PARSEVAL FRAMES OF LOCALIZED WANNIER FUNCTIONS

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ABSTRACT. Let $d \leq 3$ and consider a real analytic and $\mathbb{Z}^d$-periodic family $\{P(\mathbf{k})\}_{\mathbf{k}\in\mathbb{R}^d}$ of orthogonal projections of rank m. A moving *orthonormal basis* of $\operatorname{Ran} P(\mathbf{k})$ consisting of real analytic and $\mathbb{Z}^d$-periodic Bloch vectors can be constructed if and only if the first Chern number(s) of P vanish(es). Here we are mainly interested in the topologically obstructed case.

First, by dropping the generating condition, we can construct a collection of $m-1$ *orthonormal*, real analytic, and $\mathbb{Z}^d$-periodic Bloch vectors. Second, by dropping the orthonormality condition, we can construct a *Parseval frame* of $m+1$ real analytic and $\mathbb{Z}^d$-periodic Bloch vectors which generate $\operatorname{Ran} P(\mathbf{k})$. Both constructions are based on a two-step logarithm method which produces a moving orthonormal basis in the topologically trivial case.

In applications to condensed matter systems, a moving Parseval frame of analytic, $\mathbb{Z}^d$-periodic Bloch vectors generates a Parseval frame of exponentially localized composite Wannier functions for the occupied states of a gapped periodic Hamiltonian.

KEYWORDS. Wannier functions, Parseval frames, constructive algorithms.

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CONTENTS

1. INTRODUCTION

We study families of rank-m orthogonal projections $\{P(\mathbf{k})\}_{\mathbf{k}\in\mathbb{R}^d}$, $P(\mathbf{k}) = P(\mathbf{k})^2 = P(\mathbf{k})^*$, acting on some Hilbert space $\mathcal{H}$, which are subject to the following conditions:

(i) the map $P\colon \mathbb{R}^d \to \mathcal{B}(\mathcal{H})$, $\mathbf{k} \mapsto P(\mathbf{k})$, is smooth (at least of class C^1);
(ii) the map $P\colon \mathbb{R}^d \to \mathcal{B}(\mathcal{H})$, $\mathbf{k} \mapsto P(\mathbf{k})$, is $\mathbb{Z}^d$-periodic, that is, $P(\mathbf{k}) = P(\mathbf{k}+\mathbf{n})$ for all $\mathbf{n} \in \mathbb{Z}^d$.

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Such families of projections arise in condensed matter physics from the Bloch-Floquet transform of a gapped periodic Hamiltonian. We refer the reader to [4] for more details.

Definition 1.1. A *Bloch vector* for the family of projections $\{P(\mathbf{k})\}_{\mathbf{k}\in\mathbb{R}^d}$ is a map $\xi\colon \mathbb{R}^d \to \mathcal{H}$ such that

$$P(\mathbf{k})\xi(\mathbf{k}) = \xi(\mathbf{k}) \quad \text{for all } \mathbf{k} \in \mathbb{R}^d.$$

A Bloch vector ξ is called

(i) *continuous* if the map $\xi\colon \mathbb{R}^d \to \mathcal{H}$ is continuous;
(ii) *periodic* if the map $\xi\colon \mathbb{R}^d \to \mathcal{H}$ is $\mathbb{Z}^d$-periodic, that is, $\xi(\mathbf{k}) = \xi(\mathbf{k}+\mathbf{n})$ for all $\mathbf{n} \in \mathbb{Z}^d$;
(iii) *normalized* if $\|\xi(\mathbf{k})\| = 1$ for all $\mathbf{k} \in \mathbb{R}^2$.

A collection of M Bloch vectors $\{\xi_a\}_{a=1}^M$ is said to be

(i) *independent* (respectively *orthonormal*) if the vectors $\{\xi_a(\mathbf{k})\}_{a=1}^M \subset \mathcal{H}$ are linearly independent (respectively orthonormal) for all $\mathbf{k} \in \mathbb{R}^d$;
(ii) a *moving Parseval M-frame* (or M-frame in short) if $M \geq m$ and for every $\psi \in \operatorname{Ran} P(\mathbf{k})$ we have

$$\psi = \sum_{a=1}^{M} \langle \xi_a(\mathbf{k}), \psi\rangle\, \xi_a(\mathbf{k}) \quad \text{or equivalently} \quad \|\psi\|^2 = \sum_{a=1}^{M} |\langle \xi_a(\mathbf{k}), \psi\rangle|^2 . \tag{1.1}$$

If $M = m$, we call $\{\xi_a\}_{a=1}^m$ a *Bloch basis*.

In general, all the above conditions on a collection of Bloch vectors compete against each other, and one has to give up some of them in order to enforce the others. This is well-known in differential geometry: Indeed, given a smooth, periodic family of projections, one can construct the associated *Bloch bundle* $\mathcal{E} \to \mathbb{T}^d$ [18], which is an Hermitian vector bundle over the (Brillouin) d-torus, and Bloch vectors are nothing but *sections* for this vector bundle. The *topological obstruction* to construct sections of a vector bundle reflects in the impossibility to construct collections of Bloch vectors with the required properties. For example:

- in general, a Bloch vector can be continuous but *not* periodic, or viceversa periodic but *not* continuous: in the latter case, one then speaks of *local sections* of the associated Bloch bundle, defined in the patches where they are continuous;
- global (continuous and periodic) sections may exists, but they may *vanish* in $\mathbb{T}^d$, thus violating the normalization condition for a Bloch vector;
- when $d \leq 3$, the topological obstruction to construct a (possibly orthonormal) Bloch basis consisting of continuous, periodic Bloch vectors is encoded in the *Chern numbers* [18, 16]

$$c_1(P)_{ij} = \frac{1}{2\pi \mathrm{i}} \int_{\mathbb{T}^2_{ij}} \mathrm{d}k_i\, \mathrm{d}k_j\ \mathrm{Tr}_{\mathcal{H}}\left(P(\mathbf{k})\,[\partial_i P(\mathbf{k}), \partial_j P(\mathbf{k})]\right) \quad \in \mathbb{Z}, \quad 1 \leq i < j \leq d, \tag{1.2}$$

where $\mathbb{T}^2_{ij} \subset \mathbb{T}^d$ is the 2-torus where the coordinates different from k_i and k_j are set equal to zero. Only when the Chern numbers vanish does a Bloch basis exist, in which case the Bloch bundle is *trivial*, *i.e.* isomorphic to $\mathbb{T}^d \times \mathbb{C}^m$.

In this paper, we are interested in studying the possibility of relaxing the condition to be a continuous, periodic, and orthonormal Bloch basis in two possible ways, by considering instead collections of M Bloch vectors such that

(i) $M < m$, and the continuous, periodic Bloch vectors are still *orthonormal*;
(ii) $M > m$, and the continuous, periodic Bloch vectors are still *generating* (hence constitute an M-frame).

Moreover, we are interested in finding the optimal value M in each of the two situations (the maximal M in the first, and the minimal M in the second).

Results concerning the *existence* of such collections of Bloch vectors can be found in the literature on vector bundles, for example:

(i) by [12, Chap. 9, Thm. 1.2], there exist $m-\ell_d$ continuous and periodic *independent* sections of the Bloch bundle, where[1] $\ell_d = \lceil (d-1)/2 \rceil$;
(ii) by [12, Chap. 8, Thm. 7.2], there exists an $(m + r_d)$*-frame* for the Bloch bundle, where $r_d = \lceil d/2 \rceil$.

Remark 1.2. The second of the above statements can be rephrased by saying that there exists a *trivial* vector bundle $\mathcal{T}$ of rank $m + r_d$ that contains $\mathcal{E}$ as a subbundle. Indeed, if $\{\psi_a\}_{a=1}^{m+r_d}$ is a moving basis for $\mathcal{T}$, then setting $\xi_a(\mathbf{k}) := P(\mathbf{k})\,\psi_a(\mathbf{k})$, $a \in \{1,\dots,m+r_d\}$, defines an $(m + r_d)$-frame for $\mathcal{E}$ (see also [9]).

Related results in the specific case of Bloch bundles were obtained in [13], where an upper bound of the form $M \le 2^d\, m$ was given for the number of Bloch vectors needed to span $\operatorname{Ran} P(\mathbf{k})$. Improved estimates on M for Bloch bundles in $d \le 3$ were announced in [14] (see also [1]), yielding $M = m + 1$.

We are instead interested in proving *constructively* the existence of the above objects. We will do so in $d = 2$ and $d = 3$. We thus formulate our main result.

Theorem 1.3. *Let $d \le 3$, and let $\{P(\mathbf{k})\}_{\mathbf{k}\in\mathbb{R}^d}$ be a smooth, $\mathbb{Z}^d$-periodic family of orthogonal projections of rank m.*

(i) *One can* construct *at least $m - 1$ independent Bloch vectors which are continuous and $\mathbb{Z}^d$-periodic.*
(ii) *One can* construct *a Parseval $(m+1)$-frame of continuous and $\mathbb{Z}^d$-periodic Bloch vectors (see* (1.1)*).*
(iii) *Assume furthermore that $c_1(P)_{ij} = 0 \in \mathbb{Z}$ for all $1 \le i < j \le d$, where $c_1(P)_{ij}$ is defined in* (1.2). *Then, one can* construct *an* orthonormal Bloch basis *of continuous and $\mathbb{Z}^d$-periodic Bloch vectors.*

Notice that the above result for $d = 3$ yields an optimal number ($M = m + 1$) of vectors in a Parseval frame, which is actually smaller than the number $M = m + r_{d=3} = m + 2$ predicted by the general, bundle-theoretic result quoted above [12, Chap. 8, Thm. 7.2].

Remark 1.4. By standard arguments, which we reproduce in Appendix A.1 for the reader's convenience, it is possible to improve the regularity of Bloch vectors if the family of projections is more regular: the only obstruction is to continuity. In other words, if for example the map $\mathbf{k} \mapsto P(\mathbf{k})$ is smooth or analytic, then a continuous Bloch vector yields a smooth or analytic one by convolution with a sufficiently regular kernel. Moreover, one can always make sure that all the other properties (periodicity, orthogonality...) are preserved by this smoothing procedure.

Notice in particular that, by the above considerations, Theorem 1.3(iii) provides a constructive proof of the results of [18, 15], which are instead obtained by abstract bundle-theoretic methods. There, the condition of vanishing Chern numbers is obtained as a consequence of *time-reversal symmetry*. Constructive algorithms for Bloch bases under this symmetry assumption have been recently investigated in [7, 8, 3, 4, 5, 6].

In problems coming from condensed matter physics, modelled by a gapped periodic Hamiltonian H, the construction of (smooth) Bloch vectors translates in the construction of *localized composite Wannier functions* for the occupied states of H, by transforming the frame back from the $\mathbf{k}$-space representation to the position representation via the Bloch–Floquet transform. The second part of the above Theorem can then be rephrased as the possibility to *construct Parseval frames in $L^2(\mathbb{R}^d)$ consisting of $m+1$ exponentially localized Wannier functions, together with their translates by lattice shifts.*

Parseval frames have found many applications in both pure and applied mathematics, in particular in signal processing and Gabor analysis [11]. We hope that our constructions could help to gain more insight on related problems in periodic systems.

[1] We denote by $\lceil x \rceil$ the smallest integer n such that $x \le n$.

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2. The topologically trivial case

We begin by proving Theorem 1.3(iii) since elements of this proof will be essential for the other two parts of Theorem 1.3. Thus we assume throughout this Section that $\{P(\mathbf{k})\}_{\mathbf{k}\in\mathbb{R}^d}$, $d \le 3$, is a smooth and $\mathbb{Z}^d$-periodic family of rank-m projections with vanishing Chern numbers. We will construct an orthonormal Bloch basis (so, a m-tuple of orthogonal Bloch vectors) which is continuous and $\mathbb{Z}^d$-periodic.

2.1. The 1D case.

We start from the case $d = 1$. Notice that any 1-dimensional family of projections $\{P(k)\}_{k\in\mathbb{R}}$ is topologically trivial, that is, it has vanishing Chern numbers (as there are no non-zero differential 2-forms on the circle $\mathbb{T}$).

Let $T(k, 0)$ denote the parallel transport unitary along the segment from the point 0 to the point k associated to $\{P(k)\}_{k\in\mathbb{R}}$ (see Appendix A.2 for more details). At $k = 1$, write $T(1, 0) = \mathrm{e}^{\mathrm{i}M}$, where $M = M^* \in \mathcal{B}(\mathcal{H})$ is self-adjoint.

Pick an orthonormal basis $\{\xi_a(0)\}_{a=1}^m$ in $\operatorname{Ran} P(0) \simeq \mathbb{C}^m \subset \mathcal{H}$, and define for $a \in \{1, \dots, m\}$ and $k \in \mathbb{R}$

$$\xi_a(k) := W(k)\, \xi_a(0), \quad W(k) := T(k, 0)\mathrm{e}^{-\mathrm{i}kM}.$$

Then $\{\xi_a\}_{a=1}^m$ gives a continuous, $\mathbb{Z}^2$-periodic, and orthonormal Bloch basis for the 1-dimensional family of projections $\{P(k)\}_{k\in\mathbb{R}}$ (compare [4, 5]). This proves Theorem 1.3 in $d = 1$ (where the only non-trivial statement is part (iii)).

2.2. The induction argument in the dimension.

Consider a smooth and periodic family of projections $\{P(k_1, \mathbf{k})\}_{(k_1,\mathbf{k})\in\mathbb{R}^d}$, and let $D := d - 1$. Assume that the D-dimensional restriction $\{P(0, \mathbf{k})\}_{\mathbf{k}\in\mathbb{R}^D}$ admits a continuous and $\mathbb{Z}^D$-periodic orthonormal Bloch basis $\{\xi_a(0, \cdot)\}_{a=1}^m$. Consider now the parallel transport unitary $T_{\mathbf{k}}(k_1, 0)$ along the straight line from the point $(0, \mathbf{k})$ to the point $(k_1, \mathbf{k})$. At $k_1 = 1$, denote $\mathcal{T}(\mathbf{k}) := T_{\mathbf{k}}(1, 0)$. Define

$$\psi_a(k_1, \mathbf{k}) := T_{\mathbf{k}}(k_1, 0)\, \xi_a(0, \mathbf{k}), \quad a \in \{1, \dots, m\}\,,\ (k_1, \mathbf{k}) \in \mathbb{R}^d. \tag{2.1}$$

The above defines a collection of m Bloch vectors for $\{P(k_1, \mathbf{k})\}_{(k_1,\mathbf{k})\in\mathbb{R}^d}$ which are continuous, orthonormal, and $\mathbb{Z}^D$-periodic in the variable $\mathbf{k}$, but in general fail to be $\mathbb{Z}$-periodic in the variable k_1. Indeed, one can check that

$$\psi_b(k_1 + 1, \mathbf{k}) = \sum_{a=1}^m \psi_a(k_1, \mathbf{k})\, \alpha(\mathbf{k})_{ab}, \quad \text{where} \quad \alpha(\mathbf{k})_{ab} := \langle \xi_a(0, \mathbf{k}),\, \mathcal{T}(\mathbf{k})\, \xi_b(0, \mathbf{k})\rangle \tag{2.2}$$

(compare [5, Eqn.s (3.4) and (3.5)]). The family $\{\alpha(\mathbf{k})\}_{\mathbf{k}\in\mathbb{R}^D}$ defined above is a continuous and $\mathbb{Z}^D$-periodic family of $m \times m$ unitary matrices.

The possibility of "rotating" $\alpha(\mathbf{k})$ to the identity entails thus the construction of a Bloch basis which is also periodic in k_1. Formally, we have the following statement (compare also [6, Thm.s 2.4 and 2.6]).

Proposition 2.1. *For the continuous and periodic family $\{\alpha(\mathbf{k})\}_{\mathbf{k}\in\mathbb{R}^D}$ defined in (2.2), the following are equivalent:*

(i) *the family is* null-homotopic*, namely there exists a collection of continuous and $\mathbb{Z}^D$-periodic family of unitary matrices $\{\alpha_t(\mathbf{k})\}_{\mathbf{k}\in\mathbb{R}^D}$, depending continuously on $t \in [0, 1]$, and such that $\alpha_{t=0}(\mathbf{k}) \equiv \mathbf{1}$ while $\alpha_{t=1}(\mathbf{k}) = \alpha(\mathbf{k})$ for all $\mathbf{k} \in \mathbb{R}$;*

(ii) *assuming* $D \le 2$, *we have* $\deg_j(\det\alpha) = 0$ *for all* $j \in \{1, \dots, D\}$. *In the smooth case, this is the same as:*

$$\deg_j(\det\alpha) = \frac{1}{2\pi\mathrm{i}} \int_0^1 \mathrm{d}k_j \ \mathrm{tr}_{\mathbb{C}^m} \left(\alpha(\mathbf{k})^* \frac{\partial\alpha}{\partial k_j}(\mathbf{k}) \right) = 0 \quad \text{for all } j \in \{1, \dots, D\}\,; \tag{2.3}$$

(iii) *the family admits a continuous and* $\mathbb{Z}^D$*-periodic* N-step logarithm, *namely there exist* N *continuous and* $\mathbb{Z}^D$*-periodic families of self-adjoint matrices* $\{h_i(\mathbf{k})\}_{\mathbf{k}\in\mathbb{R}^D}$, $i \in \{1, \dots, N\}$, *such that*

$$\alpha(\mathbf{k}) = \mathrm{e}^{\mathrm{i}h_1(\mathbf{k})} \cdots \mathrm{e}^{\mathrm{i}h_N(\mathbf{k})}, \quad \mathbf{k} \in \mathbb{R}^D; \tag{2.4}$$

(iv) *there exists a continuous family of unitary matrices* $\{\beta(k_1, \mathbf{k})\}_{(k_1,\mathbf{k})\in\mathbb{R}^d}$, $d = D+1$, *which is* $\mathbb{Z}^D$*-periodic in* $\mathbf{k}$, *with* $\beta(0, \mathbf{k}) \equiv \mathbf{1}$ *for all* $\mathbf{k} \in \mathbb{R}^D$, *and such that*

$$\alpha(\mathbf{k}) = \beta(k_1, \mathbf{k})\, \beta(k_1 + 1, \mathbf{k})^{-1}, \quad (k_1, \mathbf{k}) \in \mathbb{R}^d;$$

(v) *there exists a continuous and* $\mathbb{Z}^d$*-periodic Bloch basis* $\{\xi_a\}_{a=1}^m$ *for* $\{P(\mathbf{k})\}_{\mathbf{k}\in\mathbb{R}^d}$.

Proof. (i) $\iff$ (ii). The integer $\deg_j(\det\alpha)$ defined in (2.3) computes the winding number of the continuous and periodic function $k_j \mapsto \det\alpha(\cdots, k_j, \cdots) \colon \mathbb{R} \to U(1)$, $j \in \{1, \dots, D\}$. It is a well-known fact in topology that $\pi_1(U(m)) \simeq \pi_1(U(1)) \simeq \mathbb{Z}$, with the first isomorphism implemented by the map $[\alpha] \mapsto [\det\alpha]$ and the second one implemented by the map $[\varphi] \mapsto \deg(\varphi) := (2\pi\mathrm{i})^{-1} \int_0^1 \varphi^{-1}\, \mathrm{d}\varphi$. It can be then argued that these winding numbers constitute complete homotopy invariants for continuous, periodic maps $\alpha \colon \mathbb{R}^D \to U(m)$ when $D \le 2$ (see *e.g* [17, App. A]).

(i) $\iff$ (iii). Let $\{\alpha_t(\mathbf{k})\}_{\mathbf{k}\in\mathbb{R}^D}$ be an homotopy between $\mathbf{1}$ and α, as in the statement. Since $[0, 1]$ is a compact interval and α_t is $\mathbb{Z}^D$-periodic, by uniform continuity there exists $\delta > 0$ such that

$$\sup_{\mathbf{k}\in\mathbb{R}^D} \|\alpha_s(\mathbf{k}) - \alpha_t(\mathbf{k})\| < 2 \quad \text{whenever} \quad |s - t| < \delta. \tag{2.5}$$

Let $N \in \mathbb{N}$ be such that $1/N < \delta$. Then in particular

$$\sup_{\mathbf{k}\in\mathbb{R}^D} \left\|\alpha_{1/N}(\mathbf{k}) - \mathbf{1}\right\| < 2$$

so that the Cayley transform (see Appendix A.3) provides a "good" logarithm for $\alpha_{1/N}(\mathbf{k})$, *i.e.* $\alpha_{1/N}(\mathbf{k}) = \mathrm{e}^{\mathrm{i}h_N(\mathbf{k})}$, with $h_N(\mathbf{k}) = h_N(\mathbf{k})^*$ continuous and $\mathbb{Z}^D$-periodic.

Using again (2.5) we have that

$$\sup_{\mathbf{k}\in\mathbb{R}^D} \left\|\alpha_{2/N}(\mathbf{k})\, \mathrm{e}^{-\mathrm{i}h_N(\mathbf{k})} - \mathbf{1}\right\| = \sup_{\mathbf{k}\in\mathbb{R}^D} \left\|\alpha_{2/N}(\mathbf{k}) - \alpha_{1/N}(\mathbf{k})\right\| < 2$$

so that by the same argument

$$\alpha_{2/N}(\mathbf{k})\, \mathrm{e}^{-\mathrm{i}h_N(\mathbf{k})} = \mathrm{e}^{\mathrm{i}h_{N-1}(\mathbf{k})}, \quad \text{or} \quad \alpha_{2/N}(\mathbf{k}) = \mathrm{e}^{\mathrm{i}h_{N-1}(\mathbf{k})}\, \mathrm{e}^{\mathrm{i}h_N(\mathbf{k})}.$$

Repeating the same line of reasoning N times, we end up exactly with (2.4).

Conversely, if $\alpha(\mathbf{k})$ is as in (2.4), then

$$\alpha_t(\mathbf{k}) := \mathrm{e}^{\mathrm{i}\,th_1(\mathbf{k})} \dots \mathrm{e}^{\mathrm{i}\,th_N(\mathbf{k})}, \quad t \in [0, 1],\ \mathbf{k} \in \mathbb{R}^D,$$

defines the required homotopy between $\alpha_0(\mathbf{k}) \equiv \mathbf{1}$ and $\alpha_1(\mathbf{k}) = \alpha(\mathbf{k})$.

(i) $\iff$ (iv). Let $\{\alpha_t(\mathbf{k})\}_{\mathbf{k}\in\mathbb{R}^D}$ be an homotopy between $\mathbf{1}$ and α. We set

$$\beta(k_1, \mathbf{k}) := \alpha_{k_1}(\mathbf{k})^{-1}, \quad k_1 \in [0, 1],\ \mathbf{k} \in \mathbb{R}^D,$$

and extend this definition to positive $k_1 > 0$ via

$$\beta(k_1 + 1, \mathbf{k}) := \alpha(\mathbf{k})^{-1}\, \beta(k_1, \mathbf{k})$$

and to negative $k_1 < 0$ via

$$\beta(k_1, \mathbf{k}) := \alpha(\mathbf{k})\, \beta(k_1 + 1, \mathbf{k}).$$

We just need to show that this definition yields a continuous function of k_1. We have $\beta(0^+, \mathbf{k}) = \mathbf{1}$ and $\beta(1^-, \mathbf{k}) = \alpha(\mathbf{k})^{-1}$ by definition. Let $\epsilon > 0$. If $k_1 = -\epsilon$ is negative but close to zero, we have due to the definition

$$\beta(-\epsilon, \mathbf{k}) = \alpha(\mathbf{k})\, \beta(1-\epsilon, \mathbf{k}) \to \alpha(\mathbf{k})\, \beta(1^-, \mathbf{k}) = \mathbf{1} \quad \text{as } \epsilon \to 0.$$

Hence β is continuous at $k_1 = 0$. At $k_1 = 1$ we have instead

$$\beta(1+\epsilon, \mathbf{k}) = \alpha(\mathbf{k})^{-1}\, \beta(\epsilon, \mathbf{k}) \to \alpha(\mathbf{k})^{-1}\, \beta(0^+, \mathbf{k}) = \alpha(\mathbf{k})^{-1} \quad \text{as } \epsilon \to 0$$

and β is also continuous there. In a similar way one can prove continuity at every integer, thus on $\mathbb{R}$.

Conversely, if $\{\beta(k_1, \mathbf{k})\}_{(k_1, \mathbf{k}) \in \mathbb{R}^2}$ is as in the statement, then the required homotopy α_t between $\mathbf{1}$ and α is provided by setting

$$\alpha_t(\mathbf{k}) := \beta(-t/2, \mathbf{k})\, \beta(t/2, \mathbf{k})^{-1}, \quad t \in [0,1],\ \mathbf{k} \in \mathbb{R}^D.$$

(iv) $\iff$ (v). It suffices to set

$$\xi_a(k_1, \mathbf{k}) := \sum_{b=1}^{m} \psi_b(k_1, \mathbf{k})\, \beta(k_1, \mathbf{k})_{ba}, \quad a \in \{1, \dots, m\},$$

or equivalently

$$\beta(k_1, \mathbf{k})_{ba} := \langle \psi_b(k_1, \mathbf{k}),\, \xi_a(k_1, \mathbf{k}) \rangle, \quad a, b \in \{1, \dots, m\},$$

for $\{\psi_b\}_{b=1}^m$ as in (2.1) and $(k_1, \mathbf{k}) \in \mathbb{R}^d$. □

To turn the above proof into a constructive argument, we need to construct the "good" logarithms in (2.4).

Proposition 2.2. *For $D \le 2$, let $\{\alpha(\mathbf{k})\}_{\mathbf{k} \in \mathbb{R}^D}$ be a continuous and $\mathbb{Z}^D$-periodic family of unitary matrices. Assume that α is null-homotopic. Then it is possible to* construct *a two-step "good" logarithm for α, i.e. $N = 2$ in Proposition 2.1(iii).*

Proof. Step 1 : the generic form. We first need to know that one can construct a sequence of continuous, $\mathbb{Z}^D$-periodic families of unitary matrices $\{\alpha_n(\mathbf{k})\}_{\mathbf{k} \in \mathbb{R}^D}$, $n \in \mathbb{N}$, such that

- $\sup_{\mathbf{k} \in \mathbb{R}^D} \|\alpha_n(\mathbf{k}) - \alpha(\mathbf{k})\| \to 0$ as $n \to \infty$, and
- the spectrum of $\alpha_n(\mathbf{k})$ is completely non-degenerate for all $n \in \mathbb{N}$ and $\mathbf{k} \in \mathbb{R}^D$.

The proof of this fact is rather techical, and is deferred to Appendix A.4. In the following, we denote $\alpha'(\mathbf{k}) := \alpha_n(\mathbf{k})$ where $n \in \mathbb{N}$ is large enough so that

$$\sup_{\mathbf{k} \in \mathbb{R}} \|\alpha'(\mathbf{k}) - \alpha(\mathbf{k})\| < 2.$$

Step 2 : α' is homotopic to α. Since

$$\sup_{\mathbf{k} \in \mathbb{R}^D} \left\| \alpha'(\mathbf{k})\, \alpha(\mathbf{k})^{-1} - \mathbf{1} \right\| = \sup_{\mathbf{k} \in \mathbb{R}^D} \|\alpha'(\mathbf{k}) - \alpha(\mathbf{k})\| < 2$$

we have that -1 always lies in the resolvent set of $\alpha'(\mathbf{k})\, \alpha(\mathbf{k})^{-1}$, which then admits a continuous and $\mathbb{Z}^D$-periodic logarithm defined via the Cayley transform:

$$\alpha'(\mathbf{k})\, \alpha(\mathbf{k})^{-1} = \mathrm{e}^{\mathrm{i} h''(\mathbf{k})}, \quad h''(\mathbf{k})^* = h''(\mathbf{k}) = h''(\mathbf{k} + \mathbf{n}) \text{ for } \mathbf{n} \in \mathbb{Z}^D. \tag{2.6}$$

Therefore

$$\alpha_t(\mathbf{k}) := \alpha'(\mathbf{k})\, \mathrm{e}^{\mathrm{i}\, t h''(\mathbf{k})}, \quad t \in [0,1],\ \mathbf{k} \in \mathbb{R}^D,$$

gives a continuous homotopy between $\alpha_0(\mathbf{k}) = \alpha'(\mathbf{k})$ and $\alpha_1(\mathbf{k}) = \alpha(\mathbf{k})$. As a consequence, we have that α' is null-homotopic, since α is by assumption.

Step 3 : a logarithm for α'. Denote by $\{\lambda_1(\mathbf{k}), \dots, \lambda_m(\mathbf{k})\}$ a continuous labelling of the periodic, non-degenerate eigenvalues of $\alpha'(\mathbf{k})$.

If $m = 1$, then $\alpha'(\mathbf{k}) \equiv \det(\alpha'(\mathbf{k})) \equiv \lambda_1(\mathbf{k})$ cannot wind around the circle, due to the hypothesis that α' is null-homotopic. This implies that one can choose a continuous *and periodic* argument for λ_1, namely $\lambda_1(\mathbf{k}) = \mathrm{e}^{\mathrm{i}\phi_1(\mathbf{k})}$ with $\phi_1 \colon \mathbb{R}^D \to \mathbb{R}$ continuous and $\mathbb{Z}^D$-periodic (compare e.g. [4, Lemma 2.13]).

If $m \geq 2$, then the same is true for each of the eigenvalues $\lambda_j(\mathbf{k})$, $j \in \{1, \ldots, m\}$. Indeed, let $\phi_j : \mathbb{R}^D \to \mathbb{R}$ be a continuous argument of the eigenvalue λ_j. The function ϕ_j will satisfy

$$\phi_j(\mathbf{k} + \mathbf{e}_l) = \phi_j(\mathbf{k}) + 2\pi n_j^{(l)}, \quad l \in \{1, \ldots, D\}, \quad n_j^{(l)} \in \mathbb{Z},$$

where $\mathbf{e}_l = (0, \ldots, 1, \ldots, 0)$ is the l-th vector in the standard basis of $\mathbb{R}^D$ and the integer $n_j^{(l)}$ is the winding number of the periodic function $\mathbb{R} \to U(1)$, $k_l \mapsto \lambda_j(\cdots, k_l, \cdots)$. Fix $l \in \{1, \ldots, D\}$, and assume that there exist $i, j \in \{1, \ldots, m\}$ for which $n_i^{(l)} \neq n_j^{(l)}$. Define $\phi(\mathbf{k}) := \phi_j(\mathbf{k}) - \phi_i(\mathbf{k})$; then

$$\phi(\mathbf{k} + \mathbf{e}_j) = \phi(\mathbf{k}) + 2\pi \left(n_j^{(l)} - n_i^{(l)} \right).$$

Since $n_j^{(l)} - n_i^{(l)} \neq 0$, the periodic function $\lambda(\mathbf{k}) := \mathrm{e}^{\mathrm{i}\phi(\mathbf{k})}$ winds around the circle $U(1)$ at least once as a function of the l-th component, and in particular covers the whole circle. So there must exist $\mathbf{k}_0 \in \mathbb{R}^D$ such that $\lambda(\mathbf{k}_0) = 1$, or equivalently $\lambda_i(\mathbf{k}_0) = \mathrm{e}^{\mathrm{i}\phi_i(\mathbf{k}_0)} = \mathrm{e}^{\mathrm{i}\phi_j(\mathbf{k}_0)} = \lambda_j(\mathbf{k}_0)$, in contradiction with the non-degeneracy of the eigenvalues of $\alpha'(\mathbf{k})$.

We deduce then that $n_i^{(l)} = n_j^{(l)} \equiv n^{(l)}$ for all $i, j \in \{1, \ldots, m\}$. Set now $\det(\alpha'(\mathbf{k})) = \mathrm{e}^{\mathrm{i}\Phi(\mathbf{k})}$ for $\Phi(\mathbf{k}) = \phi_1(\mathbf{k}) + \cdots + \phi_m(\mathbf{k})$. Then the equality

$$\Phi(\mathbf{k} + \mathbf{e}_l) = \Phi(\mathbf{k}) + 2\pi \sum_{j=1}^{m} n_j^{(l)} = \Phi(\mathbf{k}) + 2\pi m n^{(l)}$$

shows that necessarily $n^{(l)} = 0$ for all $l \in \{1, \ldots, D\}$, as otherwise the determinant of α' would wind around the circle contrary to the hypothesis of null-homotopy of α'.

Finally, denote by $0 < g \leq 2$ the minimal distance between any two eigenvalues of $\alpha'(\mathbf{k})$, and define the continuous and periodic function $\rho(\mathbf{k}) := \phi_1(\mathbf{k}) + g/100$. Then $\mathrm{e}^{\mathrm{i}\,\rho(\mathbf{k})}$ lies in the resolvent set of $\alpha'(\mathbf{k})$ for all $\mathbf{k} \in \mathbb{R}$. As a consequence, -1 is always in the resolvent set of the continuous and periodic family of unitary matrices $\widetilde{\alpha}(\mathbf{k}) := \mathrm{e}^{-\mathrm{i}\,(\rho(\mathbf{k})+\pi)}\,\alpha'(\mathbf{k})$, which then admits a continuous and periodic logarithm via the Cayley transform: $\widetilde{\alpha}(\mathbf{k}) = \mathrm{e}^{\mathrm{i}\,\widetilde{h}(\mathbf{k})}$. We conclude that

$$\alpha'(\mathbf{k}) = \mathrm{e}^{\mathrm{i}h'(\mathbf{k})} \quad \text{with} \quad h'(\mathbf{k}) := \widetilde{h}(\mathbf{k}) + (\rho(\mathbf{k}) + \pi)\mathbf{1}. \tag{2.7}$$

The family of self-adjoint matrices $\{h'(\mathbf{k})\}_{\mathbf{k}\in\mathbb{R}^D}$ is still continuous and periodic by definition.

Step 4 : a two-step logarithm for α. In view of (2.6) and (2.7) we have $\mathrm{e}^{\mathrm{i}h'(\mathbf{k})}\,\alpha(\mathbf{k})^{-1} = \mathrm{e}^{\mathrm{i}h''(\mathbf{k})}$ for continuous and periodic families of self-adjoint matrices $\{h'(\mathbf{k})\}_{\mathbf{k}\in\mathbb{R}^D}$ and $\{h''(\mathbf{k})\}_{\mathbf{k}\in\mathbb{R}^D}$. This can be rewritten as $\alpha(\mathbf{k}) = \mathrm{e}^{-\mathrm{i}h''(\mathbf{k})}\,\mathrm{e}^{\mathrm{i}h'(\mathbf{k})}$, which is (2.4) for $N = 2$. □

2.3. The link between the topology of α and that of P.

We now come back to Theorem 1.3(iii). First we consider the case $d = 2$ (so that $D = d - 1 = 1$). We have constructed in (2.2) a continuous and $\mathbb{Z}$-periodic family of unitary matrices $\{\alpha(k_2)\}_{k_2\in\mathbb{R}}$, starting from a smooth, periodic family of projections $\{P(k_1, k_2)\}_{(k_1,k_2)\in\mathbb{R}^2}$ and an orthonormal Bloch basis for the restriction $\{P(0, k_2)\}_{k_2\in\mathbb{R}}$. The next result links the topology of α with the one of P.

Proposition 2.3. *Let $\{\alpha(k_2)\}_{k_2\in\mathbb{R}}$ and $\{P(\mathbf{k})\}_{\mathbf{k}\in\mathbb{R}^2}$ be as above. Then*

$$\deg(\det \alpha) = c_1(P).$$

Proof. The equality in the statement follows at once from the following chain of equalities:

$$\mathrm{tr}_{\mathbb{C}^m}\left(\alpha(k_2)^* \partial_{k_2} \alpha(k_2)\right) = \mathrm{Tr}_{\mathcal{H}}\left(P(0, k_2)\, \mathcal{T}(k_2)^* \partial_{k_2} \mathcal{T}(k_2)\right) = \int_0^1 \mathrm{d}k_1\ \mathrm{Tr}_{\mathcal{H}}\left(P(\mathbf{k})\ [\partial_1 P(\mathbf{k}), \partial_2 P(\mathbf{k})]\right).$$

Their proof can be found in Appendix A.2 (compare [5, Sec. 6.3]). □

We are finally able to conclude the proof of Theorem 1.3(iii).

Proof of Theorem 1.3(iii), ($d = 2$). Given our initial hypothesis that $c_1(P) = 0$, the combination of Propositions 2.1 and 2.3 gives that α is null-homotopic, and hence admits a two-step logarithm which can be constructed via Proposition 2.2. This construction then yields the desired continuous and periodic Bloch basis, again via Proposition 2.1. □

Proof of Theorem 1.3(iii), (d = 3). Let $\{P(k_1,k_2,k_3)\}_{(k_1,k_2,k_3)\in\mathbb{R}^3}$ be a smooth and periodic family of projections. Under the assumption that $c_1(P)_{23}=0$, the 2-dimensional result we just proved provides an orthonormal Bloch basis for the restriction $\{P(0,k_2,k_3)\}_{(k_2,k_3)\in\mathbb{R}^2}$, which can be parallel-transported to $\{k_1=1\}$ and hence defines $\{\alpha(k_2,k_3)\}_{(k_2,k_3)\in\mathbb{R}^2}$, as in (2.2). We now apply Proposition 2.3, to the 2-dimensional restrictions $\{P(k_1,0,k_3)\}_{(k_1,k_3)\in\mathbb{R}^2}$ and $\{P(k_1,k_2,0)\}_{(k_1,k_2)\in\mathbb{R}^2}$ instead, and obtain that

(2.8)
$$\deg_2(\det\alpha)=\deg(\det\alpha(\cdot,0))=c_1(P)_{12}=0,\quad \deg_3(\det\alpha)=\deg(\det\alpha(0,\cdot))=c_1(P)_{13}=0$$

(compare Appendix A.2). Again by Proposition 2.1 the family α is then null-homotopic, and one can construct its two-step logarithm via Proposition 2.2. Proposition 2.1 illustrates how to produce the required continuous and $\mathbb{Z}^3$-periodic Bloch basis. □

3. Maximal number of orthonormal Bloch vectors

We come to the proof of Theorem 1.3(i), concerning the existence of $m-1$ orthonormal Bloch vectors for a smooth and $\mathbb{Z}^d$-periodic family of projections $\{P(\mathbf{k})\}_{\mathbf{k}\in\mathbb{R}^d}$ with $2\le d\le 3$. As usual, we have denoted by m the rank of $P(\mathbf{k})$.

3.1. **Pseudo-periodic families of matrices.**

Before giving the proof of Theorem 1.3(i), we need some generalizations of the results in Section 2.2.

Definition 3.1. Let $\{\gamma(k_3)\}_{k_3\in\mathbb{R}}$ be a continuous and $\mathbb{Z}$-periodic family of unitary matrices. We say that a continuous family of matrices $\{\mu(k_2,k_3)\}_{(k_2,k_3)\in\mathbb{R}^2}$ is *γ-periodic* if it satisfies the following conditions:

$$\mu(k_2+1,k_3)=\gamma(k_3)\,\mu(k_2,k_3)\,\gamma(k_3)^{-1},\quad \mu(k_2,k_3+1)=\mu(k_2,k_3),\quad (k_2,k_3)\in\mathbb{R}^2.$$

We say that two continuous and γ-periodic families $\{\mu_0(\mathbf{k})\}_{\mathbf{k}\in\mathbb{R}^2}$ and $\{\mu_1(\mathbf{k})\}_{\mathbf{k}\in\mathbb{R}^2}$ are *γ-homotopic* if there exists a collection of continuous and γ-periodic families $\{\mu_t(\mathbf{k})\}_{\mathbf{k}\in\mathbb{R}^2}$, depending continuously on $t\in[0,1]$, such that $\mu_{t=0}(\mathbf{k})=\mu_0(\mathbf{k})$ and $\mu_{t=1}(\mathbf{k})=\mu_1(\mathbf{k})$ for all $\mathbf{k}\in\mathbb{R}^2$.

Notice that a γ-periodic family of matrices is periodic in k_3 and only pseudo-periodic in k_2: the family γ encodes the failure of k_2-periodicity.

Proposition 3.2. *Let $\{\alpha(k_2,k_3)\}_{(k_2,k_3)\in\mathbb{R}^2}$ be a continuous and γ-periodic family of unitary matrices, and assume that* $\deg_2(\det\alpha)=\deg_3(\det\alpha)=0$. *Then one can* construct *a continuous and γ-periodic two-step logarithm for α, namely there exist continuous and γ-periodic families of self-adjoint matrices $\{h_i(\mathbf{k})\}_{\mathbf{k}\in\mathbb{R}^2}$, $i\in\{1,2\}$, such that*

$$\alpha(k_2,k_3)=\mathrm{e}^{\mathrm{i}h_1(k_2,k_3)}\,\mathrm{e}^{\mathrm{i}h_2(k_2,k_3)},\quad (k_2,k_3)\in\mathbb{R}^2.$$

Proof. The argument goes as in the proof of Proposition 2.2. One just needs to modify Step 1 there, where the approximants of α with completely non-degenerate spectrum are constructed obeying γ-periodicity rather than mere periodicity (compare Appendix A.4). It is also worth noting that both the spectrum and the norm of $\mu(k_2+1,k_3)$ coincide with the spectrum and the norm of $\mu(k_2,k_3)$ for any γ-periodic family of matrices μ, and that the Cayley transform of a γ-periodic family of unitary matrices $\{\alpha(k_2,k_3)\}_{(k_2,k_3)\in\mathbb{R}^2}$ is also γ-periodic. Hence, logarithms constructed via functional calculus on the Cayley transform are automatically γ-periodic (see Appendix A.3). Finally, observing that the spectrum of a γ-periodic family of matrices is $\mathbb{Z}^2$-periodic, the rest of the argument for Proposition 2.2 goes through unchanged. □

The next result generalizes Proposition 2.1 considerably.

Proposition 3.3. *Assume that $D\le 2$. Let $\{\alpha_0(\mathbf{k})\}_{\mathbf{k}\in\mathbb{R}^D}$ and $\{\alpha_1(\mathbf{k})\}_{\mathbf{k}\in\mathbb{R}^D}$ be continuous and periodic families of unitary matrices. Then the following are equivalent:*

(i) *the families are homotopic;*
(ii) $\deg_j(\det\alpha_0)=\deg_j(\det\alpha_1)$ *for all* $j\in\{1,\dots,D\}$, *where* $\deg_j(\det\cdot)$ *is defined in* (2.3)*;*

(iii) *one can* construct *a continuous family of unitary matrices* $\{\beta(k_1,\mathbf{k})\}_{(k_1,\mathbf{k})\in\mathbb{R}^d}$, $d = D+1$, *which is periodic in* $\mathbf{k}$, *with* $\beta(0,\mathbf{k}) \equiv \mathbf{1}$ *for all* $\mathbf{k} \in \mathbb{R}^D$, *and such that*

$$\alpha_1(\mathbf{k}) = \beta(k_1,\mathbf{k})\,\alpha_0(\mathbf{k})\,\beta(k_1+1,\mathbf{k})^{-1}, \quad (k_1,\mathbf{k}) \in \mathbb{R}^d.$$

If $D = 2$*, then the above three statements remain equivalent even if one replaces periodicity by* γ*-periodicity and homotopy by* γ*-homotopy.*

Proof. Since periodicity is a particular case of γ-periodicity, we give the proof in the γ-periodic framework. Set

$$\alpha'(\mathbf{k}) := \alpha_1(\mathbf{k})^{-1}\,\alpha_0(\mathbf{k}), \quad \mathbf{k} \in \mathbb{R}^D.$$

Then $\{\alpha'(\mathbf{k})\}_{\mathbf{k}\in\mathbb{R}^D}$ is a continuous and γ-periodic family of unitary matrices, satifying moreover $\deg_j(\det\alpha') = \deg_j(\det\alpha_0) - \deg_j(\det\alpha_1) = 0$ for $j \in \{1,\dots,D\}$. In view of Proposition 3.2, one can construct a continuous and γ-periodic two-step logarithm for α':

$$\alpha'(\mathbf{k}) = \mathrm{e}^{\mathrm{i}h_2(\mathbf{k})}\,\mathrm{e}^{\mathrm{i}h_1(\mathbf{k})}.$$

Define

$$\beta(k_1,\mathbf{k}) := \mathrm{e}^{\mathrm{i}\,k_1\,h_2(\mathbf{k})}\,\mathrm{e}^{\mathrm{i}\,k_1\,h_1(\mathbf{k})}, \quad k_1 \in [0,1],\ \mathbf{k} \in \mathbb{R}^D,$$

and extend this definition to positive $k_1 > 0$ by

$$\beta(k_1+1,\mathbf{k}) := \alpha_1(\mathbf{k})^{-1}\,\beta(k_1,\mathbf{k})\,\alpha_0(\mathbf{k})$$

and to negative $k_1 < 0$ by

$$\beta(k_1,\mathbf{k}) := \alpha_1(\mathbf{k})\,\beta(k_1+1,\mathbf{k})\,\alpha_0(\mathbf{k})^{-1}.$$

Notice first that the above defines a family of unitary matrices which is γ-periodic in $\mathbf{k}$. We just need to show that this definition yields also a continuous function of k_1. We have $\beta(0^+,\mathbf{k}) = \mathbf{1}$ and $\beta(1^-,k_2) = \alpha_1(\mathbf{k})^{-1}\,\alpha_0(\mathbf{k})$ by definition. Let $\epsilon > 0$. If $k_1 = -\epsilon$ is negative but close to zero, we have due to the definition

$$\beta(-\epsilon,\mathbf{k}) = \alpha_1(\mathbf{k})\,\beta(1-\epsilon,\mathbf{k})\,\alpha_0(\mathbf{k})^{-1} \to \alpha_1(\mathbf{k})\,\beta(1^-,\mathbf{k})\,\alpha_0(\mathbf{k})^{-1} = \mathbf{1} \quad \text{as } \epsilon \to 0.$$

Hence β is continuous at $k_1 = 0$. At $k_1 = 1$ we have instead

$$\beta(1+\epsilon,\mathbf{k}) = \alpha_1(\mathbf{k})^{-1}\,\beta(\epsilon,\mathbf{k})\,\alpha_0(\mathbf{k}) \to \alpha_1(\mathbf{k})^{-1}\,\beta(0^+,\mathbf{k})\,\alpha_0(\mathbf{k}) = \alpha_1(\mathbf{k})^{-1}\,\alpha_0(\mathbf{k}) \quad \text{as } \epsilon \to 0$$

and β is also continuous there.

Conversely, if we are given $\{\beta(k_1,\mathbf{k})\}_{(k_1,\mathbf{k})\in\mathbb{R}^3}$ as in the statement, then

$$\alpha_t(\mathbf{k}) := \beta(-t/2,\mathbf{k})\alpha_0(\mathbf{k})\,\beta(t/2,\mathbf{k})^{-1}, \quad t \in [0,1],\ \mathbf{k} \in \mathbb{R}^2,$$

gives the desired γ-homotopy between α_0 and α_1. □

3.2. **Orthonormal Bloch vectors.**
We now come back to the proof of Theorem 1.3(i).

Proof of Theorem 1.3(i). Let us start from a 2-dimensional smooth and $\mathbb{Z}^2$-periodic family of rank-m projections $\{P(\mathbf{k})\}_{\mathbf{k}\in\mathbb{R}^2}$. We replicate the construction at the beginning of Section 2 (see Equation (2.1)) to obtain an orthonormal collection of m Bloch vectors $\{\psi_a\}_{a=1}^m$ for $\{P(\mathbf{k})\}_{\mathbf{k}\in\mathbb{R}^2}$ which are continuous and $\mathbb{Z}$-periodic in the variable k_2. The continuous and periodic family of unitary matrices $\{\alpha_{2\mathrm{D}}(k_2)\}_{k_2\in\mathbb{R}}$, defined as in (2.2), measures the failure of $\{\psi_a\}_{a=1}^m$ to be periodic in k_1.

Define

$$\widetilde{\alpha}_{2\mathrm{D}}(k_2) := \begin{pmatrix} \det\alpha_{2\mathrm{D}}(k_2) & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 \end{pmatrix}. \tag{3.1}$$

Clearly $\det \alpha_{2D}(k_2) = \det \widetilde{\alpha}_{2D}(k_2)$, so that in particular α_{2D} and $\widetilde{\alpha}_{2D}$ are homotopic. Proposition 3.3 applies and produces a family of unitary matrices $\{\beta_{2D}(k_1,k_2)\}_{(k_1,k_2)\in\mathbb{R}^2}$ which is periodic in k_2 and such that

$$\alpha_{2D}(k_2) = \beta_{2D}(k_1,k_2)\,\widetilde{\alpha}_{2D}(k_2)\,\beta_{2D}(k_1+1,k_2)^{-1}$$

holds for all $(k_1,k_2)\in\mathbb{R}^2$.

With $\{\psi_a\}_{a=1}^m$ as in (2.1) and $\{\beta_{2D}(\mathbf{k})\}_{\mathbf{k}\in\mathbb{R}^2}$ as above, define

$$\xi_a(\mathbf{k}) := \sum_{b=1}^m \psi_b(\mathbf{k})\,\beta_{2D}(\mathbf{k})_{ba}, \quad a\in\{1,\dots,m\}\,,\ \mathbf{k}\in\mathbb{R}^2.$$

Then we see that for $a\in\{1,\dots,m\}$ and $(k_1,k_2)\in\mathbb{R}^2$

(3.2)

$$\begin{aligned}\xi_a(k_1+1,k_2) &= \sum_{b=1}^m \psi_b(k_1+1,k_2)\,\beta_{2D}(k_1+1,k_2)_{ba} = \sum_{b,c=1}^m \psi_c(k_1,k_2)\,\alpha_{2D}(k_2)_{cb}\,\beta_{2D}(k_1+1,k_2)_{ba} \\ &= \sum_{c=1}^m \psi_c(k_1,k_2)\,\left[\alpha_{2D}(k_2)\,\beta_{2D}(k_1+1,k_2)\right]_{ca} = \sum_{c=1}^m \psi_c(k_1,k_2)\,\left[\beta_{2D}(k_1,k_2)\,\widetilde{\alpha}_{2D}(k_2)\right]_{ca} \\ &= \sum_{b=1}^m\sum_{c=1}^m \psi_c(k_1,k_2)\,\beta_{2D}(k_1,k_2)_{cb}\,\widetilde{\alpha}_{2D}(k_2)_{ba} = \sum_{b=1}^m \xi_b(k_1,k_2)\,\widetilde{\alpha}_{2D}(k_2)_{ba}.\end{aligned}$$

Since $\widetilde{\alpha}_{2D}(k_2)$ is in the form (3.1), when we set $a\in\{2,\dots,m\}$ in the above equation this reads $\xi_a(k_1+1,k_2)=\xi_a(k_1,k_2)$, that is, $\{\xi_a\}_{a=2}^m$ is an orthonormal collection of $(m-1)$ Bloch vectors which are continuous *and $\mathbb{Z}^2$-periodic*. This concludes the proof of Theorem 1.3(i) in the 2-dimensional case.

We now move to the case $d=3$. Let $\{P(\mathbf{k})\}_{\mathbf{k}\in\mathbb{R}^3}$ be a family of rank-m projections which is smooth and $\mathbb{Z}^3$-periodic. In view of what we have just proved, the 2-dimensional restriction $\{P(0,k_2,k_3)\}_{(k_2,k_3)\in\mathbb{R}^2}$ admits a collection of m orthonormal Bloch vectors $\{\xi_a(0,\cdot,\cdot)\}_{a=1}^m$ satisfying

$$\begin{aligned}&\xi_1(0,k_2+1,k_3) = \det\alpha_{2D}(k_3)\,\xi_1(0,k_2,k_3),\\ &\xi_b(0,k_2+1,k_3) = \xi_b(0,k_2,k_3) \text{ for all } b\in\{2,\dots,m\}\,,\\ &\xi_a(0,k_2,k_3+1) = \xi_a(0,k_2,k_3) \text{ for all } a\in\{1,\dots,m\}\,.\end{aligned} \tag{3.3}$$

Parallel-transport these Bloch vectors along the k_1-direction, and define $\{\psi_a\}_{a=1}^m$ as in (2.1) and $\{\alpha(k_2,k_3)\}_{(k_2,k_3)\in\mathbb{R}^2}$ as in (2.2). The latter matrices are still unitary, depend continuously on (k_2,k_3), are periodic in k_3, but

$$\alpha(k_2+1,k_3) = \widetilde{\alpha}_{2D}(k_3)\,\alpha(k_2,k_3)\,\widetilde{\alpha}_{2D}(k_3)^{-1},$$

as can be checked from (3.3). Thus, the family $\{\alpha(k_2,k_3)\}_{(k_2,k_3)\in\mathbb{R}^2}$ is $\widetilde{\alpha}_{2D}$-periodic, and consequently so is the family defined by

$$\widetilde{\alpha}(k_2,k_3) := \begin{pmatrix}\det\alpha(k_2,k_3) & 0 & \cdots & 0\\ 0 & 1 & \cdots & 0\\ \vdots & \vdots & \ddots & \vdots\\ 0 & 0 & \cdots & 1\end{pmatrix}$$

(actually, since $\widetilde{\alpha}$ and $\widetilde{\alpha}_{2D}$ commute, in this case $\widetilde{\alpha}_{2D}$-periodicity reduces to mere periodicity). Since α and $\widetilde{\alpha}$ share the same determinant, Proposition 3.3 again produces a continuous, $\widetilde{\alpha}_{2D}$-periodic family of unitary matrices $\{\beta(k_1,\mathbf{k})\}_{(k_1,\mathbf{k})\in\mathbb{R}^3}$ such that for all $(k_1,\mathbf{k})\in\mathbb{R}^3$

$$\alpha(\mathbf{k}) = \beta(k_1,\mathbf{k})\,\widetilde{\alpha}(\mathbf{k})\,\beta(k_1+1,\mathbf{k})^{-1}.$$

Arguing as above (compare (3.2)), the collection of Bloch vectors defined by

$$\xi_a(k_1,\mathbf{k}) := \sum_{b=1}^m \psi_b(k_1,\mathbf{k})\,\beta(k_1,\mathbf{k})_{ba}, \quad a\in\{1,\dots,m\}\,,\ (k_1,\mathbf{k})\in\mathbb{R}^3$$

satisfies

$$\xi_a(k_1+1,\mathbf{k}) = \sum_{b=1}^{m} \xi_b(k_1,\mathbf{k})\, \widetilde{\alpha}(\mathbf{k})_{ba}.$$

Due to the form of $\widetilde{\alpha}$, this implies again that $\{\xi_a\}_{a=2}^m$ are continuous, orthonormal, *and* $\mathbb{Z}^3$*-periodic* Bloch vectors for $\{P(\mathbf{k})\}_{\mathbf{k}\in\mathbb{R}^3}$, thus concluding the proof. □

4. Moving Parseval frames of Bloch vectors

In this Section, we finally prove Theorem 1.3(ii), and complete the proof of our main result. The central step consists in proving the result for families of rank 1, which we will do first.

4.1. **The rank-1 case.**

Proof of Theorem 1.3(ii) (rank-1 case). Let $d \le 3$. We consider first a smooth and $\mathbb{Z}^d$-periodic family of projections $\{P_1(\mathbf{k})\}_{\mathbf{k}\in\mathbb{R}^d}$ of rank $m = 1$. We want to show that there exists two Bloch vectors $\{\xi_1, \xi_2\}$ which are continuous, $\mathbb{Z}^d$-periodic, and generate the 1-dimensional space $\operatorname{Ran} P_1(\mathbf{k}) \subset \mathcal{H}$ at each $\mathbf{k} \in \mathbb{R}^d$.

To do so, fix a complex conjugation C on the Hilbert space $\mathcal{H}$ (which is tantamount to the choice of an orthonormal basis). Define

$$Q(\mathbf{k}) := C\, P_1(-\mathbf{k})\, C^{-1}.$$

Using the fact that C is an antiunitary operator such that $C^2 = \mathbf{1}$, one can check that $\{Q(\mathbf{k})\}_{\mathbf{k}\in\mathbb{R}^d}$ defines a smooth and $\mathbb{Z}^d$-periodic family of orthogonal projectors. Moreover, one also has that $c_1(Q)_{ij} = -c_1(P)_{ij}$ for all $1 \le i < j \le d$, as can be seen by integrating the identity

$$\operatorname{Tr}_{\mathcal{H}}\left(Q(\mathbf{k})\, [\partial_i Q(\mathbf{k}), \partial_j Q(\mathbf{k})]\right) = -\operatorname{Tr}_{\mathcal{H}}\left(P_1(-\mathbf{k})\, [\partial_i P_1(-\mathbf{k}), \partial_j P_1(-\mathbf{k})]\right)$$

over $\mathbb{T}^2_{ij}$ (compare [18]).

Set now $P(\mathbf{k}) := P_1(\mathbf{k}) \oplus Q(\mathbf{k})$ for $\mathbf{k} \in \mathbb{R}^d$. The rank-2 family of projections $\{P(\mathbf{k})\}_{\mathbf{k}\in\mathbb{R}^d}$ on $\mathcal{H} \oplus \mathcal{H}$ satisfies then

$$c_1(P)_{ij} = c_1(P_1)_{ij} + c_1(Q)_{ij} = 0 \quad \text{for all } 1 \le i < j \le d.$$

Hence, in view of the results of Section 2, it admits a Bloch basis $\{\psi_1, \psi_2\}$. Let $\pi_j \colon \mathcal{H} \oplus \mathcal{H} \to \mathcal{H}$ be the projection on the j-th factor, $j \in \{1, 2\}$. Set finally

$$\xi_a(\mathbf{k}) := \pi_1\left((P_1(\mathbf{k}) \oplus 0)\ \psi_a(\mathbf{k})\right), \quad a \in \{1,2\}\,,\ \mathbf{k} \in \mathbb{R}^d.$$

Let us show that $\{\xi_a(\mathbf{k})\}_{a=1}^2$ gives a (continuous and $\mathbb{Z}^d$-periodic) Parseval frame in $\operatorname{Ran} P_1(\mathbf{k})$. Indeed, let $\psi \in \operatorname{Ran} P_1(\mathbf{k})$: then automatically $\psi \oplus 0 \in \operatorname{Ran} P(\mathbf{k})$. Since $\{\psi_a(\mathbf{k})\}_{a=1}^2$ is an orthonormal basis for $\operatorname{Ran} P(\mathbf{k})$, we obtain that

$$\psi \oplus 0 = \sum_{a=1}^{2} \langle \psi_a(\mathbf{k}),\, \psi \oplus 0\rangle_{\mathcal{H}\oplus\mathcal{H}}\, \psi_a(\mathbf{k}) = \sum_{a=1}^{2} \langle \xi_a(\mathbf{k}),\, \psi\rangle_{\mathcal{H}}\, \psi_a(\mathbf{k}).$$

Finally, we apply $\pi_1 \circ (P_1(\mathbf{k}) \oplus 0)$ on both sides and obtain

$$\psi = \sum_{a=1}^{2} \langle \xi_a(\mathbf{k}),\, \psi\rangle_{\mathcal{H}}\, \xi_a(\mathbf{k})$$

which is the defining condition for $\{\xi_a(\mathbf{k})\}_{a=1}^2$ to be a Parseval frame in $\operatorname{Ran} P_1(\mathbf{k})$. □

4.2. **The higher rank case:** $m > 1$.

Proof of Theorem 1.3(ii) (rank-m case, $m > 1$). Let $d \leq 3$, and consider a smooth and $\mathbb{Z}^d$-periodic family of rank-m projections $\{P(\mathbf{k})\}_{\mathbf{k}\in\mathbb{R}^d}$. In view of Theorem 1.3(i), which we already proved, it admits $m-1$ orthonormal Bloch vectors $\{\xi_a\}_{a=1}^{m-1}$: they are $\mathbb{Z}^d$-periodic, and without loss of generality (see Appendix A.1) we assume them to be smooth. Denote by

$$P_{m-1}(\mathbf{k}) := \sum_{a=1}^{m-1} |\xi_a(\mathbf{k})\rangle \langle \xi_a(\mathbf{k})| , \quad \mathbf{k} \in \mathbb{R}^2,$$

the rank-$(m-1)$ projection onto the space spanned by $\{\xi_a(\mathbf{k})\}_{a=1}^{m-1}$. Since the latter are smooth and periodic Bloch vectors for $\{P(\mathbf{k})\}_{\mathbf{k}\in\mathbb{R}^d}$, the family $\{P_{m-1}(\mathbf{k})\}_{\mathbf{k}\in\mathbb{R}^d}$ is smooth, $\mathbb{Z}^d$-periodic, and satisfies $P_{m-1}(\mathbf{k})\,P(\mathbf{k}) = P(\mathbf{k})\,P_{m-1}(\mathbf{k}) = P_{m-1}(\mathbf{k})$.

Denote by $P_1(\mathbf{k})$ the orthogonal projection onto the orthogonal complement of $\operatorname{Ran} P_{m-1}(\mathbf{k})$ inside $\operatorname{Ran} P(\mathbf{k})$. Then $\{P_1(\mathbf{k})\}_{\mathbf{k}\in\mathbb{R}^d}$ is a smooth and $\mathbb{Z}^d$-periodic family of rank-1 projections, and furthermore $P_1(\mathbf{k})\,P(\mathbf{k}) = P(\mathbf{k})\,P_1(\mathbf{k}) = P_1(\mathbf{k})$. In view of the results of the previous Subsections, we can construct two continuous and $\mathbb{Z}^d$-periodic Bloch vectors $\{\xi_m, \xi_{m+1}\}$ which generate $\operatorname{Ran} P_1(\mathbf{k})$ at all $\mathbf{k} \in \mathbb{R}^d$. Since $P_1(\mathbf{k})$ is a sub-projection of $P(\mathbf{k})$, it then follows that

$$P(\mathbf{k})\,\xi_a(\mathbf{k}) = P(\mathbf{k})\,P_1(\mathbf{k})\,\xi_a(\mathbf{k}) = P_1(\mathbf{k})\,\xi_a(\mathbf{k}) = \xi_a(\mathbf{k}) \quad \text{for all } a \in \{m, m+1\}\,.$$

Besides, by construction $\{\xi_m(\mathbf{k}), \xi_{m+1}(\mathbf{k})\}$ generate the orthogonal complement in $\operatorname{Ran} P(\mathbf{k})$ to the span of $\{\xi_a(\mathbf{k})\}_{a=1}^{m-1}$, and hence the full collection of $m+1$ Bloch vectors $\{\xi_a\}_{a=1}^{m+1}$ give an $(m+1)$-frame for $\{P(\mathbf{k})\}_{\mathbf{k}\in\mathbb{R}^d}$ consisting of continuous and $\mathbb{Z}^d$-periodic vectors, as desired. □

5. Outlook

We would like to conclude by outlining two open problems related to the topics discussed in this paper.

1. The first natural challenge would be to extend Theorem 1.3 to dimensions $d \geq 4$. In this case, the topological obstruction to the triviality is no longer encoded exclusively in the first Chern class. For example, if $d = 4$ and $m \geq 2$, a Bloch bundle is trivial if and only if the first two Chern classes vanish (see [2, Eqn. (4.28)]). In our "induction in the dimension" language, the vanishing of the first Chern class would allow us to construct a smooth and periodic orthonormal basis containing m vectors $\{\xi_a(0, k_2, k_3, k_4)\}_{a=1}^{m}$ for the projection family $P(0, k_2, k_3, k_4)$, $(k_2, k_3, k_4) \in \mathbb{R}^3$. After parallel transporting these vectors along the k_1-direction we end up with a $m \times m$ family of unitary matrices $\alpha(k_2, k_3, k_4)$ which is $\mathbb{Z}^3$-periodic and smooth (compare (2.2)). Again, the vanishing of the first Chern class ensures that the determinant of α will not wind by Proposition 2.3, hence it has a periodic phase. However, the new obstacle which can appear is that we can no longer hope to always find a smooth approximation α' whose spectrum is always non-degenerate. Here is where the vanishing of the second Chern class comes into play and allows us to construct a two-step "good" logarithm for α.

Is it possible in the obstructed case to modify our method in order to produce a Parseval basis consisting of $m + r_d = m + 2 \geq 4$ smooth and periodic vectors? What about higher dimensions?

2. One interesting class of obstructed families of Bloch projections appearing in condensed matter systems is the one coming from spectral projections of $2d$ magnetic Schrödinger operators with a so-called rational flux condition. If the rank of the Bloch projection is m, we know from Theorem 1.3(ii) and (iii) that we can still construct $m-1$ orthonormal Bloch vectors, as well as a Parseval frame consisting of $m+1$ vectors. Going back from the $\mathbf{k}$-space into the position representation we generate a Parseval frame composed by $m+1$ localized composite Wannier functions together with all their translates by lattice shifts.

Now assume that the external constant magnetic field is slightly changed so that the rational flux condition is violated. Is it still possible to prove the existence of a Parseval frame for the perturbed magnetic spectral projection? We note that when the unperturbed Bloch projection is topologically trivial, then one can construct an *orthonormal basis* of m magnetic Wannier functions together with all their *magnetic* translates by lattice shifts as in [4].

Appendix A. "Black boxes"

In this Appendix we will provide more details and appropriate references for a number of tools and "black boxes" employed in the body of the paper.

A.1. **Smoothing argument.**

We start by providing a smoothing argument that allows to produce *real analytic* Bloch vectors from continuous ones.

Lemma A.1 (Smoothing argument). *Let $\{P(\mathbf{k})\}_{\mathbf{k}\in\mathbb{R}^d}$ be a family of orthogonal projections admitting an analytic, $\mathbb{Z}^d$-periodic analytic extension to a complex strip around $\mathbb{R}^d \subset \mathbb{C}^d$. Assume that there exist continuous, $\mathbb{Z}^d$-periodic, and orthogonal Bloch vectors $\{\xi_1, ..., \xi_m\}$ for $\{P(\mathbf{k})\}_{\mathbf{k}\in\mathbb{R}^d}$. Then, there exist also* real analytic*, $\mathbb{Z}^d$-periodic, and orthogonal Bloch vectors $\left\{\widehat{\xi}_1, ..., \widehat{\xi}_m\right\}$.*

The same holds true if analyticity is replaced by C^r-smoothness for some $r \in \mathbb{N} \cup \{\infty\}$.

Proof (sketch). We sketch here the proof: more details can be found in [4, Sec. 2.3].

Define

$$g(\mathbf{k}) = g(k_1, \dots, k_d) := \frac{1}{\pi^d} \prod_{j=1}^{d} \frac{1}{1+k_j^2}.$$

The function g is analytic over the strip $\left\{\mathbf{z} = (z_1, \dots, z_d) \in \mathbb{C}^d : |\mathrm{Im}\, z_j| < 1,\ j \in \{1, \dots, d\}\right\}$ and obeys $\int_{\mathbb{R}^d} g(\mathbf{k})\, \mathrm{d}\mathbf{k} = 1$. For $\delta > 0$, define $g_\delta(\mathbf{k}) := \delta^{-d} g(\mathbf{k}/\delta)$. Set

$$\psi_a^{(\delta)}(\mathbf{k}) := \int_{\mathbb{R}^d} g_\delta(\mathbf{k}-\mathbf{k}')\, \xi_a(\mathbf{k}')\, \mathrm{d}\mathbf{k}', \quad a \in \{1, ..., m\}\,,\ \mathbf{k} \in \mathbb{R}^d.$$

The above define $\mathbb{Z}^d$-periodic vectors which admit an analytic extension to a strip of half-width δ around the real axis in $\mathbb{C}^d$, and moreover converge to ξ_a uniformly as $\delta \to 0$. We note here that an alternative way of smoothing has been suggested to us by G. Panati: he proposed taking the convolution with the Fejér kernel, which has the advantage of integrating on $[-1/2, 1/2]^d$ and not on the whole $\mathbb{R}^d$.

Now denote $\phi_a^{(\delta)}(\mathbf{k}) := P(\mathbf{k})\, \psi_a^{(\delta)}(\mathbf{k})$, for $a \in \{1, ..., m\}$ and $\mathbf{k} \in \mathbb{R}^d$. Then for any $\epsilon > 0$ there exists $\delta > 0$ such that $\phi_a^{(\delta)}(\mathbf{k})$ and $\xi_a(\mathbf{k})$ are uniformly at a distance less then ϵ. Moreover, as the ξ_a's are orthogonal, we can make sure that the Gram–Schmidt matrix $h^{(\delta)}(\mathbf{k})_{ab} := \left\langle \phi_a^{(\delta)}(\mathbf{k}),\, \phi_b^{(\delta)}(\mathbf{k}) \right\rangle$ is close to the identity matrix, uniformly in $\mathbf{k}$, possibly at the price of choosing an even smaller δ. This implies that $h^{(\delta)}(\mathbf{k})^{-1/2}$ is real analytic and $\mathbb{Z}^d$-periodic, and hence the vectors

$$\widehat{\xi}_a(\mathbf{k}) := \sum_{b=1}^{m} \phi_b^{(\delta)}(\mathbf{k}) \left[h^{(\delta)}(\mathbf{k})^{-1/2}\right]_{ba}$$

define the required real analytic, $\mathbb{Z}^d$-periodic, and orthogonal Bloch vectors. □

A.2. **Parallel transport.**

We recall here the definition of *parallel transport* associated to a smooth and $\mathbb{Z}^d$-periodic family of projections $\{P(k_1, \dots, k_d)\}_{(k_1,\dots,k_d)\in\mathbb{R}^d}$ acting on an Hilbert space $\mathcal{H}$.

Fix $i \in \{1, \dots, d\}$. For $(k_1, \dots, k_d) \in \mathbb{R}^d$, denote by $\mathbf{k} \in \mathbb{R}^D$, $D = d-1$, the collection of coordinates different from the i-th. We use the shorthand notation $(k_1, \dots, k_d) \equiv (k_i, \mathbf{k})$ throughout this Subsection.

Define

$$A_{\mathbf{k}}(k_i) := \mathrm{i}\left[\partial_{k_i} P(k_i, \mathbf{k}), P(k_i, \mathbf{k})\right], \quad (k_i, \mathbf{k}) \in \mathbb{R}^d. \tag{A.1}$$

Then $A_{\mathbf{k}}(k_i)$ defines a self-adjoint operator on $\mathcal{H}$. The solution to the operator-valued Cauchy problem

$$\mathrm{i}\, \partial_{k_i} T_{\mathbf{k}}(k_i, k_i^0) = A_{\mathbf{k}}(k_i)\, T_{\mathbf{k}}(k_i, k_i^0), \quad T_{\mathbf{k}}(k_i^0, k_i^0) = \mathbf{1}, \tag{A.2}$$

defines a family of unitary operators on $\mathcal{H}$, called the *parallel transport unitaries* (along the i-th direction). In the following we will fix $k_i^0 = 0$. This notion coincides with the one in differential geometry of the parallel transport along the straight line from $(0,\mathbf{k})$ to $(k_i,\mathbf{k})$ associated to the *Berry connection* on the Bloch bundle. The parallel transport unitaries satisfy the properties listed in the following result.

Lemma A.2. *Let $\{P(\mathbf{k})\}_{\mathbf{k}\in\mathbb{R}^d}$ be a smooth (respectively analytic) and $\mathbb{Z}^d$-periodic family of orthogonal projections acting on an Hilbert space $\mathcal{H}$. Then the family of parallel transport unitaries $\{T_{\mathbf{k}}(k_i,0)\}_{k_i\in\mathbb{R},\,\mathbf{k}\in\mathbb{R}^D}$ defined in* (A.2) *satisfies the following properties:*

(i) *the map $\mathbb{R}^d \ni \mathbf{k} = (k_i,\mathbf{k}) \mapsto T_{\mathbf{k}}(k_i,0) \in \mathcal{U}(\mathcal{H})$ is smooth (respectively real analytic);*

(ii) *for all $k_i\in\mathbb{R}$ and $\mathbf{k}\in\mathbb{R}^D$*

$$T_{\mathbf{k}}(k_i+1,1) = T_{\mathbf{k}}(k_i,0)$$

and

$$T_{\mathbf{k}+\mathbf{n}}(k_i,0) = T_{\mathbf{k}}(k_i,0) \quad \textit{for } \mathbf{n}\in\mathbb{Z}^D;$$

(iii) *the intertwining property*

$$P(k_i,\mathbf{k}) = T_{\mathbf{k}}(k_i,0)\,P(0,\mathbf{k})\,T_{\mathbf{k}}(k_i,0)^{-1}$$

holds for all $k_i\in\mathbb{R}$ and $\mathbf{k}\in\mathbb{R}^D$.

A proof of all these properties can be found for example in [10] or in [4, Sec. 2.6].

In (2.2), the parallel transport unitary $\mathcal{T}(\mathbf{k}) := T_{\mathbf{k}}(1,0)$ is employed to define the continuous, $\mathbb{Z}^D$-periodic family of unitary matrices $\{\alpha(\mathbf{k})\}_{\mathbf{k}\in\mathbb{R}^D}$. Let $j\in\{1,\dots,d\}$, $j\neq i$. The integrand in the formula (2.3) for $\deg_j(\det\alpha)$ can be expressed in terms of the parallel transport unitaries as

$$\mathrm{tr}_{\mathbb{C}^m}\left(\alpha(\mathbf{k})^*\partial_{k_j}\alpha(\mathbf{k})\right) = \mathrm{Tr}_{\mathcal{H}}\left(P(0,\mathbf{k})\,\mathcal{T}(\mathbf{k})^*\partial_{k_j}\mathcal{T}(\mathbf{k})\right)$$

(compare [5, Lemma 6.1]). Besides, by the Duhamel formula we have

$$\partial_{k_j}T_{\mathbf{k}}(k_i,0) = T_{\mathbf{k}}(k_i,0)\int_0^{k_i}\mathrm{d}s\,T_{\mathbf{k}}(s,0)^*\,\partial_{k_j}A_{\mathbf{k}}(s)\,T_{\mathbf{k}}(s,0),$$

where $A_{\mathbf{k}}(s)$ is as in (A.1) (compare [5, Lemma 6.2]). On the other hand, one can also compute

$$P(k_i,\mathbf{k})\,\partial_{k_j}A_{\mathbf{k}}(k_i)\,P(k_i,\mathbf{k}) = P(k_i,\mathbf{k})\,[\partial_{k_i}P(k_i,\mathbf{k}),\partial_{k_j}P(k_i,\mathbf{k})]\,P(k_i,\mathbf{k})$$

so that, denoting $\mathbf{K} := (k_i,\mathbf{k})\in\mathbb{R}^d$,

$$\mathrm{Tr}_{\mathcal{H}}\left(P(0,\mathbf{k})\,\mathcal{T}(\mathbf{k})^*\partial_{k_j}\mathcal{T}(\mathbf{k})\right) = \int_0^1\mathrm{d}k_i\;\mathrm{Tr}_{\mathcal{H}}\left(P(\mathbf{K})\,\left[\partial_{k_i}P(\mathbf{K}),\partial_{k_j}P(\mathbf{K})\right]\right)$$

(compare [5, Eqn. (6.13)]). Putting all the above equalities together, we conclude that

$$\deg_j(\det\alpha) = \frac{1}{2\pi\mathrm{i}}\int_0^1\mathrm{d}k_j\int_0^1\mathrm{d}k_i\;\mathrm{Tr}_{\mathcal{H}}\left(P(\mathbf{K})\,\left[\partial_{k_i}P(\mathbf{K}),\partial_{k_j}P(\mathbf{K})\right]\right) = c_1(P)_{ij},$$

see (1.2). The above equality proves Proposition 2.3 as well as Equation (2.8).

A.3. **Cayley transform.**

An essential tool to produce “good” logarithms for families of unitary matrices which inherit properties like continuity and (γ-)periodicity is the *Cayley transform*. We recall here this construction.

Lemma A.3 (Cayley transform)**.** *Let $\{\alpha(\mathbf{k})\}_{\mathbf{k}\in\mathbb{R}^D}$ be a family of unitary matrices which is continuous and $\mathbb{Z}^D$-periodic. Assume that -1 lies in the resolvent set of $\alpha(\mathbf{k})$ for all $\mathbf{k}\in\mathbb{R}^D$. Then one can* construct *a family $\{h(\mathbf{k})\}_{\mathbf{k}\in\mathbb{R}^D}$ of self-adjoint matrices which is continuous, $\mathbb{Z}^D$-periodic and such that*

$$\alpha(\mathbf{k}) = \mathrm{e}^{\mathrm{i}\,h(\mathbf{k})} \quad \textit{for all } \mathbf{k}\in\mathbb{R}^D.$$

If $D=2$ and $\{\alpha(k_2,k_3)\}_{(k_2,k_3)\in\mathbb{R}^2}$ is γ-periodic (in the sense of Definition 3.1), then the above family of self-adjoint matrices can be chosen to be γ-periodic as well.

Proof. The proof adapts the one in [5, Prop. 3.5]. The Cayley transform

$$s(\mathbf{k}) := \mathrm{i}\,(\mathbf{1}-\alpha(\mathbf{k}))\,(\mathbf{1}+\alpha(\mathbf{k}))^{-1}$$

is self-adjoint, depends continuously on $\mathbf{k}$, and is $\mathbb{Z}^D$-periodic (respectively γ-periodic) if α is as well. One also immediately verifies that

$$\alpha(\mathbf{k}) = (\mathbf{1}+\mathrm{i}\,s(\mathbf{k}))\,(\mathbf{1}-\mathrm{i}\,s(\mathbf{k}))^{-1}\,.$$

Let $\mathcal{C}$ be a closed, positively-oriented contour in the complex plane which encircles the real spectrum of $s(\mathbf{k})$ for all $\mathbf{k}\in\mathbb{R}^D$. Let $\log(\cdot)$ denote the choice of the complex logarithm corresponding to the branch cut on the negative real semi-axis. Then

$$h(\mathbf{k}) := \frac{1}{2\pi}\oint_{\mathcal{C}} \log\left(\frac{1+\mathrm{i}\,z}{1-\mathrm{i}\,z}\right)(s(\mathbf{k})-z\mathbf{1})^{-1}\,\mathrm{d}z, \quad \mathbf{k}\in\mathbb{R}^D,$$

obeys all the required properties. □

A.4. **Generically non-degenerate spectrum of families of unitary matrices.**
The aim of this Subsection is to prove that

Proposition A.4. *Let $D\le 2$. Consider a continuous and $\mathbb{Z}^D$-periodic family of unitary matrices $\{\alpha(\mathbf{k})\}_{\mathbf{k}\in\mathbb{R}^D}$. Then, one can* construct *a sequence of continuous, $\mathbb{Z}^D$-periodic families of unitary matrices $\{\alpha_n(\mathbf{k})\}_{\mathbf{k}\in\mathbb{R}^D}$, $n\in\mathbb{N}$, such that*

- $\sup_{\mathbf{k}\in\mathbb{R}^D}\|\alpha_n(\mathbf{k})-\alpha(\mathbf{k})\|\to 0$ *as $n\to\infty$, and*
- *the spectrum of $\alpha_n(\mathbf{k})$ is completely non-degenerate for all $n\in\mathbb{N}$ and $\mathbf{k}\in\mathbb{R}^D$.*

In $D=2$, the same conclusion holds if periodicity and homotopy are replaced by γ-periodicity and γ-homotopy, in the sense of Definition 3.1.

The periodic case for $D\le 2$ has already been treated in [4], [5] and [6], but we will sketch below the main ideas and give details on the new, γ-periodic situation.

We will need two technical results, which we state here.

Lemma A.5 (Analytic Approximation Lemma)**.** *Consider a uniformly continuous family of unitary matrices $\alpha(k)$ where $k\in[a,b]\subset\mathbb{R}$. Let I be any compact set completely included in $[a,b]$. Then one can* construct *a sequence $\{\alpha_n(k)\}_{k\in I}$, $n\in\mathbb{N}$, of families of unitary matrices which are* real analytic *on I and such that*

$$\sup_{k\in I}\|\alpha_n(k)-\alpha(k)\|\to 0 \quad \text{as } n\to\infty.$$

If α is continuous and $\mathbb{Z}$-periodic, the same is true for α_n and the approximation is uniform on $\mathbb{R}$. This last statement can be extended to any $D\ge 1$.

Proof (sketch). The proof proceeds in the same spirit of Lemma A.1 above. First, we take the convolution with a real analytic kernel and obtain a smooth matrix $\beta(k)$ which is close in norm to $\alpha(k)$. Thus $\gamma := \beta^*\beta$ must be close to the identity matrix, it is self-adjoint and real analytic, and the same holds true for $\gamma^{1/2}$. Finally, we restore unitarity by writing $\alpha' := \beta\gamma^{1/2}$ and checking that $(\alpha')^*\alpha' = \mathbf{1}$. More details can be found in [5, Lemma A.2]. □

Lemma A.6 (Local Splitting Lemma)**.** *For $R>0$ and $\mathbf{k}_0\in\mathbb{R}^D$, denote by $B_R(\mathbf{k}_0)$ the open ball of radius R around $\mathbf{k}_0$. Let $\{\alpha(\mathbf{k})\}_{\mathbf{k}\in B_R(\mathbf{k}_0)}$ be a continuous family of unitary matrices. Then, for some $R'\le R$, one can* construct *a sequence $\{\alpha_n(\mathbf{k})\}_{\mathbf{k}\in B_{R'}(\mathbf{k}_0)}$, $n\in\mathbb{N}$, of continuous families of unitary matrices such that*

- $\sup_{\mathbf{k}\in B_R(\mathbf{k}_0)}\|\alpha_n(\mathbf{k})-\alpha(\mathbf{k})\|\to 0$ *as $n\to\infty$, and*
- *the spectrum of $\alpha_n(\mathbf{k})$ is completely non-degenerate for all $\mathbf{k}\in B_{R'}(\mathbf{k}_0)$.*

The proof of the above Lemma can be found in [5, Lemma A.1] for $D=1$ and in [6, Lemma 5.1] for $D=2$.

Proof of Proposition A.4. The main idea is to lift all the spectral degeneracies of α within the unit interval $[0,1]$ or the unit square $[0,1]\times[0,1]$, and then extend the approximants with non-degenerate spectrum to the whole $\mathbb{R}^D$ by either periodicity or γ-periodicity.

We start with $D=1$. By the Analytic Approximation Lemma we can find an approximant $\alpha^{(1)}$ of α which depends analytically on k. If $\alpha^{(1)}$ has degenerate eigenvalues, then they either cross at isolated points (a finite number of them in the compact interval $[0,1]$) or they stay degenerate for all $k\in[0,1]$. Pick a point in $[0,1]$ which is not an isolated degenerate point. Applying the Local Splitting Lemma, find a continuous approximant $\alpha^{(2)}$ of $\alpha^{(1)}$ for which the second option is ruled out, so that its eigenvalues cannot be constantly degenerate.

Let now $\alpha^{(3)}$ be an analytic approximation of $\alpha^{(2)}$, obtained by means of the Analytic Approximation Lemma. The eigenvalues of $\alpha^{(3)}$ can only be degenerate at a finite number of points $\{0<k_1<\cdots<k_S<1\}$ (we assume without loss of generality that no eigenvalue intersections occur at $k=0$: this can be achieved by means of small shift of the coordinate). By applying the Local Splitting Lemma to balls of radius $1/n$ around each such point (starting from a large enough n_0), and extending the definition of the approximants from $[0,1]$ to $\mathbb{R}$ by periodicity, we obtain the required continuous and periodic approximants α_n with completely non-degenerate spectrum. Notice that, under the assumption of null-homotopy of α, the rest of the argument of Theorem 2.2 applies: in particular, for n sufficiently large α_n admits a continuous and periodic logarithm, namely $\alpha_n(k)=\mathrm{e}^{\mathrm{i}\,h_n(k)}$.

Now we continue with $D=2$. We will only treat the γ-periodic setting, since the periodic case for $D\le 2$ has been already analyzed in [4], [5] and [6].

We start by considering the strip $[0,1]\times\mathbb{R}$. The matrix $\alpha(0,k_3)$ is periodic, hence we may find a smooth approximation $\alpha_0(k_3)$ which is always non-degenerate and periodic.

The matrix $\alpha(k_2,k_3)\alpha(0,k_3)^{-1}$ is close to the identity near $k_2=0$, and so is $\alpha(k_2,k_3)\alpha_0(k_3)^{-1}$. Hence if k_2 is close to 0 we can write (using the Cayley transform)

$$\alpha(k_2,k_3)=\mathrm{e}^{\mathrm{i}H_0(k_2,k_3)}\alpha_0(k_3)$$

where $H_0(k_2,k_3)$ is continuous, periodic in k_3, and uniformly close to zero. Due to the γ-periodicity of α, we have that $\alpha(1,k_3)$ and $\gamma(k_3)\alpha_0(k_3)\gamma(k_3)^{-1}$ are also close in norm. Reasoning in the same way as near $k_2=0$ we can write

$$\alpha(k_2,k_3)=\mathrm{e}^{\mathrm{i}H_1(k_2,k_3)}\gamma(k_3)\alpha_0(k_3)\gamma(k_3)^{-1}$$

where $H_1(k_2,k_3)$ is continuous, periodic in k_3, and uniformly close to zero near $k_2=1$.

Let $\delta<1/10$. Choose a smooth function $0\le g_\delta\le 1$ such that

$$g_\delta(k_2)=\begin{cases}1 & \text{if } k_2\in[0,\delta]\cup[1-\delta,1],\\ 0 & \text{if } 2\delta\le k_2\le 1-2\delta.\end{cases}$$

For $0\le k_2\le 1$ and $k_3\in\mathbb{R}$, define the matrix $\alpha_\delta(k_2,k_3)$ in the following way:

$$\alpha_\delta(k_2,k_3):=\begin{cases}\mathrm{e}^{\mathrm{i}(1-g_\delta(k_2))H_0(k_2,k_3)}\,\alpha_0(k_3) & \text{if } 0\le k_2\le 3\delta,\\ \alpha(k_2,k_3) & \text{if } 3\delta<k_2<1-3\delta,\\ \mathrm{e}^{\mathrm{i}(1-g_\delta(k_2))H_1(k_2,k_3)}\,\gamma(k_3)\,\alpha_0(k_3)\,\gamma(k_3)^{-1} & \text{if } 1-3\delta\le k_2\le 1.\end{cases}$$

We notice that α_δ is continuous, periodic in k_3 and converges in norm to α when δ goes to zero. Moreover,

$$\alpha_\delta(1,k_3)=\gamma(k_3)\,\alpha_\delta(0,k_3)\,\gamma(k_3)^{-1},$$

which is a crucial ingredient if we want to continuously extend it by γ-periodicity to $\mathbb{R}^2$.

We also note that $\alpha_\delta(k_2,k_3)$ is completely non-degenerate when k_2 is either 0 or 1, hence by continuity it must remain completely non-degenerate when $k_2\in[0,\epsilon]\cup[1-\epsilon,1]$ if ϵ is small enough.

Following [6], we will explain how to produce an approximation $\alpha'(k_2,k_3)$ of $\alpha_\delta(k_2,k_3)$ with the following properties:

- it coincides with $\alpha_\delta(k_2,k_3)$ if $k_2\in[0,\epsilon]\cup[1-\epsilon,1]$,
- it is continuous on $[0,1]\times\mathbb{R}$ and periodic in k_3,

- it is completely non-degenerate on the strip $[0,1]\times\mathbb{R}$.

Assuming for now that all this holds true, let us investigate the consequences. Because it coincides with α_δ near $k_2=0$ and $k_2=1$, we also have:

$$\alpha'(1,k_3)=\gamma(k_3)\alpha'(0,k_3)\gamma(k_3)^{-1}.$$

If $k_2>0$ we define recursively

$$\alpha'(k_2+1,k_3)=\gamma(k_3)\alpha'(k_2,k_3)\gamma(k_3)^{-1}$$

and if $k_2<0$

$$\alpha'(k_2,k_3)=\gamma(k_3)^{-1}\alpha'(k_2+1,k_3)\gamma(k_3).$$

Then α' has all the properties required in the statement, and the proof is complete.

Finally let us sketch the main ideas borrowed from [6] which are behind the proof of the three properties of α' listed above.

First, the construction of α' is based on continuously patching non-degenerate local logarithms, which is why the already non-degenerate region $k_2\in[0,\epsilon]\cup[1-\epsilon,1]$ is left unchanged.

Second, let us consider the finite segment defined by $k_2\in[\epsilon,1-\epsilon]$ and $k_3=0$. The family of matrices $\{\alpha_\delta(k_2,0)\}$ is 1-dimensional, with a spectrum which is completely non-degenerate near $k_2=\epsilon$ and $k_2=1-\epsilon$. Reasoning as in the case $D=1$ we can find a continuous approximation $\alpha_2(k_2)$ which is completely non-degenerate on the whole interval $k_2\in[\epsilon,1-\epsilon]$. The matrix $\alpha_\delta(k_2,k_3)\alpha_2(k_2)^{-1}$ is close to the identity matrix if $|k_3|\ll 1$, hence we may locally perturb α_δ near the segment $(\epsilon,1-\epsilon)\times\{0\}$ so that the new α'_δ is completely non-degenerate on a small tubular neighborhood of the boundary of the segment $(\epsilon,1-\epsilon)\times\{0\}$. This perturbation must be taken small enough not to destroy the initial non-degeneracy near $k_2=\epsilon$ and $k_2=1-\epsilon$.

Third, since α_δ is periodic in k_3, the local perturbation around the strip $(\epsilon,1-\epsilon)\times\{0\}$ can be repeated near all the strips $(\epsilon,1-\epsilon)\times\mathbb{Z}$. The new matrix, α''_δ, will be non-degenerate near a small tubular neighborhood of any unit square of the type $[0,1]\times[p,p+1]$, with $p\in\mathbb{Z}$. The final step is to locally perturb α''_δ inside these squares, like in [6, Prop. 5.11]. The splitting method relies in an essential way on the condition $D\le 2$, since it uses the fact that a smooth map between $\mathbb{R}^D$ and $\mathbb{R}^3$ cannot have regular values. □

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