Periodic Schrödinger operators on topological crystals: framework, analytically fibered operator, conjugate operator

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Abstract

In this conference proceeding's paper we recall several constructions related to periodic Schrödinger operators in the discrete setting. Our aim is to focus on periodic systems without being distracted by any perturbation. This material is mainly borrowed from a joint paper with D. Parra where perturbations of such periodic systems are also considered.

1 Introduction

There were two motivations for writing this review paper. Firstly, it corresponds to a paper version of a presentation made during the conference *Mathematical aspects of quantum fields and related topics* organized at Rims in Kyoto in July 2018. This paper will be published in the proceedings of this conference. The second motivation comes from discussions with Prof. K. Kurdyka which took place in September 2018. Indeed, after several unitary transformations and identifications, periodic Schrödinger operators lead naturally to a certain class of hyperbolic polynomials which have been extensively studied in [24]. For that reason, the present paper contains a thorough presentation of periodic Schrödinger operators on topological crystals, together with a detailed description of these transformations. Let us emphasize that only purely periodic systems are considered, with all perturbation arguments removed. We hope that such an uncluttered presentation will facilitate the access of this theory to a larger readership. On the other hand, note that more complete investigations on such models have been performed in [26] to which we refer for the more analytical part.

The study of Laplace operators on infinite graphs has recently attracted lots of attention. Let us mention for example the problem of essential self-adjointness for very general infinite graphs [12, 18], or the more precise study of the spectrum for bounded Laplacians [4, 25]. For periodic graphs it is well-known that this spectrum has a band structure with at most a finite number of eigenvalues of infinite multiplicity [14]. This structure is preserved if one considers periodic Schrödinger operators [20, 21, 22]. Perturbations of such systems have also been extensively considered, as for example in [3, 5, 7, 14, 16, 19] and more recently in [26].

As mentioned above, we do not consider perturbations of the purely periodic system. Consequently this paper does not contain any new result, but focus on a precise description of the framework and on the path to a new representation in terms of analytically fibered operators. In addition to this, we construct in the last section a conjugate operator for any analytically fibered matrix valued operator. Again this construction is not new and a similar construction already appeared in the seminal paper [11]. However, the version provided in the present paper is more detailed, and slightly simpler since the initial operator is bounded. Note that the interest for presenting this construction is twofold. On the one hand, a conjugate operator is an essential tool for investigating perturbed systems, as shown in [1, 7, 25, 26]. On the other hand, the construction provided is intimately linked to Rellich's theorem, a result which is also at the root of the investigations performed in [24]. A better understanding of the construction of the conjugate operator in the context of this paper would certainly be valuable.

2 Topological crystals and periodic Schrödinger operators

In this section we provide the definition of a topological crystal and define some related notions. An explicit and rather general construction of a topological crystal is introduced at the end of the section.

A graph $X = \big(V(X), E(X)\big)$ is composed of a set of vertices $V(X)$ and a set of unoriented edges $E(X)$. Graphs with loops and parallel edges are accepted. Generically we shall use the notation x, y for elements of $V(X)$, and e for elements of $E(X)$. If both $V(X)$ and $E(X)$ are finite sets, the graph X is said to be finite.

A morphism $\omega : X \to \mathfrak{X}$ between two graphs X and $\mathfrak{X}$ is composed of two maps $\omega : V(X) \to V(\mathfrak{X})$ and $\omega : E(X) \to E(\mathfrak{X})$ such that it preserves the adjacency relations between vertices and edges, namely if e is an edge in X between the vertices x and y, then $\omega(\mathrm{e})$ is an edge in $\mathfrak{X}$ between the vertices $\omega(x)$ and $\omega(y)$. Let us stress that we use the same notation for the two maps $\omega : V(X) \to V(\mathfrak{X})$ and $\omega : E(X) \to E(\mathfrak{X})$, and that this should not lead to any confusion. An isomorphism is a morphism that is a bijection on the vertices and on the edges. The group of isomorphisms of a graph X into itself is denoted by $\mathrm{Aut}(X)$. For a vertex $x \in V(X)$ we also set $E(X)_x := \{\mathrm{e} \in E(X) \mid x \in \mathrm{e}\}$. If $E(X)_x$ is finite for every $x \in V(X)$ we say that X is locally finite.

A morphism $\omega : X \to \mathfrak{X}$ between two graphs is said to be *a covering map* if

(i) $\omega : V(X) \to V(\mathfrak{X})$ is surjective,

(ii) for all $x \in V(X)$, the restriction $\omega|_{E(X)_x} : E(X)_x \to E(\mathfrak{X})_{\omega(x)}$ is a bijection.

In that case we say that X is a *covering graph* over the *base graph* $\mathfrak{X}$. For such a covering, we define the *transformation group* of the covering as the subgroup of $\mathrm{Aut}(X)$, denoted by Γ, such that for every $\mu \in \Gamma$ the equality $\omega \circ \mu = \omega$ holds. We now define a topological crystal, and refer to [30, Sec. 6.2] for more details.

Definition 2.1. *A d-dimensional topological crystal is a quadruplet* $(X, \mathfrak{X}, \omega, \Gamma)$ *such that:*

(i) X *and* $\mathfrak{X}$ *are graphs, with* $\mathfrak{X}$ *finite,*

(ii) $\omega : X \to \mathfrak{X}$ *is a covering map,*

(iii) The transformation group Γ of ω is isomorphic to $\mathbb{Z}^d$,

(iv) ω is regular, i.e. for every x, $y \in V(X)$ satisfying $\omega(x) = \omega(y)$ there exists $\mu \in \Gamma$ such that $x = \mu y$.

We usually say that X is a topological crystal if it admits a d-dimensional topological crystal structure $(X, \mathfrak{X}, \omega, \Gamma)$. Note that all topological crystal are locally finite, with an upper bound for the number of elements in $E(X)_x$ independent of x. Indeed, the local finiteness and the fixed upper bound follow from the definition of a covering and the finiteness of $\mathfrak{X}$. For shortness, we shall use the multiplicative notation for the group law in the abstract setting, but the additive notation for the group $\mathbb{Z}^d$.

Remark 2.2. *Topological crystals have been extensively studied in the monograph [30] to which we refer for many examples. Let us also mention [5] in which one can find* square, triangular, hexagonal*, and* diamond *periodic graphs. In reference [20]* body-centered cubic *and* face-centered cubic *periodic graphs have been studied, while* armchair graph *is presented in [6]. We also refer to the Remark 2.3 below for an explicit procedure generating an infinite number of topological crystals $(X, \mathfrak{X}, \omega, \Gamma)$ once a small graph $\mathfrak{X}$ has been chosen.*

For a while let us come back to an arbitrary graph X. From the set of unoriented edges $E(X)$ of the graph X we construct the set of oriented edges $A(X)$ by considering for every unoriented edge between x and y both oriented edges from x to y and from y to x. The elements of $A(X)$ are still denoted by e. The origin vertex of such an oriented edge e is denoted by $o(e)$, the terminal one by $t(e)$, and $\bar{e}$ denotes the edge obtained from e by interchanging the vertices, *i.e.* $o(\bar{e}) = t(e)$ and $t(\bar{e}) = o(e)$. For $x \in V(X)$ we set $A(X)_x \equiv A_x := \{e \in A(X) \mid o(e) = x\}$. Clearly, any morphism ω between a graph X and a graph $\mathfrak{X}$, and in particular any covering map, can be extended to a map sending oriented edges of $A(X)$ to oriented edges of $A(\mathfrak{X})$. For this extension we keep the convenient notation $\omega : A(X) \to A(\mathfrak{X})$.

A *measure* m on a graph X is a strictly positive function defined on vertices and on unoriented edges. On oriented edges, the measure satisfies $m(e) = m(\bar{e})$. From now on, let us assume that the graph X is locally finite. For such a graph the Laplace operator is defined on the space of 0-*cochains* $C^0(X) := \{f \mid V(X) \to \mathbb{C}\}$ by

$$[\Delta(X, m)f](x) := \sum_{e \in A_x} \frac{m(e)}{m(x)} \big(f\big(t(e)\big) - f(x)\big), \qquad \forall f \in C^0(X).$$

Furthermore, when

$$\deg_m : V(X) \to \mathbb{R}_+, \quad \deg_m(x) := \sum_{e \in A_x} \frac{m(e)}{m(x)} \tag{2.1}$$

is bounded, then the operator $\Delta(X, m)$ is a bounded self-adjoint operator in the Hilbert space

$$l^2(X, m) := \Big\{f \in C^0(X) \mid \|f\|^2 := \sum_{x \in V(X)} m(x)|f(x)|^2 < \infty\Big\}$$

endowed with the scalar product

$$\langle f, g \rangle := \sum_{x \in V(X)} m(x)f(x)\overline{g(x)} \qquad \forall f, g \in l^2(X, m).$$

We refer for example to [18, Thm. 2.4] for the statement about boundedness. Note also that we use the simple notation $l^2(X, m)$ for what could have been denoted by $l^2(V(X), m)$.

Let us now come back to the setting of a topological crystal $(X, \mathfrak{X}, \omega, \Gamma)$. We also consider a Γ-periodic measure m_0 and a Γ-periodic function $R_0 : V(X) \to \mathbb{R}$. The periodicity means that for every $\mu \in \Gamma$, $x \in V(X)$ and $e \in E(X)$ we have $m_0(\mu x) = m_0(x)$, $m_0(\mu e) = m_0(e)$ and $R_0(\mu x) = R_0(x)$. We can provide the definition of a *periodic Schrödinger operator*: it consists in the operator

$$H_0 := -\Delta(X, m_0) + R_0. \tag{2.2}$$

Note that we use the same notation for the function R_0 and for the corresponding multiplication operator. As a consequence of our assumptions, the expression H_0 defines a bounded self-adjoint operator in the Hilbert space $l^2(X, m_0)$.

In the paper [26] perturbations of the operators H_0 are considered, either by assuming that the measure m is only asymptotically periodic and/or by assuming that a function R is only asymptotically periodic. Perturbations theory has then to be used in order to study the corresponding operator

$$H := -\Delta(X, m) + R, \tag{2.3}$$

and for such investigations the theory of the conjugate operator plays an important role. Let us still mention that such investigations take place in a 2-Hilbert spaces setting, since the natural Hilbert space for H is $l^2(X, m)$. Various tools related to toroidal pseudo-differential operators have also to be borrowed from [28]. We do not continue in this direction in the present manuscript.

Let us now introduce a notion of norm on the set of vertices or edges. We consider again the topological crystal $(X, \mathfrak{X}, \omega, \Gamma)$. The notation x, resp. $\mathfrak{x}$, will be used for the elements of $V(X)$, resp. of $V(\mathfrak{X})$, and accordingly the notation e, resp. $\mathfrak{e}$, will be used for the elements of $E(X)$, resp. $E(\mathfrak{X})$. It follows from the assumption (iii) in Definition 2.1 that $\Gamma \backslash X \cong \mathfrak{X}$, and therefore we can identify $V(\mathfrak{X})$ as a subset of $V(X)$ by choosing a representative of each orbit. Namely, since $V(\mathfrak{X}) = \{\mathfrak{x}_1, \ldots, \mathfrak{x}_n\}$ for some $n \in \mathbb{N}$, we choose $\{x_1, \ldots, x_n\} \subset V(X)$ such that $\omega(x_j) = \mathfrak{x}_j$ for any $j \in \{1, \ldots, n\}$. For shortness we also use the notation $\check{x} := \omega(x) \in V(\mathfrak{X})$ for any $x \in V(X)$, and reciprocally for any $\mathfrak{x} \in \mathfrak{X}$ we write $\hat{\mathfrak{x}} \in \{x_1, \ldots, x_n\}$ for the unique element x_j in this set such that $\omega(x_j) = \mathfrak{x}$.

As a consequence of the previous identification we can also identify $A(\mathfrak{X})$ as a subset of $A(X)$. More precisely, we identify $A(\mathfrak{X})$ with $\cup_{j=1}^n A_{x_j} \subset A(X)$ and use notations similar to the previous ones: For any $e \in A(X)$ one sets $\check{e} := \omega(e) \in A(\mathfrak{X})$, and for any $\mathfrak{e} \in A(\mathfrak{X})$ one sets $\hat{\mathfrak{e}} \in \cup_{j=1}^n A_{x_j}$ for the unique element in $\cup_{j=1}^n A_{x_j}$ such that $\omega(\hat{\mathfrak{e}}) = \mathfrak{e}$. Let us stress that these identifications and notations depend only on the initial choice of $\{x_1, \ldots, x_n\} \subset V(X)$.

We have now enough notation for defining the *entire part* of a vertex x as the map $\lfloor \cdot \rfloor : V(X) \to \Gamma$ satisfying

$$\lfloor x \rfloor \widehat{\check{x}} = x . \tag{2.4}$$

Similarly, the entire part of an edge is defined as the map $\lfloor \cdot \rfloor : A(X) \to \Gamma$ satisfying

$$\lfloor e \rfloor \widehat{\check{e}} = e . \tag{2.5}$$

The existence of this function $\lfloor \cdot \rfloor$ follows from the assumption (iv) of Definition 2.1 on the regularity of a topological crystal. One easy consequence of the previous construction is that the equality $\lfloor e \rfloor = \lfloor o(e) \rfloor$ holds for any $e \in A(X)$.

For later use, let us finally define the map

$$\eta : A(X) \to \Gamma, \quad \eta(e) := \lfloor t(e) \rfloor \lfloor o(e) \rfloor^{-1}$$

and call $\eta(e)$ the *index* of the edge e. For any $\mu \in \Gamma$ we then infer that

$$\eta(\mu e) = \lfloor t(\mu e) \rfloor \lfloor o(\mu e) \rfloor^{-1} = \mu \lfloor t(e) \rfloor \mu^{-1} \lfloor o(e) \rfloor^{-1} = \eta(e).$$

This periodicity enables us to define unambiguously $\eta : A(\mathfrak{X}) \to \Gamma$ by the relation $\eta(\mathfrak{e}) := \eta(\hat{\mathfrak{e}})$ for every $\mathfrak{e} \in A(\mathfrak{X})$. Again, this index on $A(\mathfrak{X})$ depends only on the initial choice $\{x_1, \ldots, x_n\} \subset V(X)$ and could not be defined by considering only $A(\mathfrak{X})$.

Before moving to the next section, we provide an explicit construction of a topological crystal, starting from a given $\mathfrak{X}$.

Remark 2.3. *In this remark we provide a procedure for constructing a topological crystal $(X, \mathfrak{X}, \omega, \Gamma)$ for any given graph $\mathfrak{X}$ and almost every index function η. The construction of X mimics the construction of the universal covering of a graph provided in [30, Chp. 5]. Let $\mathfrak{X}$ be a given finite graph, and let us choose any spanning tree $\mathfrak{T}$ in $\mathfrak{X}$. The number of edges in $\mathfrak{X}\backslash\mathfrak{T}$ corresponds to the Betti number $B(\mathfrak{X})$ of $\mathfrak{X}$. Then, let us choose any integer $d \leq B(\mathfrak{X})$, which will lead to a transformation group Γ equal to $\mathbb{Z}^d$. For any edge $\mathfrak{e} \in \mathfrak{X}\backslash\mathfrak{T}$ let us associate an element $\eta(\mathfrak{e}) \in \mathbb{Z}^d$ with the single condition that the set $\{\eta(\mathfrak{e})\}_{\mathfrak{e} \in \mathfrak{X}\backslash\mathfrak{T}}$ generates $\mathbb{Z}^d$. For such an edge $\mathfrak{e} \in \mathfrak{X}\backslash\mathfrak{T}$, we also fix an orientation to $\mathfrak{e}$ by choosing $o(\mathfrak{e})$ and $t(\mathfrak{e})$. We are now ready for the construction of X: i) For any $\mu \in \mathbb{Z}^d$ we consider a copy of $\mathfrak{T}$ and denote it by $\mathfrak{T}_\mu$. ii) For any $\mathfrak{e} \in \mathfrak{X}\backslash\mathfrak{T}$ and for any $\mu \in \mathbb{Z}^d$ we set an edge between the vertex corresponding to $o(\mathfrak{e})$ in $\mathfrak{T}_\mu$ and the vertex corresponding to $t(\mathfrak{e})$ in $\mathfrak{T}_{\mu\eta(\mathfrak{e})}$. iii) We define the set $V(X)$ by collecting all vertices of $\{\mathfrak{T}_\mu\}_{\mu \in \mathbb{Z}^d}$ and for $E(X)$ all edges of $\{\mathfrak{T}_\mu\}_{\mu \in \mathbb{Z}^d}$ together with the additional edges constructed in ii). With an obvious definition for the map ω we finally observe that $(X, \mathfrak{X}, \omega, \mathbb{Z}^d)$ is a d-dimensional topological crystal. In addition, if we fix n distinct vertices $\{x_1, \ldots, x_n\}$ of $\mathfrak{T}_0$ with $0 \in \mathbb{Z}^d$ and n the cardinality of $V(\mathfrak{X})$, then any $x \in V(X)$ with $x \in \mathfrak{T}_\mu$ will satisfy $\lfloor x \rfloor = \mu$ and any $e \in A(X)$ will satisfy either $\lfloor e \rfloor = 0$ or $\lfloor e \rfloor = \pm\eta(\mathfrak{e})$ for one $\mathfrak{e}$ in our initial set $\mathfrak{X}\backslash\mathfrak{T}$.*

3   A bounded analytically fibered operator

The aim of this section is to construct another representation of the operator H_0, more suitable for further investigations. For that purpose we first introduce the dual group of Γ, denoted by $\hat{\Gamma}$. It consists of group homomorphisms from Γ to the multiplicative group $\mathbb{T} \subset \mathbb{C}$ endowed with pointwise multiplication. Since Γ is discrete, $\hat{\Gamma}$ is a compact Abelian group and comes with a normalized Haar measure $d\xi$ of volume 1 [9, Proposition 4.24]. We can then define the Fourier transform $\mathscr{F} : l^1(\Gamma) \to C(\hat{\Gamma})$ by

$$[\mathscr{F}f](\xi) \equiv \hat{f}(\xi) := \sum_{\mu \in \Gamma} \overline{\xi(\mu)} f(\mu) \tag{3.1}$$

and it is well-known that this extends to a unitary map from $l^2(\Gamma)$ to $L^2(\hat{\Gamma})$ which is still denoted by $\mathscr{F}$. The adjoint map $\mathscr{F}^* : L^2(\hat{\Gamma}) \to l^2(\Gamma)$ is defined on elements in $L^1(\hat{\Gamma})$ by the

formula $[\mathscr{F}^*u](\mu) = \int_{\hat{\Gamma}} \mathrm{d}\xi\, \xi(\mu)u(\xi)$. Furthermore, by the Fourier inversion formula for any $f \in l^1(\Gamma)$ one has [9, Theorem 4.21]:

$$f(\mu) = \int_{\hat{\Gamma}} \mathrm{d}\xi\, \xi(\mu)\hat{f}(\xi),$$

or equivalently for any $u \in L^1(\hat{\Gamma})$ such that $\mathscr{F}^*u \in l^1(\Gamma)$

$$u(\xi) = \sum_{\mu \in \Gamma} \overline{\xi(\mu)}[\mathscr{F}^*u](\mu).$$

Let us now provide a direct integral decomposition. The framework is the following: a topological crystal $(X, \mathfrak{X}, \omega, \Gamma)$ and a Γ-periodic measure m_0 on X. Because of its periodicity, this measure is also well-defined on $\mathfrak{X}$ by the relation $m_0(\mathfrak{x}) := m_0(\hat{\mathfrak{x}})$ and $m_0(\mathfrak{e}) := m_0(\hat{\mathfrak{e}})$. For simplicity, we keep the same notation for this measure on $\mathfrak{X}$. Let us consider the Hilbert spaces $l^2(X, m_0)$ and $L^2(\hat{\Gamma}; l^2(\mathfrak{X}, m_0))$, and use the shorter notation $l^2(X)$ and $L^2(\hat{\Gamma}; l^2(\mathfrak{X}))$. We also denote by $c_c(X) \subset l^2(X)$ the space of 0-cochains of finite support. We then define the map $\mathscr{U} : c_c(X) \to L^2(\hat{\Gamma}; l^2(\mathfrak{X}))$ for $f \in c_c(X)$, $\xi \in \hat{\Gamma}$, and $\mathfrak{x} \in V(\mathfrak{X})$ by

$$[\mathscr{U}f](\xi, \mathfrak{x}) := \sum_{\mu \in \Gamma} \overline{\xi(\mu)} f(\mu\hat{\mathfrak{x}}). \tag{3.2}$$

Clearly, the map $\mathscr{U}$ corresponds the composition of two maps: the identification of $l^2(X)$ with $l^2(\Gamma; l^2(\mathfrak{X}))$ and the Fourier transform introduced in (3.1). As a consequence, $\mathscr{U}$ extends to a unitary map from $l^2(X)$ to $L^2(\hat{\Gamma}; l^2(\mathfrak{X}))$, and we shall keep the same notation for this continuous extension. The formula for its adjoint is then given on any $u \in L^1(\hat{\Gamma}; l^2(\mathfrak{X}))$ by

$$[\mathscr{U}^*u](x) = \int_{\hat{\Gamma}} \mathrm{d}\xi\, \xi(\lfloor x \rfloor)u(\xi, \check{x}).$$

Lemma 3.1 (Lemma 3.2 of [26]). *Let $(X, \mathfrak{X}, \omega, \Gamma)$ be a topological crystal and let m_0 be a Γ-periodic measure on X. Then for any $u \in L^2(\hat{\Gamma}; l^2(\mathfrak{X}))$, every $\mathfrak{x} \in V(\mathfrak{X})$ and almost every $\xi \in \hat{\Gamma}$ the following equality holds:*

$$[\mathscr{U}\Delta(X, m_0)\mathscr{U}^*u](\xi, \mathfrak{x}) = \sum_{\mathfrak{e} \in A_{\mathfrak{x}}} \frac{m_0(\mathfrak{e})}{m_0(\mathfrak{x})}\Big[\xi\big(\eta(\mathfrak{e})\big)u\big(\xi, t(\mathfrak{e})\big) - u(\xi, \mathfrak{x})\Big].$$

Let us now make a connection with the so-called magnetic Laplacians. We recall that for any $\theta : A(\mathfrak{X}) \to \mathbb{T}$ satisfying $\theta(\overline{\mathfrak{e}}) = \overline{\theta(\mathfrak{e})}$ one defines a magnetic Laplace operator on $\mathfrak{X}$ by the formula

$$[\Delta_\theta(\mathfrak{X}, m_0)\varphi](\mathfrak{x}) := \sum_{\mathfrak{e} \in A_{\mathfrak{x}}} \frac{m_0(\mathfrak{e})}{m_0(\mathfrak{x})}\big(\theta(\mathfrak{e})\varphi(t(\mathfrak{e})) - \varphi(\mathfrak{x})\big) \qquad \forall \varphi \in l^2(\mathfrak{X}).$$

Thus, if for fixed $\xi \in \hat{\Gamma}$ one sets

$$\theta_\xi : A(\mathfrak{X}) \to \mathbb{T}, \quad \theta_\xi(\mathfrak{e}) := \xi\big(\eta(\mathfrak{e})\big), \tag{3.3}$$

then one infers that

$$\theta_\xi(\overline{\mathfrak{e}}) = \xi\big(\eta(\overline{\mathfrak{e}})\big) = \xi\big(\eta(\mathfrak{e})^{-1}\big) = \overline{\xi\big(\eta(\mathfrak{e})\big)} = \overline{\theta_\xi(\mathfrak{e})}.$$

As a consequence, the operator $\Delta_{\theta_\xi}(\mathfrak{X}, m_0)$ defined on any $\varphi \in l^2(\mathfrak{X})$ by

$$[\Delta_{\theta_\xi}(\mathfrak{X}, m_0)\varphi](\mathfrak{r}) := \sum_{\mathfrak{e} \in A_\mathfrak{r}} \frac{m_0(\mathfrak{e})}{m_0(\mathfrak{r})}\big(\theta_\xi(\mathfrak{e})\varphi(t(\mathfrak{e})) - \varphi(\mathfrak{r})\big)$$

$$= \sum_{\mathfrak{e} \in A_\mathfrak{r}} \frac{m_0(\mathfrak{e})}{m_0(\mathfrak{r})}\big(\xi\big(\eta(\mathfrak{e})\big)\varphi(t(\mathfrak{e})) - \varphi(\mathfrak{r})\big)$$

corresponds to a magnetic Laplace operator on $\mathfrak{X}$.

Let us now recall that $L^2\big(\hat{\Gamma}; l^2(\mathfrak{X})\big) = \int_{\hat{\Gamma}}^\oplus \mathrm{d}\xi\, l^2(\mathfrak{X})$. As a consequence of the previous lemma and of the construction made above, the operator $\mathscr{U}\Delta(X, m_0)\mathscr{U}^*$ itself can be identified with the direct integral operator $\int_{\hat{\Gamma}}^\oplus \mathrm{d}\xi\, \Delta_{\theta_\xi}(\mathfrak{X}, m_0)$. In other words, the Laplace operator $\Delta(X, m_0)$ is unitarily equivalent to a direct integral of magnetic Laplace operators acting on $\mathfrak{X}$.

It only remains to deal with the multiplication operator R_0 by a Γ-periodic function, as introduced in (2.2). For that purpose, let us observe that for any real Γ-periodic function defined on $V(X)$ one can associate a well-defined function on $V(\mathfrak{X})$ by the relation $R_0(\mathfrak{r}) := R_0(\hat{\mathfrak{r}})$. For simplicity (and as already done before) we keep the same notation for this new function. Then the following statement is obtained by a direct computation.

Lemma 3.2. *Let R_0 be a Γ-periodic function on $V(X)$. Then one has $\mathscr{U}R_0\mathscr{U}^* = R_0$, or more precisely for any $u \in L^2\big(\hat{\Gamma}; l^2(\mathfrak{X})\big)$, for all $\mathfrak{r} \in \mathfrak{X}$ and a.e. $\xi \in \hat{\Gamma}$ the following equality holds:*

$$[\mathscr{U}R_0\mathscr{U}^*u](\xi, \mathfrak{r}) = R_0(\mathfrak{r})u(\xi, \mathfrak{r}).$$

By adding the various results obtained in this section one can finally state:

Proposition 3.3. *Let $(X, \mathfrak{X}, \omega, \Gamma)$ be a topological crystal and let m_0 be a Γ-periodic measure on X. Let R_0 be a real Γ-periodic function defined on $V(X)$. Then the periodic Schrödinger operator $H_0 := -\Delta(X, m_0) + R_0$ is unitarily equivalent to the direct integral of magnetic Schrödinger operators acting on $\mathfrak{X}$ defined by*

$$\int_{\hat{\Gamma}}^\oplus \mathrm{d}\xi\, \big[-\Delta_{\theta_\xi}(\mathfrak{X}, m_0) + R_0\big]$$

with θ_ξ defined in (3.3).

We shall now show that H_0 is unitarily equivalent to an *analytically fibered operator*. We refer to [11] and [27, Sec. XIII.16] for more general information on such operators, and restrict ourselves to the simplest framework. In that respect, the next definition is adapted to our setting. Note that from now on we shall use the notation $\mathbb{T}^d$ for the d-dimensional (flat) torus, *i.e.* for $\mathbb{T}^d = \mathbb{R}^d/\mathbb{Z}^d$, with the inherited local coordinates system and differential structure. We shall also use the notation $M_n(\mathbb{C})$ for the $n \times n$ matrices over $\mathbb{C}$.

Definition 3.4. *In the Hilbert space $L^2(\mathbb{T}^d; \mathbb{C}^n)$, a bounded analytically fibered operator corresponds to a multiplication operator defined by a real analytic map $h : \mathbb{T}^d \to M_n(\mathbb{C})$.*

In order to show that the periodic operator introduced above fits into this framework, some identifications are necessary. More precisely, since Γ is isomorphic to $\mathbb{Z}^d$, as stated in the point (iii) of Definition 2.1, we know that $\hat{\Gamma}$ is isomorphic to $\mathbb{T}^d$. In fact, we consider that a

basis of Γ is chosen and then identify Γ with $\mathbb{Z}^d$, and accordingly $\hat{\Gamma}$ with $\mathbb{T}^d$. As a consequence of these identifications we shall write $\xi(\mu) = e^{2\pi i \xi \cdot \mu}$, where $\xi \cdot \mu = \sum_{j=1}^d \xi_j \mu_j$. Accordingly, the Fourier transform defined in (3.1) corresponds to $[\mathscr{F}f](\xi) \equiv \hat{f}(\xi) = \sum_{\mu \in \mathbb{Z}^d} e^{-2\pi i \xi \cdot \mu} f(\mu)$, and its inverse to $[\mathscr{F}^* u](\mu) \equiv \check{u}(\mu) = \int_{\mathbb{T}^d} d\xi\, e^{2\pi i \xi \cdot \mu} u(\xi)$, with $d\xi$ the usual measure on $\mathbb{T}^d$. Note that an other consequence of this identification is the use of the additive notation for the composition of two elements of $\mathbb{Z}^d$, instead of the multiplicative notation employed until now for the composition in Γ.

The second necessary identification is between $l^2(\mathfrak{X})$ and $\mathbb{C}^n$. Indeed, since $V(\mathfrak{X}) = \{\mathfrak{x}_1, \ldots, \mathfrak{x}_n\}$, as already mentioned in the previous section, the vector space $l^2(\mathfrak{X})$ is of dimension n. However, since the scalar product in $l^2(\mathfrak{X})$ is defined with the measure m_0 while $\mathbb{C}^n$ is endowed with the standard scalar product, one more unitary transformation has to be defined. More precisely, for any $\varphi \in l^2(\mathfrak{X})$ one sets $\mathscr{I} : l^2(\mathfrak{X}) \to \mathbb{C}^n$ with

$$\mathscr{I}\varphi := \big(m_0(\mathfrak{x}_1)^{\frac{1}{2}}\varphi(\mathfrak{x}_1), m_0(\mathfrak{x}_2)^{\frac{1}{2}}\varphi(\mathfrak{x}_2), \ldots, m_0(\mathfrak{x}_n)^{\frac{1}{2}}\varphi(\mathfrak{x}_n)\big). \tag{3.4}$$

This map defines clearly a unitary transformation between $l^2(\mathfrak{X})$ and $\mathbb{C}^n$. Note that we shall use the same notation $\mathscr{I}$ for the map $L^2\big(\mathbb{T}^d; l^2(\mathfrak{X})\big) \to L^2\big(\mathbb{T}^d; \mathbb{C}^n\big)$ acting trivially on the first variables and acting as above on the remaining variables.

We can now state and prove the main result of this section, where we use the usual notation $\delta_{j\ell}$ for the Kronecker delta function.

Proposition 3.5. *Let $(X, \mathfrak{X}, \omega, \Gamma)$ be a topological crystal and let m_0 be a Γ-periodic measure on X. Let R_0 be a real Γ-periodic function defined on $V(X)$. Then the periodic Schrödinger operator $H_0 := -\Delta(X, m_0) + R_0$ is unitarily equivalent to the bounded analytically fibered operator in $L^2(\mathbb{T}^d; \mathbb{C}^n)$ defined by the function $h_0 : \mathbb{T}^d \to M_n(\mathbb{C})$ with*

$$h_0(\xi)_{j\ell} := -\sum_{\mathfrak{e} = (\mathfrak{x}_j, \mathfrak{x}_\ell)} \frac{m_0(\mathfrak{e})}{m_0(\mathfrak{x}_j)^{\frac{1}{2}} m_0(\mathfrak{x}_\ell)^{\frac{1}{2}}} e^{2\pi i \xi \cdot \eta(\mathfrak{e})} + \big(\deg_{m_0}(\mathfrak{x}_j) + R_0(\mathfrak{x}_j)\big)\delta_{j\ell} \tag{3.5}$$

for any $\xi \in \mathbb{T}^d$ and $j, \ell \in \{1, \ldots, n\}$.

Proof. The proof consists simply in computing the operator $\mathscr{I}\,\mathscr{U} H_0 \mathscr{U}^* \mathscr{I}^*$, and in checking that the resulting operator is analytically fibered. Observe first that the product $\mathscr{U} H_0 \mathscr{U}^*$ has already been computed in Proposition 3.3. The conjugation with $\mathscr{I}$ is easily computed, and one directly obtains (3.5) if one takes the equality $\xi(\mu) = e^{2\pi i \xi \cdot \mu}$ into account. Since for each fixed $\mu \in \mathbb{Z}^d$ the map $\mathbb{T}^d \ni \xi \mapsto e^{2\pi i \xi \cdot \mu} \to \mathbb{C}$ is real analytic, the matrix-valued function defined by h_0 is real analytic. $\qquad\square$

4 Mourre theory and the conjugate operator

In this section we first recall some definitions related to Mourre theory, such as some regularity conditions as well as the meaning of a Mourre estimate. These notions will be used in the second part of the section where a conjugate operator for H_0 will be constructed. Clearly, any reader familiar with the conjugate operator method can skip Section 4.1 and directly start with Section 4.2.

4.1 Mourre theory

In this section we recall the version of Mourre theory suitable for bounded operators, and refer to [2, Sec. 7.2] for more information and details.

Let us consider a Hilbert space $\mathcal{H}$ with scalar product $\langle\,\cdot\,,\,\cdot\,\rangle$ and norm $\|\,\cdot\,\|$. Let also S and A be two self-adjoint operators in $\mathcal{H}$. The operator S is assumed to be bounded, and we write $\mathcal{D}(A)$ for the domain of A. The spectrum of S is denoted by $\sigma(S)$ and its spectral measure by $E_S(\cdot)$. For shortness, we also use the notation $E_S(\lambda;\varepsilon) := E_S\big((\lambda-\varepsilon,\lambda+\varepsilon)\big)$ for all $\lambda \in \mathbb{R}$ and $\varepsilon > 0$.

The operator S belongs to $C^1(A)$ if the map

$$\mathbb{R} \ni t \mapsto e^{-itA}Se^{itA} \in \mathcal{B}(\mathcal{H}) \tag{4.1}$$

is strongly of class C^1 in $\mathcal{H}$. Equivalently, $S \in C^1(A)$ if the quadratic form

$$\mathcal{D}(A) \ni \varphi \mapsto \langle iA\varphi, S^*\varphi\rangle - \langle iS\varphi, A\varphi\rangle \in \mathbb{C}$$

is continuous in the topology of $\mathcal{H}$. In such a case, this form extends uniquely to a continuous form on $\mathcal{H}$, and the corresponding bounded self-adjoint operator is denoted by $[iS, A]$. This $C^1(A)$-regularity of S with respect to A is the basic ingredient for any investigation in Mourre theory.

Let us also define some stronger regularity conditions. First of all, $S \in C^2(A)$ if the map (4.1) is strongly of class C^2 in $\mathcal{H}$. A weaker condition can be expressed as follows: $S \in C^{1,1}(A)$ if

$$\int_0^1 \frac{\mathrm{d}t}{t^2}\big\|e^{-itA}Se^{itA} + e^{itA}Se^{-itA} - 2S\big\| < \infty.$$

It is then well-known that the following inclusions hold: $C^2(A) \subset C^{1,1}(A) \subset C^1(A)$.

For any $S \in C^1(A)$, let us now introduce two subsets of $\mathbb{R}$ which will play a central role. Namely, one sets

$$\mu^A(S) := \big\{\lambda \in \mathbb{R} \mid \exists \varepsilon > 0, a > 0 \text{ s.t. } E_S(\lambda;\varepsilon)[iS, A]E_S(\lambda;\varepsilon) \geq aE_S(\lambda;\varepsilon)\big\}$$

as well as the larger subset of $\mathbb{R}$ defined by

$$\tilde{\mu}^A(S) := \big\{\lambda \in \mathbb{R} \mid \exists \varepsilon > 0, a > 0, K \in \mathcal{K}(\mathcal{H}) \text{ s.t.}$$
$$E_S(\lambda;\varepsilon)[iS, A]E_S(\lambda;\varepsilon) \geq aE_S(\lambda;\varepsilon) + K\big\}.$$

In order to state one of the main results in Mourre theory, let us still set $\mathfrak{K} := \big(\mathcal{D}(A), \mathcal{H}\big)_{\frac{1}{2},1}$ for the Banach space obtained by real interpolation. We refer to [2, Sec. 3.4] for more information about this space and for a general presentation of Besov spaces associated with the pair $\big(\mathcal{D}(A), \mathcal{H}\big)$. Since $\mathcal{B}(\mathcal{H}) \subset \mathcal{B}(\mathfrak{K}, \mathfrak{K}^*)$, for any $z \in \mathbb{C}\setminus\mathbb{R}$ the resolvent $(S-z)^{-1}$ of S belongs to these spaces, and the following extension holds:

Theorem 4.1 ([2, Theorem 7.3.1])**.** *Let S be a self-adjoint element of $\mathcal{B}(\mathcal{H})$ and assume that $S \in C^{1,1}(A)$. Then the holomorphic function $\mathbb{C}_\pm \ni z \to (S-z)^{-1} \in \mathcal{B}(\mathfrak{K}, \mathfrak{K}^*)$ extends to a weak* continuous function on $\mathbb{C}_\pm \cup \mu^A(S)$.*

Let us still mention how a perturbative scheme can be developed. Consider a "perturbation" $V \in \mathcal{K}(\mathcal{H})$ and assume that V is self-adjoint and belongs to $C^{1,1}(A)$ as well. Even if $\mu^A(S)$ is known, it usually quite difficult to compute the corresponding set $\mu^A(S + V)$ for the self-adjoint operator $S + V$. However, the set $\tilde{\mu}^A(S)$ is much more stable since $\tilde{\mu}^A(S) = \tilde{\mu}^A(S + V)$, as a direct consequence of [2, Thm. 7.2.9].

Based on this observation, the following adaptation of [2, Thm. 7.4.2] can be stated in our context:

Theorem 4.2. *Let S be a self-adjoint element of $\mathcal{B}(\mathcal{H})$ and assume that $S \in C^{1,1}(A)$. Let $V \in \mathcal{K}(\mathcal{H})$ and assume that V is self-adjoint and belongs to $C^{1,1}(A)$. Then, for any closed interval $I \subset \tilde{\mu}^A(S)$ the operator $S + V$ has at most a finite number of eigenvalues in I, and no singular continuous spectrum in I.*

Note that such a result plays an essential role when perturbations of the periodic systems are considered. In particular, the previous result is at the root of the results obtained in [26] for the operator H mentioned in (2.3).

4.2 The conjugate operator

In this section, we construct a conjugate operator for a self-adjoint bounded analytically fibered operator h in $L^2(\mathbb{T}^d; \mathbb{C}^n)$. At the end of the day, the operator h will be the operator h_0 introduced in Proposition 3.5, but we prefer to provide an abstract construction. Note that the following content is inspired from an analog construction of [11]. However, our setting is slightly simpler, and in addition we provide here much more details.

Let us recall that a self-adjoint bounded analytically fibered operator corresponds to a multiplication operator by a real analytic function $h : \mathbb{T}^d \to M_n(\mathbb{C})$ with $h(\xi)$ Hermitian for any $\xi \in \mathbb{T}^d$. For consistency, the multiplication operator will also be denoted by h. For such an operator we introduce some notation. For any Borel set $\mathcal{V} \subset \mathbb{R}$ and any $\xi \in \mathbb{T}^d$, let us denote by $\pi_{\mathcal{V}}(\xi)$ the spectral projection $E_{h(\xi)}(\mathcal{V})$, *i.e.* the projection in $\mathbb{C}^n$ onto the vector space generated by eigenvectors associated with the eigenvalues of $h(\xi)$ that lie in $\mathcal{V}$. We also recall that $\sigma\big(h(\xi)\big)$ denotes the set of eigenvalues of $h(\xi)$. Furthermore, we set:

- $\Sigma := \big\{ (\lambda, \xi) \in \mathbb{R} \times \mathbb{T}^d, \lambda \in \sigma\big(h(\xi)\big) \big\}$,

- $\mathrm{mul} : \mathbb{R} \times \mathbb{T}^d \to \mathbb{N}$ defined by $(\lambda, \xi) \to \dim \pi_{\{\lambda\}}(\xi)\mathbb{C}^n$,

- $\Sigma_j := \{ (\lambda, \xi) \in \mathbb{R} \times \mathbb{T}^d, \mathrm{mul}(\lambda, \xi) = j \}$ for any $j \in \{0, 1 \ldots, n\}$.

The set Σ is called the *Bloch variety* (or the set of energy-momentum) of h and will be the central object of this section. We also denote by $p_{\mathbb{R}} : \Sigma \to \mathbb{R}$ and $p_{\mathbb{T}^d} : \Sigma \to \mathbb{T}^d$ the projection on each coordinate of Σ. Some properties of h and the above related objects are gathered in the next lemma. We also refer to [11, Lemma 3.4] for a similar statement in a more general setting.

Lemma 4.3. *The application $\mathrm{mul} : \mathbb{R} \times \mathbb{T}^d \to \mathbb{N}$ is upper semicontinuous. Furthermore, for all $(\lambda_0, \xi_0) \in \mathbb{R} \times \mathbb{T}^d$, there exist an interval $I_0 \in \mathcal{V}_{\mathbb{R}}(\lambda_0)$ and $\mathfrak{T}_0 \in \mathcal{V}_{\mathbb{T}^d}(\xi_0)$ such that:*

(i) $\pi_{I_0}(\xi_0) = \pi_{\{\lambda_0\}}(\xi_0)$,

(ii) The map $\xi \to \pi_{I_0}(\xi) \in M_n(\mathbb{C})$ is real analytic in $\mathfrak{T}_0$.

Before providing the proof we want to stress that the theory of hyperbolic polynomials allows us to show that the eigenvalues behave well on ξ, and this will be used to choose some convenient neighborhoods. More precisely, for h as above, the eigenvalues of $h(\xi)$ are given by the roots of $\delta(\lambda, \xi) := \det\left(\lambda\mathbb{I}_n - h(\xi)\right)$. Since each entry of the matrix $h(\xi)$ is real analytic as function of ξ, $\delta(\lambda, \xi)$ can be written as follows:

$$\delta(\lambda, \xi) = \det\left(\lambda\mathbb{I}_n - h(\xi)\right) = \lambda^n + \sum_{j=1}^n a_{n-j}(\xi)\lambda^{n-j} \tag{4.2}$$

where each function a_{n-j} is real analytic because it is the product of finitely many real analytic functions. Let us denote by $\{\lambda_1(\xi), \ldots, \lambda_n(\xi)\}$ the family of eigenvalues of $h(\xi)$ that correspond to the roots of (4.2). Then, it can be shown that the map $\xi \to \left(\lambda_1(\xi), \ldots, \lambda_n(\xi)\right) \in \mathbb{R}^n$ is locally Lipschitz [24, Theorem 4.1].

Proof of Lemma 4.3. Let us fix $(\lambda_0, \xi_0) \in \mathbb{R} \times \mathbb{T}^d$. It is clear that if λ_0 is not an eigenvalue of $h(\xi_0)$, then both conditions hold trivially since we can find I_0 and $\mathfrak{T}_0$ such that $I_0 \cap \sigma\left(h(\xi)\right) = \emptyset$ for every $\xi \in \mathfrak{T}_0$.

Suppose now that λ_0 is an eigenvalue of $h(\xi_0)$. We choose I_0 such that its closure contains no other eigenvalue of $h(\xi_0)$, which implies in particular that $\pi_{\{\lambda_0\}}(\xi_0) = \pi_{I_0}(\xi_0)$. In fact, by choosing an interval $I_0 = (a_0, b_0)$ small enough, we can also choose a neighborhood $\mathfrak{T}_0$ of ξ_0 such that for any $\xi \in \mathfrak{T}_0$ we have $\sigma\left(h(\xi)\right) \cap \{a_0, b_0\} = \emptyset$. Around I_0 we choose a positively oriented closed curve Γ_0 in $\mathbb{C}$, sufficiently close to I_0 such that it does not intersect the spectrum of $h(\xi)$ for every $\xi \in \mathfrak{T}_0$. Hence, for every $\xi \in \mathfrak{T}_0$, the eigenvalues of $h(\xi)$ that lay inside Γ_0 correspond to λ_0, or more precisely if $\lambda_j(\xi)$ lies inside Γ_0 we have $\lambda_j(\xi_0) = \lambda_0$.

As a consequence of this construction it follows that

$$\pi_{I_0}(\xi) = \frac{1}{2\pi i} \oint_{\Gamma_0} \mathrm{d}z \left(z - h(\xi)\right)^{-1}. \tag{4.3}$$

Finally, since $(z, \xi) \to \left(z - h(\xi)\right)^{-1}$ is analytic in the two variables on any domain in which z is not equal to any eigenvalues of $h(\xi)$, as shown for example in [17, Thm II.1.5], we infer from (4.3) that the map $\xi \to \pi_{I_0}(\xi)$ is real analytic.

We now recall that a real valued function defined on a topological space $\mathcal{X}$ is said to be upper semicontinuous at x_0 if for every $\epsilon > 0$ there exists $\mathcal{U} \in \mathcal{V}_{\mathcal{X}}(x_0)$ such that $\sup_{x \in \mathcal{U}} f(x) \leq f(x_0) + \epsilon$. If we pick $I_0 \times \mathfrak{T}_0$ as neighborhood of (λ_0, ξ_0) we have for $(\lambda, \xi) \in I_0 \times \mathfrak{T}_0$ that

$$\mathrm{mul}(\lambda, \xi) = \dim \pi_{\{\lambda\}}(\xi)\mathbb{C}^n \leq \dim \pi_{I_0}(\xi)\mathbb{C}^n = \dim \pi_{I_0}(\xi_0)\mathbb{C}^n = \dim \pi_{\{\lambda_0\}}(\xi_0)\mathbb{C}^n, \tag{4.4}$$

where $\dim \pi_{I_0}(\xi)\mathbb{C}^n = \dim \pi_{I_0}(\xi_0)\mathbb{C}^n$ is due to the analyticity of the map $\xi \to \pi_{I_0}(\xi)$. $\qquad\square$

The first step towards the construction of the conjugate operator is to provide a stratification of the Bloch variety. For that goal the following theorem plays an essential role. Before its statement, observe that $\mathbb{R} \times \mathbb{T}^n$ is a $(n+1)$-dimensional real analytic manifold.

Proposition 4.4. $\{\Sigma_j\}_{j=0}^n$ *is a family of semi-analytic sets in $\mathbb{R} \times \mathbb{T}^d$.*

Proof. For any $(\lambda_0, \xi_0) \in \mathbb{R} \times \mathbb{T}^d$ we set $\mathcal{O} = I_0 \times \mathfrak{T}_0 \in \mathcal{V}_{\mathbb{R} \times \mathbb{T}^d}(\lambda_0, \xi_0)$ as in Lemma 4.3. Then, for every $j > \mathrm{mul}(\lambda_0, \xi_0)$ we have $\Sigma_j \cap \mathcal{O} = \emptyset$ by (4.4), so we only need to consider

$j \leq \mathrm{mul}(\lambda_0, \xi_0)$. Let us also recall that $\delta(\lambda, \xi) = \det\left(\lambda\mathbb{I}_n - h(\xi)\right)$. By the discussion after the statement of Lemma 4.3, δ admits real analytic derivatives on each variable. In addition, $\Sigma_j \cap \mathcal{O}$ is described as follows:

$$\Sigma_j \cap \mathcal{O} = \left\{(\lambda, \xi) \in \mathcal{O} \mid \lambda \text{ is an eigenvalue of multiplicity } j \text{ of } h(\xi)\right\}$$
$$= \left\{(\lambda, \xi) \in \mathcal{O} \mid \delta(\lambda, \xi) = \frac{\partial\delta}{\partial\lambda}(\lambda, \xi) = \cdots = \frac{\partial^{j-1}\delta}{\partial\lambda^{j-1}}(\lambda, \xi) = 0, \frac{\partial^j\delta}{\partial\lambda^j}(\lambda, \xi) \neq 0\right\}.$$

Then by the definition of a semi-analytic set we infer that each Σ_j is semi-analytic in $\mathbb{R} \times \mathbb{T}^d$. $\qquad\square$

Before the next step, let us recall the version of the theorem of stratification of Hironaka presented in [8, Thm. III.1.8], see also [13, Corol. 4.4], [15, Sec. 3]. Note that we directly impose a stronger condition on f since it simplifies the statement and since this condition will be automatically satisfied in our application.

Theorem 4.5. *Let $\mathcal{M}, \mathcal{M}'$ be two real analytic manifolds, and let $f : \mathcal{M} \to \mathcal{M}'$ be a proper real analytic map. Suppose we are given finitely many subanalytic sets $\mathcal{M}_j \subset \mathcal{M}$, and finitely many subanalytic sets $\mathcal{M}'_k \subset \mathcal{M}'$. Then there exists a subanalytic stratification $(\mathscr{S}, \mathscr{S}')$ of f such that $\mathscr{S}$ is compatible with $\{\mathcal{M}_j\}$ and $\mathscr{S}'$ is compatible with $\{\mathcal{M}'_k\}$.*

We have shown above that $\{\Sigma_j\}_{j=0}^n$ is a finite family of semi-analytic subsets of $\mathbb{R} \times \mathbb{T}^d$. Since $p_\mathbb{R} : \mathbb{R} \times \mathbb{T}^d \to \mathbb{R}$ is proper and real analytic we can apply Theorem 4.5 to get a stratification $(\mathscr{S}, \mathscr{S}')$ of $p_\mathbb{R}$ such that $\mathscr{S}$ is compatible with $\{\Sigma_j\}_{j=0}^n$. We recall that each $\mathcal{S}_\alpha \in \mathscr{S}$ is contained in only one Σ_j and that $\mathscr{S}'$ is a stratification of $\mathbb{R}$. We will denote by τ *the set of thresholds*, and this set is given by the union of the elements of dimension 0 of $\mathscr{S}'$. The thresholds are the levels of energy where one can not construct a conjugate operator.

Definition 4.6. *Let h be a real analytic function $\mathbb{T}^d \to M_n(\mathbb{C})$ with $h(\xi)$ Hermitian for any $\xi \in \mathbb{T}^d$. The set of thresholds $\tau \equiv \tau(h)$ is defined by*

$$\tau := \bigcup_{\dim \mathcal{S}'_\beta = 0} \mathcal{S}'_\beta \ ,$$

where $\mathscr{S}' = \{\mathcal{S}'_\beta\}_\beta$ is the partition of $\mathbb{R}$ given by Theorem 4.5 applied to the proper real analytic function $p_\mathbb{R}$ and the family of semi-analytic subsets $\{\Sigma_j\}_{j=0}^n$.

Note that τ is a finite subset of $\mathbb{R}$ because $\mathscr{S}'$ is locally finite, *i.e.* only a finite numbers of $\mathcal{S}'_\beta$ intersects the neighborhood of a given $\lambda \in \mathbb{R}$. It is also easily observed that τ contains the energy levels corresponding to *flat bands*, *i.e.* a value $\lambda \subset \mathbb{R}$ satisfying $\lambda_j(\xi) = \lambda$ for all ξ and some fixed $j \in \{1, \ldots, n\}$.

We start now the construction of the conjugate operator for a fixed closed interval $I \subset \mathbb{R} \setminus \tau$. This is done in three steps: first we construct A_{λ_0, ξ_0} for fixed $\lambda_0 \in I$ and $\xi_0 \in \mathbb{T}^d$; then we sum over all the eigenvalues λ of $h(\xi_0)$ that lie in I and obtain A_{ξ_0}; finally we define A_I by smoothing a finite family of such A_{ξ_0}.

Let (λ_0, ξ_0) be fixed with $\lambda_0 \in I$. We denote by $\mathcal{O}$ the neighborhood of (λ_0, ξ_0) constructed as in Lemma 4.3, *i.e.* $\mathcal{O} = I_0 \times \mathfrak{T}_0$. Then $(\lambda_0, \xi_0) \in \mathcal{S}_\alpha \subset \Sigma_j$ for a unique α. Without loss of generality we can assume that $\Sigma_j \cap \mathcal{O} = \mathcal{S}_\alpha \cap \mathcal{O}$. Let s denote the dimension of the submanifold

$\mathcal{S}_\alpha$. Furthermore, since $p_{\mathbb{T}^d}|_{\mathcal{S}_\alpha}$ is injective the subset $p_{\mathbb{T}^d}(\mathcal{S}_\alpha \cap \mathcal{O}) \subset \mathbb{T}^d$ has also dimension s. This enables us to find a neighborhood $\mathcal{W}_0$ of the origin in $\mathbb{R}^d$ diffeomorphic to $\mathfrak{T}_0$, or more precisely there exists a diffeomorphism

$$\iota_0 : \mathfrak{T}_0 \to \mathcal{W}_0 \qquad \text{with} \qquad \iota_0\big(p_{\mathbb{T}^d}(\mathcal{S}_\alpha \cap \mathcal{O})\big) \subset \mathbb{R}^s \times \mathbf{0}, \tag{4.5}$$

see for example [29, Theorem 2.10.(2)]. Let us then set $x = (x', x'') \in \mathcal{W}_0$ with $x' \in \mathbb{R}^s$ and $x'' \in \mathbb{R}^{d-s}$. We also define $f : I_0 \times \mathcal{W}_0 \to \mathbb{R}$ by

$$f(\lambda, x) := \frac{\partial^{j-1} \delta}{\partial \lambda^{j-1}}\big(\lambda, \iota_0^{-1}(x)\big) .$$

It follows from the proof of Proposition 4.4 that $f\big(\lambda, (x', 0)\big) = 0$ and $\frac{\partial f}{\partial \lambda}\big(\lambda, (x', 0)\big) \neq 0$ if λ is such that $\big(\lambda, \iota_0^{-1}(x', 0)\big) \in \mathcal{S}_\alpha$. By the implicit function theorem as for example presented in [23, Theo. 2.3.5.] and maybe in a smaller subset $\mathcal{W}_0$, we get that there exists a real analytic function $\boldsymbol{\lambda} : \mathcal{W}_0 \to \mathbb{R}$ such that $f\big(\boldsymbol{\lambda}(x), x\big) = 0$ for every $x \in \mathcal{W}_0$. Then we have

$$\mathcal{S}_\alpha \cap \mathcal{O} = \Big\{ \big(\boldsymbol{\lambda}(x', 0), \iota_0^{-1}(x', 0)\big) \mid (x', 0) \in \mathcal{W}_0 \Big\}. \tag{4.6}$$

Let us denote by $(\iota_0^{-1})^*$ the pullback by ι_0^{-1} defined for φ with support on $\mathfrak{T}_0$ and for any $x \in \mathcal{W}_0$ by $[(\iota_0^{-1})^* \varphi](x) := \varphi(\iota_0^{-1}(x))$. Analogously the pullback ι_0^* is defined by $[\iota_0^* g](\xi) := g\big(\iota_0(\xi)\big)$ for any g defined on $\mathcal{W}_0$. We denote by $D_j = -i\partial_j$ the operator of differentiation with respect to the $j-$variable in $\mathbb{R}^d$. We also set $\partial^{(s)} = (\partial_1, \ldots, \partial_s)$ and $D^{(s)} = (D_1, \ldots, D_s)$. If we keep the notation π_{I_0} for the matrix-valued multiplication operator acting on $L^2(\mathbb{T}^d; \mathbb{C}^n)$ we can define A_{λ_0, ξ_0} on $C_c^\infty(\mathfrak{T}_0; \mathbb{C}^n) \subset L^2(\mathbb{T}^d; \mathbb{C}^n)$ by

$$A_{\lambda_0, \xi_0} := -\tfrac{1}{2} \pi_{I_0} \iota_0^* \Big[(\partial^{(s)} \boldsymbol{\lambda}) \cdot D^{(s)} + D^{(s)} \cdot (\partial^{(s)} \boldsymbol{\lambda}) \Big] (\iota_0^{-1})^* \pi_{I_0}.$$

By repeating this construction for each eigenvalue λ_j of $h(\xi_0)$ lying in I we can define

$$A_{\xi_0} := \sum_{\lambda_j \in \sigma(h(\xi_0)) \cap I} A_{\lambda_j, \xi_0}. \tag{4.7}$$

It follows that for every $\xi_0 \in \mathbb{T}^d$ we can find a neighborhood $\mathfrak{T}_0$, given by the intersection of the neighborhoods constructed for each pair (λ_j, ξ_0), and an operator A_{ξ_0} defined by (4.7) on $C_c^\infty(\mathfrak{T}_0; \mathbb{C}^n)$.

We now define $\mathcal{U}_I := p_{\mathbb{T}^d}(p_{\mathbb{R}}^{-1}(I))$. Since we chose I closed, $\mathcal{U}_I$ is compact. We can then consider finitely many pairs $(\xi_\ell, \mathfrak{T}_\ell)$ such that A_{ξ_ℓ} acts on $C_c^\infty(\mathfrak{T}_\ell; \mathbb{C}^n)$ and such that $\mathcal{U}_I \subset \bigcup \mathfrak{T}_\ell$. Considering a smooth partition of unity on $\mathbb{T}^d$, we can find a family of smooth functions χ_ℓ satisfying $\sum \chi_\ell^2(\xi) = 1$ for $\xi \in \mathcal{U}_I$ and such that each χ_ℓ has support contained in $\mathfrak{T}_\ell$. The candidate for our conjugate operator is then given by

$$A_I := \sum_\ell \chi_\ell A_{\xi_\ell} \chi_\ell \tag{4.8}$$

and is defined on $C^\infty(\mathbb{T}^d; \mathbb{C}^n)$. Note that A_I depends on the covering $\{\mathfrak{T}_\ell\}$ of $\mathcal{U}_I$ and we will impose later on another condition on this covering to ensure the positivity of the commutator of $[ih, A_I]$ once suitably localized.

The next step consists in showing that the operator A_I is essentially self-adjoint on $C^\infty(\mathbb{T}^d; \mathbb{C}^n)$. This proof and the necessary background material are provided in [26, Lem. 5.6]. We do not recall the argument here, and refer to this reference for the proof.

We are now in a suitable position for proving a Mourre estimate, or in other words the positivity of $[ih, A_I]$ when suitably localized. As mentioned at the beginning of this section, a similar result already appeared in [11, Thm. 3.1], but the above construction and the following proof have been adapted to our context.

Theorem 4.7. *Let h be a real analytic function $\mathbb{T}^d \to M_n(\mathbb{C})$ with $h(\xi)$ Hermitian for any $\xi \in \mathbb{T}^d$, and let also h denote the corresponding multiplication operator in $L^2(\mathbb{T}^d; \mathbb{C}^n)$. Let τ be the set of thresholds provided by Definition 4.6 and let I be any closed interval in $\mathbb{R} \setminus \tau$. Then, there exist a finite family of pairs $\{(\mathfrak{T}_\ell, \xi_\ell)\}$ with $\xi_\ell \in \mathfrak{T}_\ell$ such that for the operator A_I defined by (4.8) the following two properties hold:*

(i) the operator h belongs to $C^2(A_I)$,

(ii) there exists a constant $a_I > 0$ such that

$$E_h(I)\,[ih, A_I]\,E_h(I) \geq a_I E_h(I) \ . \tag{4.9}$$

Before providing the proof, let us restate part of the previous statement with the notation introduced in Section 4.1. As a consequence of (4.9), for any closed interval $I \equiv [a, b] \subset \mathbb{R} \setminus \tau$, one has

$$(a, b) \subset \mu^{A_I}(h) \subset \tilde{\mu}^{A_I}(h). \tag{4.10}$$

Proof. Let $(\lambda_0, \xi_0) \in \mathbb{T}^d \times \mathbb{R}$ be fixed with $\lambda_0 \in I$, and let ι_0 be the associated diffeomorphism introduced in (4.5). For shortness we also set $\pi_0 := \pi_{I_0}$, $\tilde{\lambda}_0 := \iota_0^* \boldsymbol{\lambda}(\iota_0^{-1})^*$, $\nabla_0 = \iota_0^* D^{(s)}(\iota_0^{-1})^*$ and $\partial_0 = \iota_0^* \partial^{(s)}(\iota_0^{-1})^*$. With this notation one has

$$
\begin{aligned}
A_{\lambda_0, \xi_0} &= -\tfrac{1}{2}\pi_{I_0}\iota_0^*\left[(\partial^{(s)}\boldsymbol{\lambda}) \cdot D^{(s)} + D^{(s)} \cdot (\partial^{(s)}\boldsymbol{\lambda})\right](\iota_0^{-1})^*\pi_{I_0} \\
&= -\tfrac{1}{2}\pi_0\left[(\partial_0\tilde{\lambda}_0) \cdot \nabla_0 + \nabla_0 \cdot (\partial_0\tilde{\lambda}_0)\right]\pi_0 \\
&= -\pi_0\big((\partial_0\tilde{\lambda}_0) \cdot \nabla_0\big)\pi_0 - \tfrac{i}{2}\pi_0(\Delta_0\tilde{\lambda}_0)\pi_0
\end{aligned}
$$

where $-\Delta_0 := \iota_0^*\big(\sum_{j=0}^s \partial_j^2\big)(\iota_0^{-1})^*$.

Now, since both operators h and A_{λ_0, ξ_0} leave $C^\infty(\mathfrak{T}_0; \mathbb{C}^n)$ invariant, the commutator $[ih, A_{\lambda_0, \xi_0}]$ can be defined as an operator on $C^\infty(\mathfrak{T}_0; \mathbb{C}^n)$. On this set one has

$$[ih, A_{\lambda_0, \xi_0}] = -[ih, \pi_0\big((\partial_0\tilde{\lambda}_0) \cdot \nabla_0\big)\pi_0] + \tfrac{1}{2}[h, \pi_0(\Delta_0\tilde{\lambda}_0)\pi_0]$$

Note also that the second term in the r.h.s. vanishes since $\Delta_0\tilde{\lambda}_0$ is scalar and since h commutes with π_0. Furthermore we have for $\varphi \in C^\infty(\mathfrak{T}_0; \mathbb{C}^n)$ that

$$
\begin{aligned}
&\Big(\big[ih, \pi_0\big((\partial_0\tilde{\lambda}_0) \cdot \nabla_0\big)\pi_0\big]\varphi\Big)(\xi) \\
&= ih(\xi)\pi_0(\xi)(\partial_0\tilde{\lambda}_0)(\xi) \cdot \Big((\nabla_0\pi_0)(\xi)\pi_0(\xi)\varphi(\xi) + \pi_0(\xi)\big(\nabla_0(\pi_0\varphi)\big)(\xi)\Big) \\
&\quad - i\pi_0(\xi)(\partial_0\tilde{\lambda}_0)(\xi) \cdot \Big(\big(\nabla_0(\pi_0 h)\big)(\xi)\pi_0(\xi)\varphi(\xi) + \pi_0(\xi)h(\xi)\big(\nabla_0(\pi_0\varphi)\big)(\xi)\Big) \ .
\end{aligned}
$$

Since h commutes with each (scalar) component of $\partial_0\tilde{\lambda}_0$ the second terms of the parenthesis cancel each others. Consequently, one infers that $[h, iA_{\lambda_0,\xi_0}]$ corresponds to a bounded fibered operator B_{λ_0,ξ_0} with its fibers defined by

$$b_{\lambda_0,\xi_0}(\xi) := -i\pi_0(\xi)(\partial_0\tilde{\lambda}_0)(\xi)\cdot\Big(h(\xi)(\nabla_0\pi_0)(\xi) - \big(\nabla_0(\pi_0 h)\big)(\xi)\Big)\pi_0(\xi)\ .$$

The first term in the parenthesis vanishes because $\pi(\cdot)\pi'(\cdot)\pi(\cdot) = 0$ for any differentiable family of projections. For the second term one has by construction

$$\pi_0\big(\iota_0^{-1}(x',0)\big)h\big(\iota_0^{-1}(x',0)\big) = \tilde{\lambda}_0\big(\iota_0^{-1}(x',0)\big)\pi_0\big(\iota_0^{-1}(x',0)\big)$$

for any $(x',0) \in \mathcal{W}_0$, and therefore

$$b_{\lambda_0,\xi_0}(\xi) = i\pi_0(\xi)(\partial_0\tilde{\lambda}_0)(\xi)\cdot\big(\nabla_0(\tilde{\lambda}_0\pi_0)\big)(\xi)\pi_0(\xi) = \pi_0(\xi)|(\partial_0\tilde{\lambda}_0)(\xi)|^2\pi_0(\xi)$$

for any ξ satisfying $\iota_0(\xi) \in \mathcal{W}_0 \cap \mathbb{R}^s \times \mathbf{0}$.

Let us denote by $\mathcal{S}_\alpha \in \mathscr{S}$ the real analytic submanifold of $\mathbb{R} \times \mathbb{T}^d$ obtained by the theorem of stratification of Hironoka which satisfies $(\lambda_0, \xi_0) \in \mathcal{S}_\alpha$. By the definition of the set of thresholds τ and by the properties of the stratification one has $\dim(p_{\mathbb{R}}|_{\mathcal{S}_\alpha}) = 1$. Combining this with (4.6) one infers that

$$1 = \dim(p_{\mathbb{R}}|_{\mathcal{S}_\alpha}) = \dim\big(\boldsymbol{\lambda}\big(\{(x',0) \subset \mathcal{W}_0\}\big)\big) = \text{rank}\,\big(\partial_0\tilde{\lambda}_0|_{\iota_0^{-1}(\mathcal{W}_0 \cap \mathbb{R}^s \times \mathbf{0})}\big)$$

from which we deduce that $\partial_0\tilde{\lambda}_0$ does not vanish on $\iota_0^{-1}(\mathcal{W}_0 \cap \mathbb{R}^s \times \mathbf{0})$. As a consequence one has $b_{\lambda_0,\xi_0}(\xi_0) \geq c_{0,0}\pi_{I_0}(\xi_0)$, with $c_{0,0} > 0$, and since for fixed ξ_0 there are at most n constants we infer that

$$b_{\xi_0}(\xi_0) := \sum_{\lambda_i \in \sigma(h(\xi_0))\cap I} b_{\lambda_i,\xi_0}(\xi_0) \geq \min\{c_{i,0}\}\sum \pi_{I_i}(\xi_0) = c_0\pi_I(\xi_0) \qquad (4.11)$$

with $c_0 > 0$. By continuity of both b_{ξ_0} and π_I at ξ_0 and using (4.11) we can find a possibly smaller neighborhood $\mathfrak{T}_0$ satisfying the properties of Lemma 4.3 such that for $\xi \in \mathfrak{T}_0$ we have

$$\pi_I(\xi)b_{\xi_0}(\xi)\pi_I(\xi) \geq \tfrac{1}{2}c_0\pi_I(\xi)\ . \qquad (4.12)$$

Since we chose ξ_0 arbitrarily in $\mathbb{T}^d$, we can construct $\mathfrak{T}_0$ satisfying (4.12) for every ξ_0. It follows that one can find a covering of the closed set $\mathcal{U}_I := p_{\mathbb{T}^d}(p_{\mathbb{R}}^{-1}(I))$ composed of a finite number of such $\mathfrak{T}_0$. We have thus defined the covering $\{\mathfrak{T}_\ell\}$ already mentioned before the equation (4.8) and mentioned in the above statement. To finish, observe that $[ih, A_I]$ is a bounded fibered operator with fiber b given for any $\xi \in \mathcal{U}_I$ by

$$b(\xi) = \sum_\ell \chi_\ell(\xi)b_{\xi_\ell}(\xi)\chi_\ell(\xi)\ .$$

Therefore, the operator $E_h(I)[ih, A_I]E_h(I)$ is a bounded fibered operator with fiber equal to $\pi_I(\xi)b(\xi)\pi_I(\xi)$. We also infer that

$$\sum_\ell \pi_I(\xi)\chi_\ell(\xi)b_{\xi_\ell}(\xi)\chi_\ell(\xi)\pi_I(\xi) \geq \tfrac{1}{2}\min_\ell\{c_\ell\}\pi_I(\xi)$$

for every $\xi \in \mathbb{T}^d$. By setting $a_I = \frac{1}{2}\min_\ell\{c_\ell\}$ we conclude that

$$E_h(I)[ih, A_I]E_h(I) \geq a_I E_h(I).$$

Since the operator $B := [ih, A_I]$ has been computed on $C^\infty(\mathbb{T}^d; \mathbb{C}^n)$ which is a core for A_I, and since the resulting operator is bounded, one deduces from the results stated in Section 4.1 that h belongs to $C^1(A_I)$. Then, since the operator B is again an analytically fibered operator, the computation of $[iB, A_I]$ can be performed similarly on $C^\infty(\mathbb{T}^d; \mathbb{C}^n)$ and the resulting operator is once again bounded. It then follows that h belongs to $C^2(A_I)$. $\qquad\square$

Remark 4.8. *When studying a particular graph one can usually find analytic families of eigenvalues λ_i and associated eigenprojections Π_i outside a discrete subset of $\mathbb{T}^d$. Then, a more natural conjugate operator is given formally by $\sum \Pi_i\big((\partial\lambda_i)\cdot\nabla + \nabla\cdot(\partial\lambda_i)\big)\Pi_i$ as used for example in [3] (see also [10] for a related construction). In fact it is a classical result due to Rellich that for every one-dimensional analytic family of (not necessarily bounded) operators, such analytic eigenprojections can be found. For dimension 2, the theory of hyperbolic polynomials shows that this choice can be made outside a discrete set [24, Remark 5.6]. For arbitrary dimension, there seems to be no argument to ensure that analytic eigenprojections can be chosen and so we shall use the conjugate operator given by (4.8).*

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