \mapsto \mathrm{T}_\lambda\omega$, is an action of $\Lambda \simeq \mathbb{Z}^d$ on Ω, which is assumed to be ergodic with respect to some probability measure on Ω (used to perform averages over disorder configurations). One can then set homogeneous families of operators in a C^*-algebraic setting, defining the *noncommutative Brillouin zone* as the crossed product C^*-algebra $\mathcal{A}_{\mathrm{NCBZ}} := C(\Omega) \rtimes_{\mathrm{T}} \Lambda$; this is in turn made into a noncommutative manifold by endowing it with derivations ∂_1, ∂_2 and a trace $\mathcal{T}$ which plays the rôle of integration. With this structure, the *Connes-Chern character* (the noncommutative analogue of a Chern number) can be formulated; proving that it stays quantized (namely that it assumes only integer values) requires the use of *Fredholm modules* theory.

A tentative approach to give a generalization of the $\mathbb{Z}_2$ invariants we proposed in [5] to the framework of disordered media and homogeneous families of operators would require to borrow ideas from [1, 18] and follow a similar line of argument. First, one should define a "noncommutative effective Brillouin zone", enlarging the group of macroscopic symmetries Λ to the group $G := \Lambda \rtimes \mathbb{Z}_2$, a semidirect product of Λ (namely the group of lattice translations) with the group $\mathbb{Z}_2$ generated, in the usual k-space picture, by the involution $\theta(k) = -k$. The noncommutative effective Brillouin zone $\mathcal{A}_{\mathrm{NCEBZ}} := C(\Omega) \rtimes G$ should then be equipped with derivations and integration (trace), to mimic a formula like (3.16) in the reproduction of [5] presented in Part II. The appropriate Fredholm module should then be defined to prove quantization, this time in the $\mathbb{Z}_2$ sense.

Although promising, at present this approach remains to be fully explored.

2 Topological invariants for other symmetry classes

Another possible line of investigation concerns the geometric origin of the different topological phases in the symmetry classes of the periodic tables of topological insulators (compare Table 1 in the Introduction). Pioneering results in this direction can be found in [8, 2, 3, 4, 19, 17, 7].

The methods we proposed in Part II are amenable to wide generalizations, since they rely only on the fundamental symmetries of the quantum system at hand. In particular, by considering families of projectors $\{P(k)\}_{k \in S^d}$ which are labelled by a crystal momentum in S^d instead of $\mathbb{R}^d$ (and eliminating the periodicity condition (P_2) from Assumption 2.1 in the Introduction), and/or encoding other types of symmetries (charge conjugation, chiral symmetry) possibly in combination with one another, one should in principle be able to define topological invariants for families of projectors in the various Altland-Zirnbauer classes (both for free-fermion systems and for periodic ones), proceeding again in a step-by-step construction of a Bloch frame along the cellular decomposition of the Brillouin zone (from vertices to edges, to faces, and so on).

3 Magnetic Wannier functions

As a last possible development of the line of research covered in this dissertation, we report on some currently unpublished results, which investigate magnetic Wannier functions [12].

As was discussed in the Introduction, it is by now well established [13] that the existence of a frame composed of exponentially localized Wannier functions for a gapped periodic quantum system is equivalent to the triviality of the associated Bloch bundle, or equivalently to the vanishing of its first Chern class. The latter condition is ensured by the presence of time-reversal symmetry [13, 11]. It is natural to ask what kind of decay at infinity of the Wannier functions is to be expected when the topology is *non-trivial*, namely when the Chern class of the Bloch bundle does not vanish. This is generically the case, for example, for *magnetic* periodic Schrödinger operators, since the presence of a magnetic field breaks time-reversal symmetry. This is why we refer to Bloch and Wannier functions associated to a topologically non-trivial Bloch bundle as *magnetic* Bloch and Wannier functions, respectively.

To investigate the decay at infinity of magnetic Wannier functions, we proceed as follows. We illustrate for simplicity the 2-dimensional picture, but our argument can be adapted also to dimension $d = 3$. By employing techniques similar to those used in [5], we are able to construct a Bloch frame Φ which is smooth and τ-equivariant on the boundary $\partial\mathbb{B}$ of the fundamental unit cell. This Bloch frame is then extended to $\mathbb{B} \setminus \{(0,0)\}$ by the parallel transport techniques developed in [6]: these allow also to estimate the singularity of the resulting Bloch frame at the origin, and one is able to establish that the extended frame Φ is in $H^s(\mathbb{B};\mathcal{H})$ for all $s < 1$. This requires also some arguments similar to those presented in [10] (see Part I of this dissertation).

A separate argument shows instead that, if a more regular frame $\widetilde{\Phi} \in H^1(\mathbb{B};\mathcal{H})$ existed, then the Chern number of the Bloch bundle would vanish, thus implying that the bundle itself is trivial, contrary to the "magnetic" assumption. Notice that the existence of a frame $\widehat{\Phi} \in H^r(\mathbb{B};\mathcal{H})$ with $r > 1$ is also excluded, since by Sobolev embedding $\widehat{\Phi}$ would be continuous, contradicting the non-triviality assumption on the Bloch bundle. This shows that the Sobolev regularity of the Bloch frame Φ constructed above is the best that can be obtained. In turn, such regularity implies that the associated Wannier functions w are such that $F_{\mathrm{MV}}[w] = \infty$, where F_{MV} is the *Marzari-Vanderbilt localization functional* [9, 36], given by the variance of the position operator in the state w. The physical interpretation of this result is that, just as trivial topology is related to (exponential) localization, non-trivial topology is related to *delocalization*, establishing an even stronger bound between geometric aspects and transport properties in crystals.

References

1. BELLISSARD, J.; VAN ELST, A.; SCHULZ-BALDES, H. : The noncommutative geometry of the quantum Hall effect, *J. Math. Phys* **35**, 5373–5451 (1994).
2. DE NITTIS, G.; GOMI, K. : Classification of "Real" Bloch-bundles: Topological Quantum Systems of type AI, *J. Geom. Phys.* **86**, 303-338 (2014).
3. DE NITTIS, G.; GOMI, K. : Classification of "Quaternionic" Bloch-bundles, *Commun. Math. Phys.* **339** (2015), 1–55.
4. DE NITTIS, G.; GOMI, K. : Chiral vector bundles: A geometric model for class AIII topological quantum systems, available at `arXiv:1504.04863`.
5. FIORENZA, D.; MONACO, D.; PANATI, G. : $\mathbb{Z}_2$ invariants of topological insulators as geometric obstructions, available at `arXiv:1408.1030`.
6. FREUND, S.; TEUFEL, S. : Peierls substitution for magnetic Bloch bands, available at `arXiv:1312.5931`.
7. GROSSMANN, J.; SCHULZ-BALDES, H. : Index pairings in presence of symmetries with applications to topological insulators, available at `arXiv:1503.04834`.
8. KENNEDY, R.; ZIRNBAUER, M.R. : Bott periodicity for $\mathbb{Z}_2$ symmetric ground states of free fermion systems, available at `arXiv:1409.2537`.

9. MARZARI, N.; MOSTOFI, A.A.; YATES, J.R.; SOUZA I.; VANDERBILT, D. : Maximally localized Wannier functions: Theory and applications, *Rev. Mod. Phys.* **84**, 1419 (2012).
10. MONACO, D.; PANATI, G. : Topological invariants of eigenvalue intersections and decrease of Wannier functions in graphene, *J. Stat. Phys.* **155**, Issue 6, 1027–1071 (2014).
11. MONACO, D.; PANATI, G. : Symmetry and localization in periodic crystals: triviality of Bloch bundles with a fermionic time-reversal symmetry, *Acta Appl. Math.* **137**, Issue 1, 185–203 (2015).
12. MONACO, D.; PANATI, G.; PISANTE, A.; TEUFEL, S. : Decay of magnetic Wannier functions, in preparation.
13. PANATI, G. : Triviality of Bloch and Bloch-Dirac bundles, *Ann. Henri Poincaré* **8**, 995–1011 (2007).
14. PANATI, G.; PISANTE, A. : Bloch bundles, Marzari-Vanderbilt functional and maximally localized Wannier functions, *Commun. Math. Phys.* **322**, 835–875 (2013).
15. PRODAN, E. : Robustness of the Spin-Chern number, *Phys. Rev. B* **80**, 125327 (2009).
16. PRODAN, E. : Disordered topological insulators: A non-commutative geometry perspective, *J. Phys. A* **44**, 113001 (2011).
17. PRODAN, E. : The non-commutative geometry of the complex classes of topological insulators, *Topol. Quantum Matter* **1**, 1–16 (2014).
18. PRODAN, E.; LEUNG, B.; BELLISSARD, J. : The non-commutative nth-Chern number ($n \geq 1$), *J. Phys. A* **46** (2013), 485202.
19. PRODAN, E.; SCHULZ-BALDES, H. : Non-commutative odd Chern numbers and topological phases of disordered chiral systems, available at `arXiv:1402.5002`.