

CONSTRUCTION OF REAL-VALUED LOCALIZED COMPOSITE WANNIER FUNCTIONS FOR INSULATORS

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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 a 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.

KEYWORDS. Periodic Schrödinger operators, Wannier functions, Bloch frames.

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1. INTRODUCTION

The existence of an orthonormal basis of well-localized Wannier functions is a crucial issue in solid-state physics [MYSV]. Indeed, such a basis is the key tool to obtain effective tight-binding models for a linear or non-linear Schrödinger dynamics [PSM, PeSch, IEB₁, IEB₂, WCJ], it allows computational methods whose cost scales linearly with the size of the confining box [Go], it is useful in the rigorous analysis of perturbed periodic Hamiltonians [CaLe, LeSe, ELu], and it is crucial in the modern theory of polarization of crystalline solids [Re, KSV, PST₁] and in the pioneering research on topological insulators [Has, RSFL, Pr₁, Pr₂, SoVa₁, SoVa₂].

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 [Ko], who provided a proof in dimension $d = 1$ for an even potential. The latter assumption was later removed by J. de Cloizeaux [Cl₂], who also gave a proof valid for any $d > 1$ under the assumption that the periodic potential is centro-symmetric [Cl₁, Cl₂]. The first proof under generic assumptions, again for any $d > 1$, was provided by G. Nenciu [Ne₁], and few years later a simpler proof appeared [HeSj].

In real solids, Bloch bands intersect each other. Therefore, as early suggested [Bl, Cl₂], 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 2.2). 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 [NeNe₁, Ne₂] for $d = 1$, while a proof in the case $d \leq 3$ required more abstract bundle-theoretic methods [BPCM, Pa], 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 [NeNe₂], as well as extensions to quasi-1-dimensional systems [CNN].

Beyond the abstract existence results, computational physics strived for an explicit construction. On the one hand, Marzari and Vanderbilt [MaVa] 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 [Ki, NeNe₂]. For $d > 1$, the exponential localization of the minimizers follows instead from deeper properties of the localization functional [PaPi], 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 [MaVa, BPCM].

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 [CHN]. As a predecessor in this direction, we mention again the result in [HeSj], 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 3.4). The latter result follows from a more general theorem (Theorem 3.3), 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 an 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 3.2. 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 [Hal]. Despite the apparent similarity, the case of systems with *fermionic* (or *odd*) time-reversal symmetry, relevant in the context of topological insulators [HaKa], is radically different, as emphasized in [SoVa₃, GrPo, FMP], see Remark 3.5.

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 $d \in \mathbb{N}$ [HeSj], 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 [HeSj], 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 an eventuality, the rest of the argument fails. In [Ne₁], 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 technique.

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 briefly 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.

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⁽¹⁾ We cite textually from [Ne₁]: *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*

$$H_\Gamma = -\Delta + V_\Gamma \quad \text{acting in } L^2(\mathbb{R}^d),$$

where the potential V_Γ is periodic with respect to a lattice (called the *Bravais lattice* in the physics literature)

$$\Gamma := \text{Span}_{\mathbb{Z}} \{a_1, \dots, a_d\} \simeq \mathbb{Z}^d \subset \mathbb{R}^d, \quad \text{with } \{a_1, \dots, a_d\} \text{ a basis in } \mathbb{R}^d.$$

Assuming that

$$(2.1) \quad V_\Gamma \in L^2_{\text{loc}}(\mathbb{R}^d) \text{ for } d \leq 3, \quad \text{or} \quad V_\Gamma \in L^p_{\text{loc}}(\mathbb{R}^d) \text{ with } p > d/2 \text{ for } d \geq 4,$$

the operator H_Γ is self-adjoint on the domain $H^2(\mathbb{R}^d)$ [RS, 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

$$(2.2) \quad (\mathcal{U}_{\text{BF}} w)(k, y) := \frac{1}{|\mathbb{B}|^{1/2}} \sum_{\gamma \in \Gamma} e^{-ik \cdot (y + \gamma)} w(y + \gamma), \quad y \in \mathbb{R}^d, k \in \mathbb{R}^d.$$

Here \mathbb{B} is the fundamental unit cell for the dual lattice $\Gamma^* := \text{Span}_{\mathbb{Z}} \{b_1, \dots, b_d\} \subset \mathbb{R}^d$, determined by the basis $\{b_1, \dots, b_d\}$ which satisfies $b_i \cdot a_j = 2\pi\delta_{ij}$, namely

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

From (2.2), one immediately reads the (pseudo-)periodicity properties

$$(2.3) \quad \begin{aligned} (\mathcal{U}_{\text{BF}} w)(k, y + \gamma) &= (\mathcal{U}_{\text{BF}} w)(k, y) && \text{for all } \gamma \in \Gamma, \\ (\mathcal{U}_{\text{BF}} w)(k + \lambda, y) &= e^{-i\lambda \cdot y} (\mathcal{U}_{\text{BF}} w)(k, y) && \text{for all } \lambda \in \Gamma^*. \end{aligned}$$

The function $(\mathcal{U}_{\text{BF}} w)(k, \cdot)$, for fixed $k \in \mathbb{R}^d$, is thus periodic, so it can be interpreted as an element in the Hilbert space $\mathcal{H}_f := L^2(\mathbb{T}_Y^d)$, where $\mathbb{T}_Y^d = \mathbb{R}^d/\Gamma$ is the torus obtained by identifying opposite faces of the fundamental unit cell for Γ , given by

$$Y := \left\{ y = \sum_{j=1}^d y_j a_j \in \mathbb{R}^d : -\frac{1}{2} \leq y_j \leq \frac{1}{2} \right\}.$$

Following [PST₂], we reinterpret (2.3) in order to emphasize the role of covariance with respect to the action of the relevant symmetry group. Setting

$$(\tau(\lambda)\psi)(y) := e^{-i\lambda \cdot y} \psi(y), \quad \text{for } \psi \in \mathcal{H}_f,$$

one obtains a unitary representation $\tau: \Gamma^* \rightarrow \mathcal{U}(\mathcal{H}_f)$ of the group of translations by vectors of the dual lattice. One can then argue that \mathcal{U}_{BF} establishes a unitary transformation $\mathcal{U}_{\text{BF}}: L^2(\mathbb{R}^d) \rightarrow \mathcal{H}_\tau$, where \mathcal{H}_τ is the Hilbert space

$$\mathcal{H}_\tau := \left\{ \phi \in L^2_{\text{loc}}(\mathbb{R}^d, \mathcal{H}_f) : \phi(k + \lambda) = \tau(\lambda) \phi(k) \quad \forall \lambda \in \Gamma^*, \text{ for a.e. } k \in \mathbb{R}^d \right\}$$

equipped with the inner product

$$\langle \phi, \psi \rangle_{\mathcal{H}_\tau} = \int_{\mathbb{B}} \langle \phi(k), \psi(k) \rangle_{\mathcal{H}_f} dk.$$

Moreover, the inverse transformation $\mathcal{U}_{\text{BF}}^{-1}: \mathcal{H}_\tau \rightarrow L^2(\mathbb{R}^d)$ is explicitly given by

$$(\mathcal{U}_{\text{BF}}^{-1} \phi)(x) = \frac{1}{|\mathbb{B}|^{1/2}} \int_{\mathbb{B}} dk e^{ik \cdot x} \phi(k, x).$$

In view of the identification

$$\mathcal{H}_\tau \simeq \int_{\mathbb{B}}^{\oplus} dk \mathcal{H}_f,$$

we see that the Schrödinger operator H_Γ becomes a fibered operator in the Bloch-Floquet representation, *i. e.*

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

The fiber operator $H(k)$, $k \in \mathbb{R}^d$, acts on the k -independent domain $H^2(\mathbb{T}_Y^d) \subset \mathcal{H}_f$, 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 $E_0(k) \leq E_1(k) \leq \dots \leq E_n(k) \leq E_{n+1}(k) \leq \dots$, 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

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

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

$$H(k)u_n(k) = E_n(k)u_n(k), \quad u_n(k) \in \mathcal{H}_f, \quad \|u_n(k)\|_{\mathcal{H}_f} = 1,$$

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.*

$$(2.4) \quad w_n(x) := (\mathcal{U}_{\text{BF}}^{-1} u_n)(x) = \frac{1}{|\mathbb{B}|^{1/2}} \int_{\mathbb{B}} dk e^{ik \cdot x} u_n(k, x).$$

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 [PaPi, Sec. 2] for details):

$$(2.5) \quad \begin{aligned} w \in H^s(\mathbb{R}^d), \quad s \in \mathbb{N} &\iff u \in L^2(\mathbb{B}, H^s(\mathbb{T}_Y^d)), \\ \langle x \rangle^r w \in L^2(\mathbb{R}^d), \quad r \in \mathbb{N} &\iff u \in \mathcal{H}_\tau \cap H_{\text{loc}}^r(\mathbb{R}^d, \mathcal{H}_f), \end{aligned}$$

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 $\{E_i(k) : n \leq i \leq n + m - 1\}$, $k \in \mathbb{B}$, 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*:

$$(2.6) \quad \inf_{k \in \mathbb{B}} \text{dist}(\sigma_*(k), \sigma(H(k)) \setminus \sigma_*(k)) > 0.$$

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 [PaPi, Prop. 2.1], elaborating on a long-standing tradition of related results [RS, Ne₂], the projector $P_*(k)$ satisfies the properties listed in the following Proposition.

Proposition 2.1. *Let $P_*(k) \in \mathcal{B}(\mathcal{H}_f)$ 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:*

- (p₁) *the map $k \mapsto P_*(k)$ is smooth from \mathbb{R}^d to $\mathcal{B}(\mathcal{H}_f)$ (equipped with the operator norm);*
- (p₂) *the map $k \mapsto P_*(k)$ is τ -covariant, *i. e.**

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

(p₃) there exists an antiunitary operator⁽²⁾ C acting on \mathcal{H}_f such that

$$P_*(-k) = C P_*(k) C^{-1} \quad \text{and} \quad C^2 = 1.$$

The antiunitary operator C appearing in (p₃) is explicitly given by the complex conjugation in $\mathcal{H}_f = L^2(\mathbb{T}_Y^d)$ and, in particular, one has $C\tau(\lambda) = \tau(-\lambda)C$ for all $\lambda \in \Gamma^*$.

In the multi-band case, it is convenient [Bl, Cl₁] to relax the notion of Bloch function and to consider *quasi-Bloch functions*, defined as elements $\phi \in \mathcal{H}_\tau$ such that

$$P_*(k)\phi(k) = \phi(k), \quad \|\phi(k)\|_{\mathcal{H}_f} = 1, \quad \text{for a.e. } k \in \mathbb{B}.$$

A *Bloch frame* is, by definition, a family of quasi-Bloch functions $\{\phi_a\}_{a=1,\dots,m}$, constituting an orthonormal basis of $\text{Ran } P_*(k)$ 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 $\{\tilde{\phi}_a\}$ by setting

$$\tilde{\phi}_a(k) = \sum_{b=1}^m \phi_b(k) U_{ba}(k) \quad \text{for some unitary matrix } U(k).$$

Equipped with this terminology, we rephrase a classical definition [Cl₂] as follows:

Definition 2.2 (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

$$w_a(x) := (\mathcal{U}_{\text{BF}}^{-1} \phi_a)(x) = \frac{1}{|\mathbb{B}|^{1/2}} \int_{\mathbb{B}} dk e^{ik \cdot x} \phi_a(k, x).$$

An orthonormal basis of $\mathcal{U}_{\text{BF}}^{-1} \text{Ran } P_*$ is readily obtained by considering the translated functions

$$w_{\gamma,a}(x) := w_a(x - \gamma).$$

In view of the orthogonality of the trigonometric polynomials, the set $\{w_{\gamma,a}\}_{\gamma \in \Gamma, 1 \leq a \leq m}$ is an orthonormal basis of $\mathcal{U}_{\text{BF}}^{-1} \text{Ran } P_*$, which we refer to as a *composite Wannier basis*. The above-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 [Ko, Cl₁, Ne₂], there might be competition between the smoothness of the function $k \mapsto \phi_a(k)$ and its pseudo-periodicity properties, here

⁽²⁾ By *antiunitary* operator we mean a surjective antilinear operator $C : \mathcal{H} \rightarrow \mathcal{H}$, such that $\langle C\phi, C\psi \rangle_{\mathcal{H}} = \langle \psi, \phi \rangle_{\mathcal{H}}$ for any $\phi, \psi \in \mathcal{H}$.

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 (p₃), this obstruction is absent, yielding the existence of a C^∞ -smooth (actually, analytic) Bloch frame for any $d \leq 3$ and $m \in \mathbb{N}$ [Pa, BPCM]. The result in [Pa], however, neither provides explicitly such a 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 3.5 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 [Hal].

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:

- (P₁) *smoothness*: the map $\mathbb{R}^d \ni k \mapsto P(k) \in \mathcal{B}(\mathcal{H})$ is C^∞ -smooth;
- (P₂) *τ -covariance*: the map $k \mapsto P(k)$ is covariant with respect to a unitary representation⁽³⁾ $\tau : \Lambda \rightarrow \mathcal{U}(\mathcal{H})$, $\lambda \mapsto \tau(\lambda) \equiv \tau_\lambda$, in the sense that

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

- (P₃) *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

- (P₄) *compatibility condition*: for all $\lambda \in \Lambda$ one has $\Theta \tau_\lambda = \tau_\lambda^{-1} \Theta$. ◇

It follows from the assumption (P₁) 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 3.2 (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

⁽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 $\lambda \in \Lambda$.

$\Omega \subset \mathbb{R}^d$ is a map

$$\begin{aligned} \Phi: \Omega &\longrightarrow \mathcal{H} \oplus \dots \oplus \mathcal{H} = \mathcal{H}^m \\ k &\longmapsto (\phi_1(k), \dots, \phi_m(k)) \end{aligned}$$

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

- (F₀) *continuous* if the map $\phi_a: \mathbb{R}^d \rightarrow \mathcal{H}^m$ is continuous for all $a \in \{1, \dots, m\}$;
- (F₁) *smooth* if the map $\phi_a: \mathbb{R}^d \rightarrow \mathcal{H}^m$ is C^∞ -smooth for all $a \in \{1, \dots, m\}$;
- (F₂) *τ -equivariant* if

$$\phi_a(k + \lambda) = \tau_\lambda \phi_a(k) \quad \text{for all } k \in \mathbb{R}^d, \lambda \in \Lambda, a \in \{1, \dots, m\};$$

- (F₃) *time-reversal invariant* if

$$\phi_a(-k) = \Theta \phi_a(k) \quad \text{for all } k \in \mathbb{R}^d, a \in \{1, \dots, m\}.$$

A global Bloch frame is called **symmetric** if satisfies both (F₂) and (F₃). \diamond

Theorem 3.3 (Abstract result). *Assume $d \leq 3$. 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 3.3 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 a smooth Bloch frame also satisfies (F₃) 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 [MaVa, Section V.B]. We summarize these consequences in the following statement.

Theorem 3.4 (Application to Schrödinger operators). *Assume $d \leq 3$. 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 $\{w_{\gamma,a}\}_{\gamma \in \Gamma, 1 \leq a \leq m}$ of $\mathcal{U}_{\text{BF}}^{-1} \text{Ran } P_*$ 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

$$\int_{\mathbb{R}^d} \langle x \rangle^{2r} |w_{\gamma,a}(x)|^2 dx < +\infty \quad \text{for all } r \in \mathbb{N}.$$

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 3.3, there exists a global smooth symmetric Bloch frame in the sense of Definition 3.2. In view of (F₁) and (F₂), each ϕ_a is an element of $\mathcal{H}_\tau \cap C^\infty(\mathbb{R}^d, \mathcal{H}_f)$, and thus Φ is a smooth Bloch frame in the sense of Section 2.

By (2.5), the corresponding Wannier functions $w_a := \mathcal{U}_{\text{BF}}^{-1} \phi_a$ 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 (F₃) which in this context reads $\phi_a(-k) = C\phi_a(k) = \overline{\phi_a(k)}$, since C is just complex conjugation in $L^2(\mathbb{T}_Y^d)$. By Definition 2.2, one concludes that

$$\overline{w_a}(x) = \frac{1}{|\mathbb{B}|^{1/2}} \int_{\mathbb{B}} dk e^{-ik \cdot x} \overline{\phi_a(k, x)} = \frac{1}{|\mathbb{B}|^{1/2}} \int_{\mathbb{B}} dk e^{i(-k) \cdot x} \phi_a(-k, x) = w_a(x),$$

which yields property (i) and concludes the proof. \square

We sketch the structure of the proof of Theorem 3.3, provided in Sections 4 and 5. First, one easily notices that, in view of properties (F₂) and (F₃), a global symmetric Bloch frame $\Phi : \mathbb{R}^d \rightarrow \mathcal{H}^m$ is completely specified by the values it assumes on the *effective unit cell*

$$\mathbb{B}_{\text{eff}} := \left\{ k = \sum_j k_j e_j \in \mathbb{B} : k_1 \geq 0 \right\}.$$

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 $k' \in \mathbb{B}_{\text{eff}}$, $\lambda \in \Lambda$ and $s \in \{0, 1\}$. Then the symmetric Bloch frame Φ satisfies $\Phi(k) = \tau_\lambda \Theta^s \Phi(k')$ for $k' \in \mathbb{B}_{\text{eff}}$. Viceversa, a local Bloch frame $\Phi_{\text{eff}} : \mathbb{B}_{\text{eff}} \rightarrow \mathcal{H}^m$ can be canonically extended to a global symmetric Bloch frame Φ by posing

$$(3.1) \quad \Phi(k) = \tau_\lambda \Theta^s \Phi_{\text{eff}}(k') \quad \text{for } k = (-1)^s k' + \lambda.$$

However, to obtain a global *continuous* Bloch frame, the map $\Phi_{\text{eff}} : \mathbb{B}_{\text{eff}} \rightarrow \mathcal{H}^m$ must satisfy some non-trivial “gluing conditions” on the boundary $\partial\mathbb{B}_{\text{eff}}$, 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 $\Phi_{\text{eff}} : \mathbb{B}_{\text{eff}} \rightarrow \mathcal{H}^m$ satisfying them, provided $d \leq 3$. More specifically, we assume as given a continuous Bloch frame $\Psi : \mathbb{B}_{\text{eff}} \rightarrow \mathcal{H}^m$, called *the input frame*, which does not satisfy any special condition on the boundary of \mathbb{B}_{eff} , as e.g. the outcome of numerical computations in solid-state physics. Then we explicitly construct a unitary matrix $U_{\text{eff}}(k)$ such that the “corrected” frame

$$\Phi_{\text{eff}}(k)_a := \sum_{b=1}^m \Psi_b(k) U_{\text{eff}}(k)_{ba}$$

is still continuous and satisfies all the relevant symmetry conditions on $\partial\mathbb{B}_{\text{eff}}$. 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 satisfy 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 3.3.

Remark 3.5 (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 [HaKa], and specifically in the Kane-Mele model [KaMe₁], assumption (P_3) is replaced by

$(P_{3,-})$ *fermionic time-reversal symmetry*: there exists an antiunitary operator Θ acting on \mathcal{H} such that

$$P(-k) = \Theta P(k) \Theta^{-1} \quad \text{and} \quad \Theta^2 = -\mathbf{1}_{\mathcal{H}}.$$

Then the statement analogous to Theorem 3.3 is false: there might be topological obstruction to the existence of a continuous symmetric Bloch frame [FuKa, GrPo]. One proves [GrPo, FMP] that this 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 [FuKa, FKM]. 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 [Pa], see [MoPa] for a detailed review. \diamond

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 3.3.

Our general strategy will be the following. We consider a local continuous (resp. smooth)⁽⁴⁾ Bloch frame $\Psi : \mathbb{B}_{\text{eff}} \rightarrow \mathcal{H}^m$, which always exists since \mathbb{B}_{eff} is contractible and no special conditions on the boundary are imposed.⁽⁵⁾ We look for a unitary-matrix-valued map $U : \mathbb{B}_{\text{eff}} \rightarrow \mathcal{U}(\mathbb{C}^m)$ such that the modified local Bloch frame

$$(4.1) \quad \Phi_a(k) = \sum_{b=1}^m \Psi_b(k) U_{ba}(k), \quad U(k) \in \mathcal{U}(\mathbb{C}^m)$$

satisfies (F₂) and (F₃) 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.

4.1. The relevant group action. Properties (P₂) and (P₃) are related to some fundamental automorphisms of \mathbb{R}^d , namely the maps c and t_λ defined by

$$(4.2) \quad c(k) = -k \quad \text{and} \quad t_\lambda(k) = k + \lambda \quad \text{for } \lambda \in \Lambda.$$

Since $ct_\lambda = t_{-\lambda}c$ and $c^2 = t_0$, one concludes that the relevant symmetries are encoded in the group

$$(4.3) \quad G_d := \{t_\lambda, t_\lambda c\}_{\lambda \in \Lambda} \subset \text{Aut}(\mathbb{R}^d).$$

We notice that, assuming also (P₄), the action of G_d on \mathbb{R}^d can be lifted to an action on $\mathbb{R}^d \times \text{Fr}(m, \mathcal{H})$, where $\text{Fr}(m, \mathcal{H})$ 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 $\text{Fr}(m, \mathcal{H})$. Any bounded linear or antilinear operator $A : \mathcal{H} \rightarrow \mathcal{H}$ acts on frames componentwise, *i. e.* we set

$$A\Phi := (A\phi_1, \dots, A\phi_m).$$

⁽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}_{eff} , as detailed in Remarks 4.5 and 4.8. 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 [Ka, Sec. I.6.8] on finitely-many sufficiently small open sets covering \mathbb{B}_{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}_{eff} .

Moreover, the space $\text{Fr}(m, \mathcal{H})$ 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 [GrPo]. Notice that, by the antilinearity of the time-reversal operator Θ , one has

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

A lift of the G_d action from \mathbb{R}^d to $\mathbb{R}^d \times \text{Fr}(m, \mathcal{H})$ is obtained by considering, as generators, the automorphisms C and T_λ , defined by

$$(4.4) \quad C(k, \Phi) = (c(k), \Theta \Phi) \quad T_\lambda(k, \Phi) = (t_\lambda(k), \tau_\lambda \Phi)$$

for any $(k, \Phi) \in \mathbb{R}^d \times \text{Fr}(m, \mathcal{H})$. The relation $t_\lambda c = c t_{-\lambda}$ implies that, for every $\lambda \in \Lambda$, one has to impose the relation

$$\begin{aligned} T_\lambda C(k, \Phi) &= C T_{-\lambda}(k, \Phi) & \forall (k, \Phi) \in \mathbb{R}^d \times \text{Fr}(m, \mathcal{H}) \\ \text{i. e. } \tau_\lambda \Theta \Phi &= \Theta \tau_{-\lambda} \Phi & \forall \Phi \in \text{Fr}(m, \mathcal{H}), \end{aligned}$$

which holds true in view of (P₄). Thus the action of G_d is lifted to $\mathbb{R}^d \times \text{Fr}(m, \mathcal{H})$.

Given a family of projectors \mathcal{P} satisfying (P₂), (P₃) and (P₄), it is natural to consider the set of global Bloch frames for \mathcal{P} , here denoted by $\text{Fr}(\mathcal{P})$. Notice that

$$\text{Fr}(\mathcal{P}) \subset \{f : \mathbb{R}^d \rightarrow \text{Fr}(m, \mathcal{H})\} \subset \mathbb{R}^d \times \text{Fr}(m, \mathcal{H}).$$

It is easy to check that the action of G_d , previously extended to $\mathbb{R}^d \times \text{Fr}(m, \mathcal{H})$, restricts to $\text{Fr}(\mathcal{P})$. Indeed, whenever Φ is an orthonormal frame for $\text{Ran } P(k)$ 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 $\text{Ran}(P(t_\lambda(k)))$ and $\Theta \Phi$ is an orthonormal frame in $\text{Ran}(P(c(k)))$.

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

$$(4.5) \quad V_d = \{k \in \mathbb{R}^d : \exists g \in G_d, g \neq \mathbf{1} : g(k) = k\}.$$

⁽⁶⁾ This terminology means that $\Phi \triangleleft \mathbb{1} = \Phi$, $(\Phi \triangleleft U_1) \triangleleft U_2 = \Phi \triangleleft (U_1 U_2)$ and that if $\Phi \triangleleft U_1 = \Phi \triangleleft U_2$ then $U_1 = U_2$, for all $\Phi \in \text{Fr}(m, \mathcal{H})$ and $U_1, U_2 \in \mathcal{U}(\mathbb{C}^m)$.

Since $G_d = \{t_\lambda, t_\lambda c\}_{\lambda \in \Lambda}$ and t_λ acts freely on \mathbb{R}^d , the previous definition reads

$$\begin{aligned} V_d &= \{k \in \mathbb{R}^d : \exists \lambda \in \Lambda : t_\lambda c(k) = k\} \\ &= \{k \in \mathbb{R}^d : \exists \lambda \in \Lambda : -k + \lambda = k\} = \left\{ \frac{1}{2}\lambda \right\}_{\lambda \in \Lambda}, \end{aligned}$$

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 $k_\lambda := \frac{1}{2}\lambda$.

If Φ is a symmetric Bloch frame, then conditions (F₂) and (F₃) imply that

$$(4.6) \quad \Phi(k_\lambda) = \Phi(t_\lambda c(k_\lambda)) = \tau_\lambda \Theta \Phi(k_\lambda) \quad k_\lambda \in V_d.$$

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 $\text{Ran } P(k_\lambda)$, there exists a unique unitary matrix $U_{\text{obs}}(k_\lambda) \in \mathcal{U}(\mathbb{C}^m)$ such that

$$(4.7) \quad \Psi(k_\lambda) \triangleleft U_{\text{obs}}(k_\lambda) = \tau_\lambda \Theta \Psi(k_\lambda), \quad \lambda \in \Lambda.$$

The obstruction unitary $U_{\text{obs}}(k_\lambda)$ must satisfy a compatibility condition. Indeed, by applying $\tau_\lambda \Theta$ to both sides of (4.7) one obtains

$$\begin{aligned} \tau_\lambda \Theta (\Psi(k_\lambda) \triangleleft U_{\text{obs}}(k_\lambda)) &= \tau_\lambda \Theta \tau_\lambda \Theta \Psi(k_\lambda) \\ &= \tau_\lambda \tau_{-\lambda} \Theta^2 \Psi(k_\lambda) = \Psi(k_\lambda) \end{aligned}$$

where assumption (P₄) has been used. On the other hand, the left-hand side also reads

$$\begin{aligned} \tau_\lambda \Theta (\Psi(k_\lambda) \triangleleft U_{\text{obs}}(k_\lambda)) &= (\tau_\lambda \Theta \Psi(k_\lambda)) \triangleleft \overline{U_{\text{obs}}(k_\lambda)} = \\ &= \Psi(k_\lambda) \triangleleft (U_{\text{obs}}(k_\lambda) \overline{U_{\text{obs}}(k_\lambda)}). \end{aligned}$$

By the freeness of the action of $\mathcal{U}(\mathbb{C}^m)$ on frames, one concludes that

$$(4.8) \quad U_{\text{obs}}(k_\lambda) = U_{\text{obs}}(k_\lambda)^\top$$

where M^\top 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 $U_{\text{obs}}(k_\lambda)$. Indeed, from (4.6) and (4.1) it follows that for every $\lambda \in \Lambda$

$$\begin{aligned} \Psi(k_\lambda) \triangleleft U(k_\lambda) &= \Phi(k_\lambda) = \tau_\lambda \Theta \Phi(k_\lambda) \\ &= \tau_\lambda \Theta (\Psi(k_\lambda) \triangleleft U(k_\lambda)) \\ &= (\tau_\lambda \Theta \Psi(k_\lambda)) \triangleleft \overline{U(k_\lambda)} \\ &= \Psi(k_\lambda) \triangleleft U_{\text{obs}}(k_\lambda) \overline{U(k_\lambda)}. \end{aligned}$$

⁽⁷⁾ In the context of topological insulators, such points are called *time-reversal invariant momenta* (TRIMs) in the physics literature.

By the freeness of the $\mathcal{U}(\mathbb{C}^m)$ -action, we obtain the condition⁽⁸⁾

$$(4.9) \quad U_{\text{obs}}(k_\lambda) = U(k_\lambda)U(k_\lambda)^\top.$$

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 $V = U_{\text{obs}}(k_\lambda)$ in view of (4.8).

Lemma 4.1 (Solution to the vertex equation). *Let $V \in \mathcal{U}(\mathbb{C}^m)$ be such that $V^\top = V$. Then there exists a unitary matrix $U \in \mathcal{U}(\mathbb{C}^m)$ such that $V = UU^\top$.*

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

$$V = We^{iM}W^*$$

where $M = \text{diag}(\mu_1, \dots, \mu_m)$ and each μ_j is chosen so that⁽⁹⁾ $\mu_j \in [0, 2\pi)$. We set

$$U = We^{iM/2}W^*.$$

Since $V^\top = V$ one has $\overline{W}e^{iM}W^\top = We^{iM}W^*$, yielding

$$e^{iM}W^\top W = W^\top We^{iM},$$

i. e. the matrix e^{iM} commutes with $A := W^\top W$. Thus also $e^{iM/2}$ commutes with A (since each μ_j is in $[0, 2\pi)$), hence one has

$$UU^\top = We^{iM/2}A^{-1}e^{iM/2}AW^* = We^{iM}W^* = V.$$

□

In view of (4.8), we have the following

Corollary 4.2. *For every $k_\lambda \in V_d$ there exists a unitary matrix $U(k_\lambda)$ such that $U_{\text{obs}}(k_\lambda) = U(k_\lambda)U(k_\lambda)^\top$. In particular, the Bloch frame $\Phi(k_\lambda) = \Psi(k_\lambda) \triangleleft U(k_\lambda)$ satisfies the vertex condition (4.6) at the point $k_\lambda \in V_d$.*

⁽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 [CFMP].

⁽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.

4.3. Construction in the 1-dimensional case. In the 1-dimensional case, the boundary of \mathbb{B}_{eff} consists of two vertices $v_0 = 0$ and $v_1 = k_{e_1}$. Given, as an input, a continuous Bloch frame $\Psi : \mathbb{B}_{\text{eff}} \rightarrow \mathcal{H}^m$, equation (4.7) provides, for each vertex, an obstruction matrix $U_{\text{obs}}(v_i)$. In view of Corollary 4.2, 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 $W : [0, \frac{1}{2}] \rightarrow \mathcal{U}(\mathbb{C}^m)$ such that $W(0) = U(v_0)$ and $W(\frac{1}{2}) = U(v_1)$. Moreover, the path W can be explicitly constructed, as detailed in the following Remark.

Remark 4.3 (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 $D = \text{diag}(\delta_1, \dots, \delta_m)$ 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 $W(\frac{1}{2}) = U_*$. \diamond

We define a local continuous Bloch frame $\Phi_{\text{eff}} : \mathbb{B}_{\text{eff}} \rightarrow \mathcal{H}^m$ by setting

$$\Phi_{\text{eff}}(k) = \Psi(k) \triangleleft W(k), \quad k \in \mathbb{B}_{\text{eff}}.$$

Notice that Φ_{eff} satisfies, in view of the construction above, the vertex conditions

$$(4.10) \quad \Phi_{\text{eff}}(0) = \Theta \Phi_{\text{eff}}(0) \quad \text{and} \quad \Phi_{\text{eff}}(k_{e_1}) = \tau_{e_1} \Theta \Phi_{\text{eff}}(k_{e_1}),$$

which are special cases of condition (4.6). We extend Φ_{eff} to a global Bloch frame $\Phi : \mathbb{R}^1 \rightarrow \mathcal{H}^m$ by using equation (3.1). We claim that Φ is a *continuous* symmetric Bloch frame. Indeed, it satisfies (F₂) and (F₃) 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 3.3 for $d = 1$.

4.4. Construction in the 2-dimensional case. The reduced unit cell \mathbb{B}_{eff} contains exactly six elements in V_2 . In adapted coordinates, so that (k_1, k_2) represents the point $k_1e_1 + k_2e_2$ for $\Lambda = \text{Span}_{\mathbb{Z}}\{e_1, e_2\}$, they are labelled as follows (Figure 1):

$$(4.11) \quad \begin{aligned} v_1 &= (0, 0), & v_2 &= \left(0, -\frac{1}{2}\right), & v_3 &= \left(\frac{1}{2}, -\frac{1}{2}\right), \\ v_4 &= \left(\frac{1}{2}, 0\right), & v_5 &= \left(\frac{1}{2}, \frac{1}{2}\right), & v_6 &= \left(0, \frac{1}{2}\right). \end{aligned}$$

The oriented segment joining v_i to v_{i+1} (with $v_7 \equiv v_1$) is labelled by E_i .

We start from a local continuous (resp. smooth) Bloch frame $\Psi : \mathbb{B}_{\text{eff}} \rightarrow \mathcal{H}^m$. Given Ψ , the obstruction matrix defined in (4.7) yields, via Corollary 4.2, a unitary matrix $U(v_i)$ solving equation (4.9), for $i \in \{1, \dots, 4\}$.

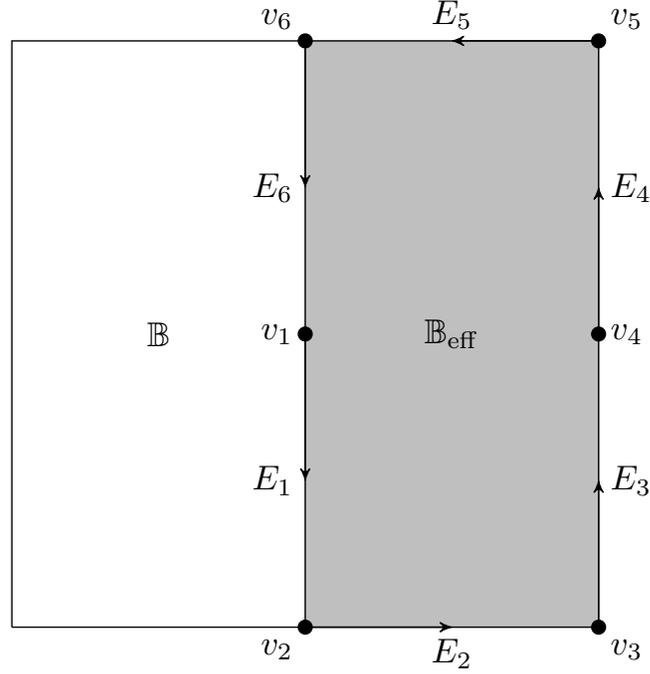


FIGURE 1. The effective unit cell (shaded area), its vertices and its edges. We use adapted coordinates (k_1, k_2) such that $k = k_1 e_1 + k_2 e_2$.

4.4.1. *Construction of the frame on the 1-skeleton.* As in the 1-dimensional case, we exploit the constructive existence of a smooth path $W_i : [0, 1/2] \rightarrow \mathcal{U}(\mathbb{C}^m)$ 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

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

so to obtain a piecewise-smooth map $\tilde{U} : E_1 \cup E_2 \cup E_3 \rightarrow \mathcal{U}(\mathbb{C}^m)$. Let

$$\tilde{\Phi}(k) := \Psi(k) \triangleleft \tilde{U}(k) \quad \text{for } k \in E_1 \cup E_2 \cup E_3.$$

We extend the map $\tilde{\Phi}$ to a continuous (resp. piecewise-smooth) symmetric Bloch frame $\hat{\Phi}$ on $\partial\mathbb{B}_{\text{eff}}$ by imposing properties (F₂) and (F₃), i. e. by setting

$$(4.12) \quad \hat{\Phi}(k) := \begin{cases} \tilde{\Phi}(k) & \text{if } k \in E_1 \cup E_2 \cup E_3 \\ \tau_{e_1} \Theta \tilde{\Phi}(t_{e_1} c(k)) & \text{if } k \in E_4 \\ \tau_{e_2} \tilde{\Phi}(t_{e_2}^{-1}(k)) & \text{if } k \in E_5 \\ \Theta \tilde{\Phi}(c(k)) & \text{if } k \in E_6. \end{cases}$$

By construction $\widehat{\Phi}$ satisfies all the *edge symmetries* for a symmetric Bloch frame Φ listed below:

$$(4.13) \quad \begin{aligned} \Phi(c(k)) &= \Theta \Phi(k) && \text{for } k \in E_1 \cup E_6 \\ \Phi(t_{e_2}(k)) &= \tau_{e_2} \Phi(k) && \text{for } k \in E_2 \\ \Phi(t_{e_1}c(k)) &= \tau_{e_1} \Theta \Phi(k) && \text{for } k \in E_3 \cup E_4 \\ \Phi(t_{e_2}^{-1}(k)) &= \tau_{e_2}^{-1} \Phi(k) && \text{for } k \in E_5. \end{aligned}$$

The map $\widehat{\Phi} : \partial\mathbb{B}_{\text{eff}} \rightarrow \mathcal{H}^m$ is continuous (resp. piecewise-smooth), since $\widetilde{\Phi}$ is continuous (resp. piecewise-smooth) and satisfies by construction the vertex conditions at v_i for $i \in \{1, 4\}$.

4.4.2. *Extension to the 2-torus.* Since both $\widehat{\Phi}(k)$ and the input frame $\Psi(k)$ are orthonormal frames in $\text{Ran } P(k)$, for every $k \in \partial\mathbb{B}_{\text{eff}}$, there exists a unique unitary matrix $\widehat{U}(k)$ such that

$$(4.14) \quad \widehat{\Phi}(k) = \Psi(k) \triangleleft \widehat{U}(k) \quad \text{for } k \in \partial\mathbb{B}_{\text{eff}}.$$

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 $U_{\text{eff}} : \mathbb{B}_{\text{eff}} \rightarrow \mathcal{U}(\mathbb{C}^m)$ 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 $f : S^1 \rightarrow X$ extends to a continuous map $F : D^2 \rightarrow X$, where D^2 is the 2-dimensional disc enclosed by the circle S^1 , if and only if 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

$$(4.15) \quad \text{deg} : \pi_1(U(1)) \xrightarrow{\sim} \mathbb{Z}, \quad [\varphi : S^1 \rightarrow U(1)] \mapsto \frac{1}{2\pi i} \oint_{S^1} \varphi(z)^{-1} \partial_z \varphi(z) dz$$

establishes an isomorphism of groups $\pi_1(U(1)) \simeq \mathbb{Z}$. We conclude that a continuous map $f : \partial\mathbb{B}_{\text{eff}} \rightarrow \mathcal{U}(\mathbb{C}^m)$ can be continuously extended to $F : \mathbb{B}_{\text{eff}} \rightarrow \mathcal{U}(\mathbb{C}^m)$ if and only if $\text{deg}([\det f]) \in \mathbb{Z}$ is zero.

The following Lemma is the crucial step in the 2-dimensional construction. It shows that, even if $\text{deg}([\det \widehat{U}]) = r \neq 0$, it is always possible to construct a continuous map $X : \partial\mathbb{B}_{\text{eff}} \rightarrow \mathcal{U}(\mathbb{C}^m)$ such that $\text{deg}([\det \widehat{U} X]) = 0$ and $\widehat{\Phi} \triangleleft X$ still satisfies the edge symmetries.⁽¹⁰⁾

⁽¹⁰⁾ This is a special feature of systems with *bosonic* TR-symmetry: if assumption (P₃) is replaced by (P_{3,-}), the analogous statement does not hold true [FMP].

Lemma 4.4 (Solution to the face-extension problem). *Let $r \in \mathbb{Z}$. There exists a piecewise-smooth map $X : \partial\mathbb{B}_{\text{eff}} \rightarrow \mathcal{U}(\mathbb{C}^m)$ 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) $X(k) \neq \mathbb{I}$ 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

$$\begin{aligned} (\Phi \triangleleft X)(-k) &= \Theta (\Phi \triangleleft X)(k) \\ &\Updownarrow \\ \Phi(-k) \triangleleft X(-k) &= \Theta (\Phi(k) \triangleleft X(k)) \\ &\Updownarrow \\ (\Theta \Phi(k)) \triangleleft X(-k) &= (\Theta \Phi(k)) \triangleleft \bar{X}(k), \end{aligned}$$

yielding the explicit condition

$$(4.16) \quad X(-k) = \bar{X}(k), \quad k \in E_1 \cup E_6.$$

Similarly, one obtains

$$(4.17) \quad X(t_{e_1} c(k)) = \bar{X}(k) \quad \text{for } k \in E_3 \cup E_4$$

$$(4.18) \quad X(t_{e_2}(k)) = X(k) \quad \text{for } k \in E_2$$

$$(4.19) \quad X(t_{e_2}^{-1}(k)) = X(k) \quad \text{for } k \in E_5.$$

Thus condition (ii) on X is equivalent to the relations (4.16), (4.17), (4.18) and (4.19).

We now exhibit a map $X : \partial\mathbb{B}_{\text{eff}} \rightarrow \mathcal{U}(\mathbb{C}^m)$ which satisfies the previous relations, and such that $\deg([\det X]) = -r$. Define $\xi : \partial\mathbb{B}_{\text{eff}} \rightarrow \mathbb{C}$ by

$$(4.20) \quad \xi(k) := \begin{cases} e^{-i2\pi r(k_2 + \frac{1}{2})} & \text{for } k \in E_3 \cup E_4 \\ 1 & \text{otherwise,} \end{cases}$$

and set $X(k) := \text{diag}(\xi(k), 1, \dots, 1) \in \mathcal{U}(\mathbb{C}^m)$ 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 $\deg([\det X]) = \deg([\xi]) = -r$.
- (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 $k = (\frac{1}{2}, k_2) \in$

$E_3 \cup E_4$. Since $t_{e_1}c(k) = (\frac{1}{2}, -k_2)$, one has

$$\begin{aligned} X(t_{e_1}c(k)) = X(\tfrac{1}{2}, -k_2) &= \text{diag}(\xi(\tfrac{1}{2}, -k_2), 1, \dots, 1) \\ &= \text{diag}(\overline{\xi(\tfrac{1}{2}, k_2)}, 1, \dots, 1) = \overline{X}(k). \end{aligned}$$

(iii) property (iii) is satisfied by construction. □

Set $r := \deg([\det \widehat{U}])$. In view of Lemma 4.4, the continuous (resp. piecewise-smooth) map $U := \widehat{U}X : \partial\mathbb{B}_{\text{eff}} \rightarrow \mathcal{U}(\mathbb{C}^m)$ satisfies $\deg([\det U]) = 0$ and hence extends to a continuous (resp. piecewise-smooth) map $U_{\text{eff}} : \mathbb{B}_{\text{eff}} \rightarrow \mathcal{U}(\mathbb{C}^m)$. Moreover, the extension procedure is explicitly constructive whenever U is piecewise-smooth, as detailed in Remark 4.5. By setting $\Phi_{\text{eff}}(k) := \Psi(k) \triangleleft U_{\text{eff}}(k)$, we obtain a continuous symmetric Bloch frame on the whole reduced unit cell \mathbb{B}_{eff} , which moreover satisfies the edge symmetries (4.13) in view of item (ii) in Lemma 4.4. 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 3.3 for $d = 2$.

Remark 4.5 (Explicit extension to the whole effective cell, $d = 2$). We emphasize that the extension of the *piecewise-smooth* map $U : \partial\mathbb{B}_{\text{eff}} \rightarrow \mathcal{U}(\mathbb{C}^m)$, with $\deg[\det U] = 0$, to a continuous (actually, piecewise-smooth) map $U_{\text{eff}} : \mathbb{B}_{\text{eff}} \rightarrow \mathcal{U}(\mathbb{C}^m)$ 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

$$W \mapsto (\det W, W^b) \in \mathcal{U}(1) \times \mathcal{SU}(m) \quad \text{with } W^b = \text{diag}(\det W^{-1}, 1, \dots, 1)W.$$

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 $f^b : k \mapsto U^b(k) \in \mathcal{SU}(m)$.

As for problem (a), let $f : \partial\mathbb{B}_{\text{eff}} \rightarrow \mathcal{U}(1)$ be a degree-zero piecewise-smooth function. Then, a piecewise-smooth extension $F : \mathbb{B}_{\text{eff}} \rightarrow \mathcal{U}(1)$ is constructed as follows. Let $\theta_0 \in \mathbb{R}$ be such that $f(0, -1/2) = e^{i2\pi\theta_0}$. Define the piecewise-smooth function $\varphi : [0, 3] \rightarrow \mathcal{U}(1)$ as

$$(4.21) \quad \varphi(t) = \begin{cases} f(t, -1/2) & \text{if } 0 \leq t \leq 1/2 \\ f(1/2, -1+t) & \text{if } 1/2 \leq t \leq 3/2 \\ f(2-t, 1/2) & \text{if } 3/2 \leq t \leq 2 \\ f(0, 5/2-t) & \text{if } 2 \leq t \leq 3 \end{cases}$$

and set

$$\theta(t) = \theta_0 + \frac{1}{2\pi i} \int_0^t \varphi(\tau)^{-1} \varphi'(\tau) d\tau, \quad \text{for } t \in [0, 3].$$

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

$$\omega(k_1, k_2) := \begin{cases} -2k_2 \theta\left(\frac{k_2 - 2k_1 + 1/2}{4k_2}\right) & \text{if } k_2 \leq -|2k_1 - 1/2|, \\ (4k_1 - 1) \theta\left(1 + \frac{k_2}{4k_1 - 1}\right) & \text{if } -|2k_1 - 1/2| \leq k_2 \leq |2k_1 - 1/2|, \text{ with } k_1 \geq 1/4, \\ 2k_2 \theta\left(2 - \frac{k_2 + 2k_1 - 1/2}{4k_2}\right) & \text{if } k_2 \geq |2k_1 - 1/2|, \\ (-4k_1 + 1) \theta\left(\frac{5}{2} - \frac{k_2}{-4k_1 + 1}\right) & \text{if } -|2k_1 - 1/2| \leq y \leq |2k_1 - 1/2|, \text{ with } k_1 \leq 1/4. \end{cases}$$

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 $|\theta(t)| \leq |\theta|_{\max}$ 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 [Hal], 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 $\mathcal{S}U(m-1) \rightarrow \mathcal{S}U(m) \rightarrow S^{2m-1}$.

Let $f^b : k \mapsto U^b(k) \in \mathcal{S}U(2)$ be a piecewise-smooth function. Then a piecewise-smooth extension $F^b : \mathbb{B}_{\text{eff}} \rightarrow \mathcal{S}U(2)$ is constructed as follows. First, we use the standard identification of $\mathcal{S}U(2)$ with the 3-sphere of unit norm vectors in \mathbb{R}^4 to look at f^b as to a piecewise-smooth function $f^b : \partial\mathbb{B}_{\text{eff}} \rightarrow S^3$. Let $p \in S^3$ be a point not in the range⁽¹¹⁾ of f^b , and let $\psi_p : S^3 \setminus \{p\} \rightarrow \{p\}^\perp$ 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

$$(4.22) \quad \begin{aligned} \psi_p(v) &= p - \frac{1}{\langle v-p|p \rangle} (v-p) \\ \psi_p^{-1}(w) &= p + \frac{2}{\|w-p\|^2} (w-p). \end{aligned}$$

⁽¹¹⁾ Such a point does exist since the map f^b is piecewise-smooth. Indeed, by an argument analogous to the Sard lemma, one can show that the range of f^b 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 .

Second, we define a piecewise-smooth function $\varphi^b : [0, 3] \rightarrow S^3$ by using the same formula as in (4.21), with f replaced by f^b .

Then, a piecewise-smooth extension of f^b to a function $F^b : \mathbb{B}_{\text{eff}} \rightarrow S^3$ is given by

$$F^b(k_1, k_2) = \begin{cases} \psi_p^{-1} \left(-2k_2 \psi_p \left(\varphi \left(\frac{k_2 - 2k_1 + 1/2}{4k_2} \right) \right) \right) & \text{if } k_2 \leq -|2k_1 - 1/2|, \\ \psi_p^{-1} \left((4k_1 - 1) \psi_p \left(\varphi \left(1 + \frac{k_2}{4k_1 - 1} \right) \right) \right) & \text{if } -|2k_1 - 1/2| \leq k_2 \leq |2k_1 - 1/2| \text{ and } k_1 \geq 1/4, \\ \psi_p^{-1} \left(2k_2 \psi_p \left(\varphi \left(2 - \frac{k_2 + 2k_1 - 1/2}{4k_2} \right) \right) \right) & \text{if } k_2 \geq |2k_1 - 1/2|, \\ \psi_p^{-1} \left((-4k_1 + 1) \psi_p \left(\varphi \left(\frac{5}{2} - \frac{k_2}{-4k_1 + 1} \right) \right) \right) & \text{if } -|2k_1 - 1/2| \leq k_2 \leq |2k_1 - 1/2| \text{ and } k_1 \leq 1/4. \end{cases}$$

Notice that F^b is continuous at $(1/4, 0)$ with $F^b(1/4, 0) = -p$, since $\psi_p \circ \varphi : [0, 3] \rightarrow p^\perp \subseteq \mathbb{R}^4$ is continuous on $[0, 3]$. This provides an explicit piecewise-smooth extension of f^b for the case $m = 2$. \diamond

4.5. Interlude: abstracting from the 1- and 2-dimensional case. Abstracting from the proofs in Subsections 4.3 and 4.4, we distill two Lemmas which will become the “building bricks” of the higher dimensional construction. To streamline the statements, we denote by $\mathbb{B}^{(d)}$ (resp. $\mathbb{B}_{\text{eff}}^{(d)}$) the d -dimensional unit cell (resp. effective unit cell) and we adhere to the following convention:

$$(4.23) \quad \begin{aligned} \mathbb{B}^{(0)} &\simeq \{0\}, & \mathbb{B}_{\text{eff}}^{(1)} &\simeq [0, \frac{1}{2}], \\ \mathbb{B}_{\text{eff}}^{(d+1)} &\simeq \mathbb{B}_{\text{eff}}^{(1)} \times \mathbb{B}^{(d)} = \left\{ \underbrace{(k_1, k_2, \dots, k_{d+1})}_{k_{\perp}} : k_1 \in [0, \frac{1}{2}], k_{\perp} \in \mathbb{B}^{(d)} \right\} & \text{for } d \geq 1. \end{aligned}$$

We also refer to the following statement as the **d -dimensional problem**:

Given a continuous Bloch frame $\Psi : \mathbb{B}_{\text{eff}}^{(d)} \rightarrow \mathcal{H}^m$, construct a continuous Bloch frame $\Phi_{\text{eff}} : \mathbb{B}_{\text{eff}}^{(d)} \rightarrow \mathcal{H}^m$ which, via (3.1), continuously extends to a global continuous symmetric Bloch frame $\Phi : \mathbb{R}^d \rightarrow \mathcal{H}^m$.

In other words, Φ_{eff} is defined only on the effective unit cell $\mathbb{B}_{\text{eff}}^{(d)}$, but satisfies all the relations on $\partial\mathbb{B}_{\text{eff}}^{(d)}$ (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 4.8.

Notice that Subsection 4.2 already contains a solution to the 0-dimensional problem: indeed, in view of Corollary 4.2, 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 4.6 (Macro 1). *Let $\Phi_{\text{one}} : \mathbb{B}^{(0)} \simeq \{0\} \rightarrow \mathcal{H}^m$ be a Bloch frame satisfying*

$$(4.24) \quad \Phi_{\text{one}}(0) = \Theta \Phi_{\text{one}}(0).$$

Then one constructs a continuous Bloch frame $\Phi_{\text{two}} : \mathbb{B}_{\text{eff}}^{(1)} \simeq [0, \frac{1}{2}] \rightarrow \mathcal{H}^m$ such that

$$(4.25) \quad \begin{cases} \Phi_{\text{two}}(0) = \Phi_{\text{one}}(0) \\ \Phi_{\text{two}}(\frac{1}{2}) = \tau_{e_2} \Theta \Phi_{\text{two}}(\frac{1}{2}). \end{cases}$$

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 distill a general procedure. For convenience, we relabel the edges of $\mathbb{B}_{\text{eff}}^{(2)}$ as follows:

$$(4.26) \quad E_{j,0} = \left\{ k = \sum_i k_i e_i \in \mathbb{B}_{\text{eff}}^{(2)} : k_j = 0 \right\}$$

$$(4.27) \quad E_{j,\pm} = \left\{ k = \sum_i k_i e_i \in \mathbb{B}_{\text{eff}}^{(2)} : k_j = \pm \frac{1}{2} \right\}$$

From the construction in Subsection 4.4, based on Lemma 4.4, one easily deduces the following result.

Lemma 4.7 (Macro 2). *Assume that $\Phi_S : S \rightarrow \mathcal{H}^m$, with $S = E_{1,0} \cup E_{2,-} \cup E_{2,+} \subset \partial\mathbb{B}_{\text{eff}}^{(2)}$, is continuous and satisfies the following edge symmetries:*

$$(4.28) \quad \begin{cases} \Phi_S(t_{e_2}(k)) = \tau_{e_2} \Phi_S(k) & \text{for } k \in E_{2,-} \\ \Phi_S(t_{e_2}^{-1}(k)) = \tau_{e_2}^{-1} \Phi_S(k) & \text{for } k \in E_{2,+} \\ \Phi_S(c(k)) = \Theta \Phi_S(k) & \text{for } k \in E_{1,0}. \end{cases}$$

Then one constructs a continuous Bloch frame $\Phi_{\text{eff}} : \mathbb{B}_{\text{eff}}^{(2)} \rightarrow \text{Fr}(m, \mathcal{H})$ such that

$$(4.29) \quad \begin{cases} \Phi_{\text{eff}}(k) = \Phi_S(k) & \text{for } k \in S \\ \Phi_{\text{eff}}(t_{e_1} c(k)) = \tau_{e_1} \Theta \Phi_{\text{eff}}(k) & \text{for } k \in E_{1,+}. \end{cases}$$

To obtain (4.29) we implicitly used property (iii) in Lemma 4.4, 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 4.6 and 4.7 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 $\partial\mathbb{B}_{\text{eff}}^{(3)}$ are labelled according to the following convention : for $j \in \{1, 2, 3\}$ we set

$$(4.30) \quad F_{j,0} = \left\{ k = \sum_{i=1}^3 k_i e_i : k_j = 0 \right\}$$

$$(4.31) \quad F_{j,\pm} = \left\{ k = \sum_{i=1}^3 k_i e_i : k_j = \pm \frac{1}{2} \right\}$$

Notice that two faces of $\partial\mathbb{B}_{\text{eff}}^{(3)}$, 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 $\mathbb{B}_{\text{eff}}^{(2)}$.

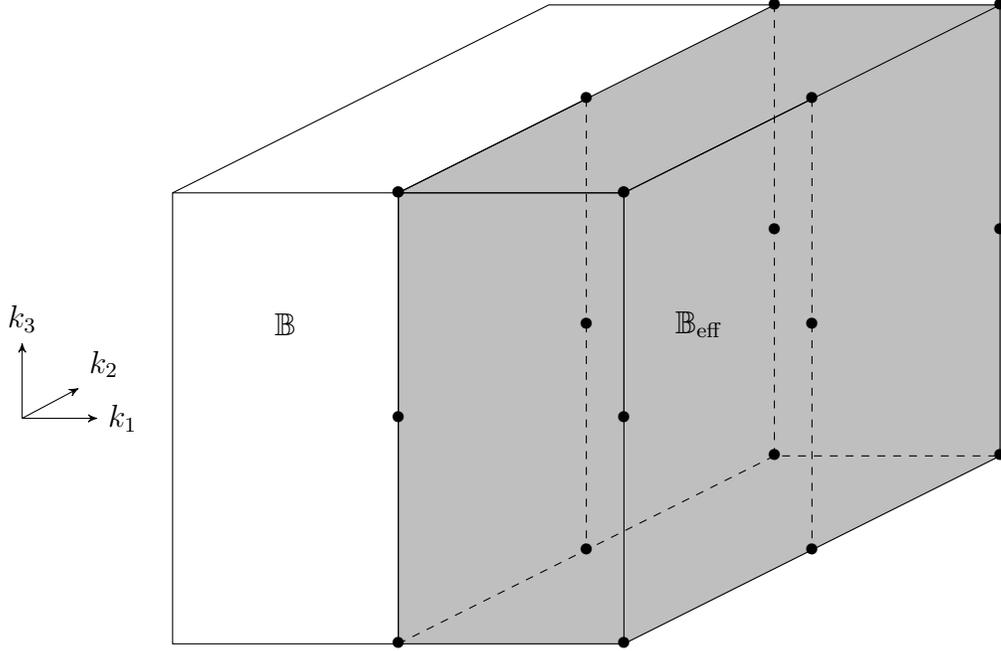


FIGURE 2. The 3-dimensional (effective) unit cell.

We assume as given a continuous Bloch frame $\Psi : \mathbb{B}_{\text{eff}}^{(3)} \rightarrow \mathcal{H}^m$ (the *input frame*) which does not satisfy any particular symmetry on the boundary $\partial\mathbb{B}_{\text{eff}}^{(3)}$. 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 $\Phi_{\text{one}} : F_{1,0} \rightarrow \mathcal{H}^m$, $\Phi_{\text{one}} = \Psi \triangleleft U_{\text{one}}$, 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 $\partial\mathbb{B}_{\text{eff}}^{(3)}$ contained in $F_{1,+}$, and let v_0 be the corresponding vertex on $F_{1,0}$. For the sake of concreteness, we choose $v_* = (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$, so that $v_0 = (0, \frac{1}{2}, \frac{1}{2})$. Then Lemma 4.6 (Macro 1) yields the existence of a continuous Bloch frame $\Phi_{\text{two}} : [v_0, v_*] \simeq \mathbb{B}_{\text{eff}}^{(1)} \rightarrow \mathcal{H}^m$ such that $\Phi_{\text{two}}(v_0) = \Phi_{\text{one}}(v_0)$ and $\Phi_{\text{two}}(v_*)$ satisfies the vertex condition (4.6) at v_* .

- *Step 2. Extend by τ -equivariance.* By imposing property (F₂), Φ_{two} naturally extends to the edges $t_{e_2}^{-1}([v_0, v_*])$ and $t_{e_3}^{-1}([v_0, v_*])$. Since Φ_{one} is τ -equivariant on $F_{1,0} \simeq \mathbb{B}^{(2)}$, one has that $\Phi_{\text{two}}(t_{e_j}^{-1}(v_0)) = \Phi_{\text{one}}(t_{e_j}^{-1}(v_0))$ for $j \in \{2, 3\}$. In view of that,

we obtain a continuous Bloch frame by setting

$$(4.32) \quad \Phi_{\text{three}}(k) := \begin{cases} \Phi_{\text{one}}(k) & \text{for } k \in F_{1,0}, \\ \Phi_{\text{two}}(k) & \text{for } k \in t_\lambda([v_0, v_*]) \text{ for } \lambda \in \{0, -e_2, -e_3\}. \end{cases}$$

• *Step 3. Extend to small faces by Macro 2.* Notice that Φ_{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 4.7 (Macro 2), and there satisfies the relations analogous to (4.28). Then Φ_{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. $j = 2$).

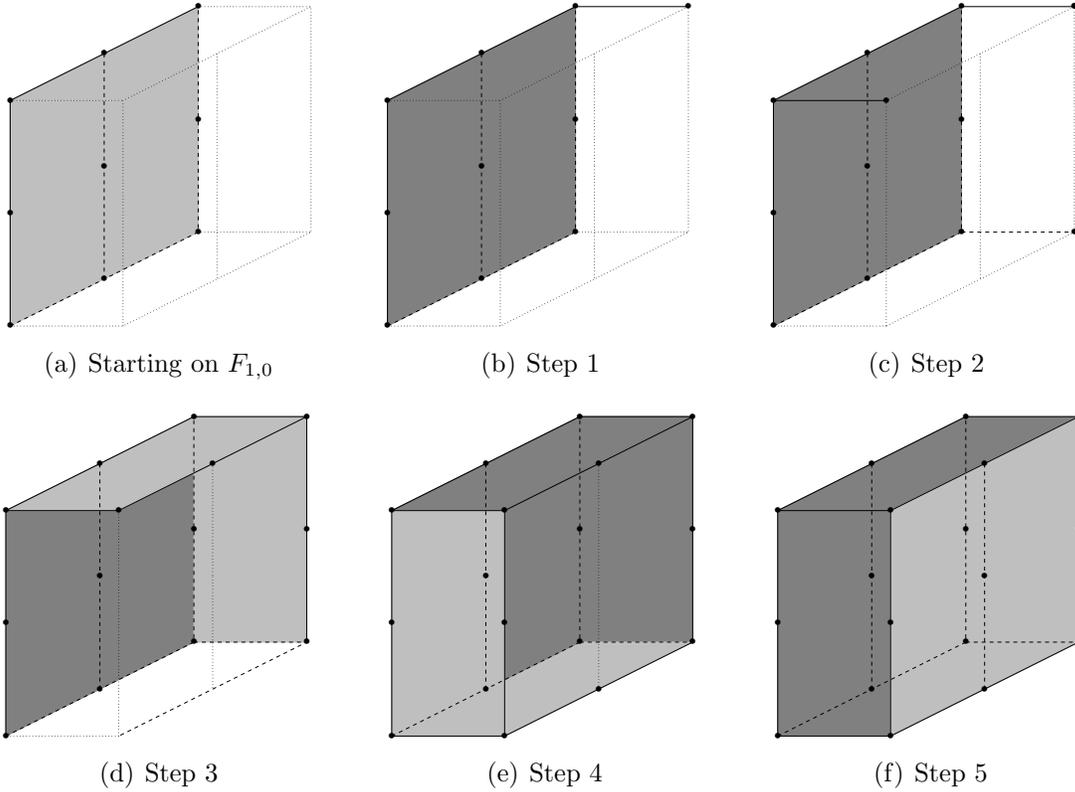


FIGURE 3. Steps in the construction.

• *Step 4. Extend by τ -equivariance.* By imposing τ -equivariance (property (F_2)), Φ_{three} naturally extends to the faces $F_{3,-}$ and $F_{2,-}$, thus yielding a continuous Bloch frame Φ_{four} defined on the set ⁽¹²⁾ $\partial \mathbb{B}_{\text{eff}}^{(3)} \setminus F_{1,+} =: K_0$.

⁽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⁾

$$(4.33) \quad T_{\pm} = \{k \in F_{1,+} : \pm k_2 \geq 0\}$$

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 4.7 (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 $\widehat{\Phi} : \partial \mathbb{B}_{\text{eff}}^{(3)} \rightarrow \text{Fr}(m, \mathcal{H})$ we set

$$(4.34) \quad \widehat{\Phi}(k) := \begin{cases} \Phi_{\text{four}}(k) & \text{for } k \in K_0 \\ \Phi_{\text{five}}(k) & \text{for } k \in T_+ \\ \Phi_{\text{five}}(t_{e_1}c(k)) & \text{for } k \in T_- \end{cases}$$

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

$$(4.35) \quad \widehat{\Phi}(k) = \Psi(k) \triangleleft \widehat{U}(k) \quad k \in \partial \mathbb{B}_{\text{eff}}^{(3)},$$

which yields a continuous map $\widehat{U} : \partial \mathbb{B}_{\text{eff}}^{(3)} \rightarrow \mathcal{U}(\mathbb{C}^m)$.

We show that such a map extends to a continuous map $U_{\text{eff}} : \mathbb{B}_{\text{eff}}^{(3)} \rightarrow \mathcal{U}(\mathbb{C}^m)$. Indeed, a continuous function f from $\partial \mathbb{B}_{\text{eff}}^{(3)} \approx S^2$ to the topological space X can be continuously extended to $\mathbb{B}_{\text{eff}}^{(3)} \approx D^3$ 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 4.8.

Equipped with such a continuous extension, we obtain a continuous symmetric Bloch frame $\Phi_{\text{eff}} : \mathbb{B}_{\text{eff}}^{(3)} \rightarrow \mathcal{H}^m$ by setting

$$(4.36) \quad \Phi_{\text{eff}}(k) = \Psi(k) \triangleleft U_{\text{eff}}(k) \quad k \in \mathbb{B}_{\text{eff}}^{(3)}.$$

• *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.

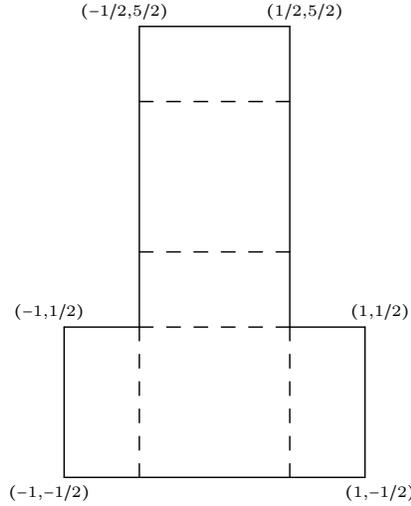
This concludes the proof of Theorem 3.3 for $d = 3$.

⁽¹³⁾ Obviously, these subsets are *die Türen*, so they are denoted by T_{\pm} .

Remark 4.8 (Explicit extension to the whole effective cell, $d = 3$). As in the 2-dimensional case (Remark 4.5), we notice that the extension of the *piecewise-smooth*⁽¹⁴⁾ function $\widehat{U} : \partial\mathbb{B}_{\text{eff}}^{(3)} \rightarrow \mathcal{U}(\mathbb{C}^m)$ to $\mathbb{B}_{\text{eff}}^{(3)}$ is completely explicit. The problem is again reduced to the following two subproblems, namely to construct a continuous extension from $\partial\mathbb{B}_{\text{eff}}^{(3)}$ to $\mathbb{B}_{\text{eff}}^{(3)}$ of:

- (a) a map $f : k \mapsto \det U(k) \in \mathcal{U}(1)$, and
- (b) a map $f^b : k \mapsto U^b(k) \in \mathcal{SU}(m)$.

As for subproblem (a), given a degree-zero piecewise-smooth function $f : \partial\mathbb{B}_{\text{eff}}^{(3)} \rightarrow \mathcal{U}(1)$, a piecewise-smooth extension $F : \mathbb{B}_{\text{eff}}^{(3)} \rightarrow \mathcal{U}(1)$ is constructed as follows. Consider the region $\mathbb{D} \subseteq \mathbb{R}^2$ depicted below



and let $\varphi : \mathbb{D} \rightarrow \mathcal{U}(1)$ be the piecewise-smooth function defined by

$$(4.37) \quad \varphi(s, t) := \begin{cases} f(-s - \frac{1}{2}, -\frac{1}{2}, t) & \text{if } (s, t) \in [-1, -\frac{1}{2}] \times [-\frac{1}{2}, \frac{1}{2}] \\ f(0, s, t) & \text{if } (s, t) \in [-\frac{1}{2}, \frac{1}{2}] \times [-\frac{1}{2}, \frac{1}{2}] \\ f(s - \frac{1}{2}, \frac{1}{2}, t) & \text{if } (s, t) \in [\frac{1}{2}, 1] \times [-\frac{1}{2}, \frac{1}{2}] \\ f(t - \frac{1}{2}, s, \frac{1}{2}) & \text{if } (s, t) \in [-\frac{1}{2}, \frac{1}{2}] \times [\frac{1}{2}, 1] \\ f(\frac{1}{2}, s, -t + \frac{3}{2}) & \text{if } (s, t) \in [-\frac{1}{2}, \frac{1}{2}] \times [1, 2] \\ f(-t + \frac{5}{2}, s, -\frac{1}{2}) & \text{if } (s, t) \in [-\frac{1}{2}, \frac{1}{2}] \times [2, \frac{5}{2}] \end{cases}$$

Choose $\theta_0 \in \mathbb{R}$ be such that $f(0, 0, 0) = e^{2\pi i \theta_0}$ and set

$$\theta(s, t) = \theta_0 + \frac{1}{2\pi i} \int_0^1 \varphi(\lambda s, \lambda t)^{-1} (s\varphi_s(\lambda s, \lambda t) + t\varphi_t(\lambda s, \lambda t)) d\lambda,$$

⁽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.

where φ_s and φ_t denote the partial derivatives of φ with respect to s and t , respectively. One has

$$e^{2\pi i\theta(s,t)} = \varphi(s,t)$$

for any $(s,t) \in \mathbb{D}$. Moreover,

$$\begin{cases} \theta(s, -\frac{1}{2}) = \theta(s, \frac{5}{2}) & \text{for } -\frac{1}{2} \leq s \leq \frac{1}{2} \\ \theta(s, -\frac{1}{2}) = \theta(-\frac{1}{2}, 3+s) & \text{for } -1 \leq s \leq -\frac{1}{2} \\ \theta(s, -\frac{1}{2}) = \theta(\frac{1}{2}, 3-s) & \text{for } \frac{1}{2} \leq s \leq 1 \\ \theta(s, \frac{1}{2}) = \theta(-\frac{1}{2}, \frac{1}{2}-s) & \text{for } -1 \leq s \leq -\frac{1}{2} \\ \theta(s, \frac{1}{2}) = \theta(\frac{1}{2}, \frac{1}{2}+s) & \text{for } \frac{1}{2} \leq s \leq 1 \\ \theta(-1, t) = \theta(-\frac{1}{2}, \frac{3}{2}-t) & \text{for } -\frac{1}{2} \leq t \leq \frac{1}{2} \\ \theta(1, t) = \theta(\frac{1}{2}, \frac{3}{2}-t) & \text{for } \frac{1}{2} \leq t \leq \frac{1}{2} \end{cases}$$

so that θ actually lifts f to a piecewise-smooth function $\theta : \partial\mathbb{B}_{\text{eff}}^{(3)} \rightarrow \mathbb{R}$. Then, one can choose $F(k_1, k_2, k_3) = e^{2\pi i\omega(k_1, k_2, k_3)}$, where

$$\omega(k_1, k_2, k_3) = \begin{cases} (-4k_1 + 1) \theta\left(-\frac{k_3}{4k_1-1}, -\frac{k_2}{4k_1-1}\right) & \text{if } 0 \leq k_1 \leq \min\left\{\left|\frac{1}{2}|k_2| - \frac{1}{4}\right|, \left|\frac{1}{2}|k_3| - \frac{1}{4}\right|\right\}, \\ 2k_3 \theta\left(\frac{1}{2} + \frac{k_3+2k_1-1/2}{4k_3}, \frac{k_2}{2k_3}\right) & \text{if } \max\left\{\left|2k_1 - \frac{1}{2}\right|, |k_2|\right\} \leq k_3 \leq \frac{1}{2}, \\ 2k_2 \theta\left(\frac{k_3}{2k_2}, \frac{1}{2} + \frac{k_2+2k_1-1/2}{4k_2}\right) & \text{if } \max\left\{\left|2k_1 - \frac{1}{2}\right|, |k_3|\right\} \leq k_2 \leq \frac{1}{2}, \\ (4k_1 - 1) \theta\left(\frac{k_3}{4k_1-1}, \frac{3}{2} - \frac{k_2}{4k_1-1}\right) & \text{if } \max\left\{\left|\frac{1}{2}|k_2| + \frac{1}{4}\right|, \left|\frac{1}{2}|k_3| + \frac{1}{4}\right|\right\} \leq k_1 \leq \frac{1}{2}, \\ -2k_3 \theta\left(-\frac{1}{2} - \frac{k_3-2k_1+1/2}{4k_3}, -\frac{k_2}{2k_3}\right) & \text{if } -\frac{1}{2} \leq k_3 \leq \min\left\{-\left|2k_1 - \frac{1}{2}\right|, -|k_2|\right\}, \\ -2k_2 \theta\left(-\frac{k_3}{2k_2}, \frac{5}{2} - \frac{k_2-2k_1+1/2}{4k_2}\right) & \text{if } -\frac{1}{2} \leq k_2 \leq \min\left\{-\left|2k_1 - \frac{1}{2}\right|, -|k_3|\right\}. \end{cases}$$

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 4.5, 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^b . By using Equation (4.37), with f replaced by f^b , one defines a piecewise-smooth function $\varphi : \mathbb{D} \rightarrow S^3$. Then, a piecewise-smooth extension of f^b to a function

⁽¹⁵⁾ This point does exist since the map f^b is piecewise-smooth, as argued in footnote (11).

$F^b : \mathbb{B}_{\text{eff}}^{(3)} \rightarrow S^3$ is explicitly given by

$$F(k_1, k_2, k_3) = \begin{cases} \psi_p^{-1} \left((-4k_1 + 1) \psi_p \left(\varphi \left(-\frac{k_3}{4k_1-1}, -\frac{k_2}{4k_1-1} \right) \right) \right) & \text{if } 0 \leq k_1 \leq \min\left\{ \left| \frac{1}{2}|k_2| - \frac{1}{4} \right|, \left| \frac{1}{2}|k_3| - \frac{1}{4} \right| \right\}, \\ \psi_p^{-1} \left(2k_3 \psi_p \left(\varphi \left(\frac{1}{2} + \frac{k_3+2k_1-1/2}{4k_3}, \frac{k_2}{2k_3} \right) \right) \right) & \text{if } \max\left\{ \left| 2k_1 - \frac{1}{2} \right|, |k_2| \right\} \leq k_3 \leq \frac{1}{2}, \\ \psi_p^{-1} \left(2k_2 \psi_p \left(\varphi \left(\frac{k_3}{2k_2}, \frac{1}{2} + \frac{k_2+2k_1-1/2}{4k_2} \right) \right) \right) & \text{if } \max\left\{ \left| 2k_1 - \frac{1}{2} \right|, |k_3| \right\} \leq k_2 \leq \frac{1}{2}, \\ \psi_p^{-1} \left((4k_1 - 1) \psi_p \left(\varphi \left(\frac{k_3}{4k_1-1}, \frac{3}{2} - \frac{k_2}{4k_1-1} \right) \right) \right) & \text{if } \max\left\{ \left| \frac{1}{2}|k_2| + \frac{1}{4} \right|, \left| \frac{1}{2}|k_3| + \frac{1}{4} \right| \right\} \leq k_1 \leq \frac{1}{2}, \\ \psi_p^{-1} \left(-2k_3 \psi_p \left(\varphi \left(-\frac{1}{2} - \frac{k_3-2k_1+1/2}{4k_3}, -\frac{k_2}{2k_3} \right) \right) \right) & \text{if } -\frac{1}{2} \leq k_3 \leq \min\left\{ \left| -2k_1 - \frac{1}{2} \right|, \left| -k_2 \right| \right\}, \\ \psi_p^{-1} \left(-2k_2 \psi_p \left(\varphi \left(-\frac{k_3}{2k_2}, \frac{5}{2} - \frac{k_2-2k_1+1/2}{4k_2} \right) \right) \right) & \text{if } -\frac{1}{2} \leq k_2 \leq \min\left\{ \left| -2k_1 - \frac{1}{2} \right|, \left| -k_3 \right| \right\}. \end{cases}$$

Note that F is continuous at $(1/4, 0, 0)$ with $F(1/4, 0, 0) = -p$, since $\psi_p \circ \varphi : \mathbb{D} \rightarrow p^\perp \subseteq \mathbb{R}^4$ is continuous on the compact domain \mathbb{D} . The map above provides an explicit continuous extension to $\mathbb{B}_{\text{eff}}^{(3)}$ for $m = 2$. \diamond

4.7. A glimpse to the higher-dimensional cases. The fundamental “building bricks” used to solve the 3-dimensional problem (Lemma 4.6 and 4.7) 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 $k \geq 3$, 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 4.6 and 4.7, yields a continuous Bloch frame $\widehat{\Phi} : \partial\mathbb{B}_{\text{eff}}^{(4)} \rightarrow \mathcal{H}^m$ satisfying all the relevant symmetries (on vertices, edges, faces and 3-dimensional hyperfaces). By comparison with the input frame $\Psi : \mathbb{B}_{\text{eff}}^{(4)} \rightarrow \mathcal{H}^m$, one obtains a continuous map $\widehat{U} : \partial\mathbb{B}_{\text{eff}}^{(4)} \rightarrow \mathcal{U}(\mathbb{C}^m)$ such that $\widehat{\Phi}(k) = \Psi(k) \triangleleft \widehat{U}(k)$ for all $k \in \partial\mathbb{B}_{\text{eff}}^{(4)}$. Arguing as in Subsection 4.6, one concludes that the existence of a continuous extension $U_{\text{eff}} : \mathbb{B}_{\text{eff}}^{(4)} \rightarrow \mathcal{U}(\mathbb{C}^m)$ 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 [Pa, MoPa], to the appearance for $d \geq 4$ of the second Chern class of the Bloch bundle, which always vanishes for $d \leq 3$ or $m = 1$.

On the other hand, our constructive algorithm works without obstruction in the case $m = 1$, since $\pi_k(\mathcal{U}(\mathbb{C}^1)) = 0$ for all $k \geq 2$, 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 $d \in \mathbb{N}$ [HeSj], 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 $\Phi : \mathbb{R}^d \rightarrow \mathcal{H}^m$ is a global continuous symmetric Bloch frame, i. e. it satisfies properties (F₀), (F₂) and (F₃).*

Choose $\varepsilon > 0$. Then one constructs a global smooth symmetric Bloch frame Φ_{sm} such that

$$(5.1) \quad \sup_{k \in \mathbb{R}^d} \text{dist}(\Phi(k), \Phi_{\text{sm}}(k)) < \varepsilon$$

where $\text{dist}(\Phi, \Psi) = \left(\sum_a \|\phi_a - \psi_a\|_{\mathcal{H}}^2\right)^{1/2}$ is the distance in $\text{Fr}(m, \mathcal{H})$.

Notice that, for any $\Phi \in \text{Fr}(m, \mathcal{H})$ and $U, W \in \mathcal{U}(m)$, one has

$$(5.2) \quad \text{dist}(\Phi \triangleleft U, \Phi \triangleleft W) = \|U - W\|_{\text{HS}}$$

where $\|U\|_{\text{HS}}^2 = \sum_{a,b=1}^m |U_{ab}|^2$ 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 $F_k := \text{Fr Ran } P(k) \simeq \mathcal{U}(m)$ inherits from $\mathcal{U}(m)$ a Riemannian structure⁽¹⁶⁾, and the corresponding geodesic distance $d(U, W)$ 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

$$(5.3) \quad \frac{1}{2} d(\mathbb{I}, U) \leq \|\mathbb{I} - U\|_{\text{HS}} \leq d(\mathbb{I}, U) \quad \forall U \in \mathcal{U}(M) : \|\mathbb{I} - U\|_{\text{HS}} < \frac{1}{2} \tau_m,$$

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 [NSW, Prop. 6.3], where also the relation between τ_m and the principal curvature of $\mathcal{U}(m)$ is discussed.

Proof. Following [Pa], we recall that, to a family of projectors \mathcal{P} satisfying properties (P₁) and (P₂), one can canonically associate a smooth Hermitian vector bundle $\mathcal{E}_{\mathcal{P}} =$

⁽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 $\langle A, B \rangle_{\text{HS}} = \text{tr}(A^* B)$.

$(E_{\mathcal{P}} \rightarrow \mathbb{T}_*^d)$, where $\mathbb{T}_*^d = \mathbb{R}^d/\Lambda$. In particular, $\mathcal{E}_{\mathcal{P}}$ is defined by using an equivalence relation \sim_{τ} on $\mathbb{R}^d \times \mathcal{H}$, namely

$$(k, \phi) \sim_{\tau} (k', \phi') \quad \text{if and only if} \quad \exists \lambda \in \Lambda : k' = k + \lambda, \phi' = \tau_{\lambda} \phi.$$

An equivalence class is denoted by $[k, \phi]_{\tau}$. Then, the total space is defined by

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

and the projection $\pi : E_{\mathcal{P}} \rightarrow \mathbb{T}_*^d$ 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 [Pa, PaPi] 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 $\Phi : \mathbb{R}^d \rightarrow \mathcal{H}^m$ 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 $\text{Fr } \mathcal{E}_{\mathcal{P}}$. The identification is given by

$$\sigma_{\Phi}(x) = ([k, \phi_1(k)]_{\tau}, \dots, [k, \phi_m(k)]_{\tau}) \in (\text{Fr } E_{\mathcal{P}})_x \quad \text{for } x = k \pmod{\Lambda}.$$

According to a classical result, the Steenrod's Approximation Theorem ([St]; see [Wo] for recent generalizations), there exists a smooth global section $\sigma'_{\Phi} : \mathbb{T}_*^d \rightarrow \text{Fr } E_{\mathcal{P}}$ such that

$$\sup_{x \in \mathbb{T}_*^d} \text{dist}(\sigma_{\Phi}(x), \sigma'_{\Phi}(x)) < \frac{1}{2} \varepsilon.$$

Going back to the language of Bloch frames, one concludes the existence of a global smooth τ -equivariant Bloch frame $\Phi'_{\text{sm}} : \mathbb{R}^d \rightarrow \mathcal{H}^m$, such that

$$(5.4) \quad \sup_{k \in \mathbb{R}^d} \text{dist}(\Phi(k), \Phi'_{\text{sm}}(k)) < \frac{1}{2} \varepsilon.$$

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 $\exp : \mathfrak{u}(m) \rightarrow \mathcal{U}(m)$ is a diffeomorphism from the ball $B_{\delta}(0) \subset \mathfrak{u}(m)$ to the geodesic ball $B_{\delta}(\mathbb{I}) \subset \mathcal{U}(m)$, see e. g. [He, Chapter II] or [Si, Chapter VII]. In particular, for any $U \in B_{\delta}(\mathbb{I})$, there exists a unique $A_U \in B_{\delta}(0)$ such that

$$(5.5) \quad U = \exp(A_U), \quad U \in B_{\delta}(\mathbb{I}),$$

and, moreover, the map $U \mapsto A_U$ is C^{∞} -smooth on $B_{\delta}(\mathbb{I})$. Since the exponential map is normalized so that $d(\mathbb{I}, U) = \|A_U\|_{\text{HS}}$, then $d(\mathbb{I}, \bar{U}) = d(\mathbb{I}, U) = d(\mathbb{I}, U^{-1})$. In particular, both \bar{U} and U^{-1} are in the geodesic ball $B_{\delta}(\mathbb{I})$, whenever $U \in B_{\delta}(\mathbb{I})$.

For $U \in B_\delta(\mathbb{I})$, the midpoint $M(\mathbb{I}, U)$ between \mathbb{I} and U is defined by⁽¹⁷⁾

$$(5.6) \quad M(\mathbb{I}, U) := \exp\left(\frac{1}{2}A_U\right) \in B_\delta(\mathbb{I}) \subset \mathcal{U}(m).$$

One immediately checks that, for $U \in B_\delta(\mathbb{I})$,

$$(5.7) \quad M(\mathbb{I}, \overline{U}) = \exp\left(\frac{1}{2}\overline{A_U}\right) = \overline{M(\mathbb{I}, U)}$$

$$(5.8) \quad M(\mathbb{I}, U^{-1}) = \exp\left(-\frac{1}{2}A_U\right) = U^{-1}M(\mathbb{I}, U).$$

Moreover,

$$(5.9) \quad d(\mathbb{I}, M(\mathbb{I}, U)) = \frac{1}{2}d(\mathbb{I}, U).$$

Consider now two orthonormal frames $\Phi, \Psi \in \text{Fr Ran } P(k)$, such that $\text{dist}(\Phi, \Psi) < \varepsilon$. For ε sufficiently small, we define the **midpoint** $\widehat{M}(\Phi, \Psi) \in \text{Fr Ran } P(k)$ 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 $(U_{\Phi, \Psi})_{ab} = \langle \phi_a, \psi_b \rangle$. Taking (5.2) and (5.3) into account, one has

$$\varepsilon > \text{dist}(\Phi, \Psi) = \text{dist}(\Phi, \Phi \triangleleft U_{\Phi, \Psi}) = \|\mathbb{I} - U_{\Phi, \Psi}\|_{\text{HS}} \geq \frac{1}{2} d(\mathbb{I}, U_{\Phi, \Psi}).$$

Choose ε sufficiently small, namely $\varepsilon < \delta/2$. Then $U_{\Phi, \Psi}$ is in the geodesic ball $B_\delta(\mathbb{I}) \subset \mathcal{U}(m)$. By using (5.6), we define

$$(5.10) \quad \widehat{M}(\Phi, \Psi) := \Phi \triangleleft M(\mathbb{I}, U_{\Phi, \Psi}) \in \text{Fr Ran } P(k).$$

We show that

$$(5.11) \quad \widehat{M}(\Theta\Phi, \Theta\Psi) = \Theta\widehat{M}(\Phi, \Psi)$$

$$(5.12) \quad \widehat{M}(\tau_\lambda\Phi, \tau_\lambda\Psi) = \tau_\lambda\widehat{M}(\Phi, \Psi).$$

Notice preliminarily that, since both Θ and τ_λ are isometries of \mathcal{H} , one has

$$(5.13) \quad \text{dist}(\Theta\Phi, \Theta\Psi) = \text{dist}(\Phi, \Psi) = \text{dist}(\tau_\lambda\Phi, \tau_\lambda\Psi)$$

for all $\Phi, \Psi \in \text{Fr}(m, \mathcal{H})$. Thus, the midpoints appearing on the left-hand sides of (5.11) and (5.12) are well-defined, whenever $\text{dist}(\Phi, \Psi) < \frac{1}{2}\delta$.

Equation (5.11) follows from (5.7) and from the fact that $\Theta(\Phi \triangleleft U_{\Phi, \Psi}) = (\Theta\Phi) \triangleleft \overline{U_{\Phi, \Psi}}$. Indeed, one has

$$\begin{aligned} \widehat{M}(\Theta\Phi, \Theta\Psi) &= \widehat{M}(\Theta\Phi, \Theta(\Phi \triangleleft U_{\Phi, \Psi})) = \widehat{M}(\Theta\Phi, (\Theta\Phi) \triangleleft \overline{U_{\Phi, \Psi}}) \\ &= (\Theta\Phi) \triangleleft M(\mathbb{I}, \overline{U_{\Phi, \Psi}}) = (\Theta\Phi) \triangleleft \overline{M(\mathbb{I}, U_{\Phi, \Psi})} \\ &= \Theta(\Phi \triangleleft M(\mathbb{I}, U_{\Phi, \Psi})) = \Theta\widehat{M}(\Phi, \Psi). \end{aligned}$$

Analogously, equation (5.12) follows from the fact that $\tau_\lambda(\Phi \triangleleft U_{\Phi, \Psi}) = (\tau_\lambda\Phi) \triangleleft U_{\Phi, \Psi}$.

⁽¹⁷⁾ Definition (5.6) agrees with the geodesic midpoint between \mathbb{I} and U in the Riemannian manifold $\mathcal{U}(m)$, since the exponential map is normalized so that $d(\mathbb{I}, \exp(sN)) = s$, for $s < \delta$ and $\|N\|_{\text{HS}} = 1$.

We focus now on the smooth τ -equivariant Bloch frame $\Phi'_{\text{sm}} : \mathbb{R}^d \rightarrow \mathcal{H}^m$ obtained, via Steenrod's theorem, from the continuous symmetric frame Φ . Since $\text{Ran } P(k) = \Theta \text{Ran } P(-k)$, one has that $\Theta \Phi'_{\text{sm}}(-k)$ is in $F_k = \text{Fr Ran } P(k)$. Thus, we set

$$(5.14) \quad \Phi_{\text{sm}}(k) := \widehat{M}(\Phi'_{\text{sm}}(k), \Theta \Phi'_{\text{sm}}(-k)) \in F_k.$$

The definition (5.14) is well-posed. Indeed, taking (5.4) and (5.13) into account, one has

$$(5.15) \quad \begin{aligned} & \text{dist}(\Phi'_{\text{sm}}(k), \Theta \Phi'_{\text{sm}}(-k)) \\ & \leq \text{dist}(\Phi'_{\text{sm}}(k), \Phi(k)) + \text{dist}(\Phi(k), \Theta \Phi(-k)) + \text{dist}(\Theta \Phi(-k), \Theta \Phi'_{\text{sm}}(-k)) \\ & = \text{dist}(\Phi'_{\text{sm}}(k), \Phi(k)) + \text{dist}(\Phi(-k), \Phi'_{\text{sm}}(-k)) < \varepsilon < \frac{1}{2}\delta, \end{aligned}$$

where we used the fact that the central addendum (in the second line) vanishes since Φ satisfies (F₃).

We claim that (5.14) defines a smooth symmetric global Bloch frame satisfying (5.1). We explicitly check that:

1. the map $k \mapsto \Phi_{\text{sm}}(k)$ is smooth. Indeed, since Θ is an isometry of \mathcal{H} , the map $k \mapsto \Theta \Phi'_{\text{sm}}(-k) =: \Psi'_{\text{sm}}(k)$ is smooth. Hence $k \mapsto U_{\Phi'_{\text{sm}}(k), \Psi'_{\text{sm}}(k)} \in \mathcal{U}(m)$ is smooth, since $(U_{\Phi, \Psi})_{ab} = \langle \phi_a, \psi_b \rangle$. In view of (5.15) and (5.3), $U_{\Phi'_{\text{sm}}(k), \Psi'_{\text{sm}}(k)}$ is, for every $k \in \mathbb{R}^d$, in the geodesic ball $B_\delta(\mathbb{I})$ where the exponential map defines a diffeomorphism. As a consequence,

$$k \mapsto \Phi'_{\text{sm}}(k) \triangleleft M(\mathbb{I}, U_{\Phi'_{\text{sm}}(k), \Psi'_{\text{sm}}(k)}) = \Phi_{\text{sm}}(k)$$

is smooth from \mathbb{R}^d to \mathcal{H}^m .

2. the Bloch frame Φ_{sm} satisfies (F₂). Indeed, by using (P₄) and (5.12), one obtains

$$\begin{aligned} \Phi_{\text{sm}}(k + \lambda) &= \widehat{M}(\Phi'_{\text{sm}}(k + \lambda), \Theta \Phi'_{\text{sm}}(-k - \lambda)) \\ &= \widehat{M}(\tau_\lambda \Phi'_{\text{sm}}(k), \Theta \tau_{-\lambda} \Phi'_{\text{sm}}(-k)) \\ &= \widehat{M}(\tau_\lambda \Phi'_{\text{sm}}(k), \tau_\lambda \Theta \Phi'_{\text{sm}}(-k)) \\ &= \tau_\lambda \widehat{M}(\Phi'_{\text{sm}}(k), \Theta \Phi'_{\text{sm}}(-k)) = \tau_\lambda \Phi_{\text{sm}}(k). \end{aligned}$$

3. the Bloch frame Φ_{sm} satisfies (F₃). Indeed, by using $\Theta^2 = \mathbb{1}$ and (5.11), one has

$$\begin{aligned} \Phi_{\text{sm}}(-k) &= \widehat{M}(\Theta^2 \Phi'_{\text{sm}}(-k), \Theta \Phi'_{\text{sm}}(k)) \\ &= \Theta \widehat{M}(\Theta \Phi'_{\text{sm}}(-k), \Phi'_{\text{sm}}(k)) \\ &= \Theta \widehat{M}(\Phi'_{\text{sm}}(k), \Theta \Phi'_{\text{sm}}(-k)) = \Theta \Phi_{\text{sm}}(k), \end{aligned}$$

where we used the fact that $\widehat{M}(\Phi, \Psi) = \widehat{M}(\Psi, \Phi)$, whenever $\text{dist}(\Phi, \Psi) < \delta/2$. The latter fact is a direct consequence of (5.8), since

$$\begin{aligned} \widehat{M}(\Phi, \Psi) &= \Phi \triangleleft M(\mathbb{I}, U_{\Phi, \Psi}) = (\Psi \triangleleft U_{\Phi, \Psi}^{-1}) \triangleleft M(\mathbb{I}, U_{\Phi, \Psi}) \\ &= \Psi \triangleleft (U_{\Phi, \Psi}^{-1} M(\mathbb{I}, U_{\Phi, \Psi})) = \Psi \triangleleft M(\mathbb{I}, U_{\Phi, \Psi}^{-1}) \\ &= \Psi \triangleleft M(\mathbb{I}, U_{\Psi, \Phi}) = \widehat{M}(\Psi, \Phi). \end{aligned}$$

4. equation (5.1) is satisfied in view of (5.15). Indeed, setting $U_{\Phi'_{\text{sm}}(k), \Psi'_{\text{sm}}(k)} \equiv U(k)$ for notational convenience and using (5.2), (5.3) and (5.9), one obtains

$$\begin{aligned} \text{dist}(\Phi'_{\text{sm}}(k), \Phi_{\text{sm}}(k)) &= \text{dist}(\Phi'_{\text{sm}}(k), \Phi'_{\text{sm}}(k) \triangleleft M(\mathbb{I}, U(k))) \\ &= \|\mathbb{I} - M(\mathbb{I}, U(k))\|_{\text{HS}} \leq d(\mathbb{I}, M(\mathbb{I}, U(k))) = \frac{1}{2} d(\mathbb{I}, U(k)) \\ &\leq \|\mathbb{I} - U(k)\|_{\text{HS}} = \text{dist}(\Phi'_{\text{sm}}(k), \Theta \Phi'_{\text{sm}}(-k)) < \varepsilon. \end{aligned}$$

This concludes the proof of the Proposition. \square

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