

Floquet theory - a quantum mechanical point of view.

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(corrected version)

PLAN

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1 Introduction.

In this talk we discuss a subject at the confluence of the theory of induced group representations and spectral theory in Hilbert spaces, concentrating on the problem of the periodic Schrödinger Hamiltonians, of interest for mathematical physics.

The abstract Problem: Suppose given a real affine space \mathcal{X} of finite dimension $d \in \mathbb{N} \setminus \{0\}$; let us denote by $\mathcal{T} : \mathbb{R}^d \rightarrow \mathcal{D}iff(\mathcal{X})$ the natural action of the group \mathbb{R}^d on \mathcal{X} by translations. Let us denote by $BC^\infty(\mathcal{X}; \mathbb{C}^N)$ the space of smooth functions $\mathcal{X} \rightarrow \mathbb{C}^N$ that are bounded together with all their derivatives. Suppose fixed some linear differential operator

$$L(x, \nabla) := \sum_{|\alpha| \leq p} a_\alpha(x) \partial^\alpha : BC^\infty(\mathcal{X}; \mathbb{C}^N) \rightarrow BC^\infty(\mathcal{X}; \mathbb{C}^N) \quad (1.1)$$

having coefficients $\{a_\alpha : \mathcal{X} \rightarrow \mathbb{C}\}_{|\alpha| \leq p}$ that are invariant under the action by translations of the discrete subgroup $\mathbb{Z}^d \subset \mathbb{R}^d$.

We used the usual multi-index notations $\partial^\alpha := \prod_{1 \leq j \leq d} \partial_{x_j}^{\alpha_j}$, $|\alpha| := \sum_{1 \leq j \leq d} \alpha_j$.

What can one say about the structure and spectral properties of such an operator?

Historical References:

- Gustave Floquet (1883), *Sur les équations différentielles linéaires coefficients périodiques*, Annales de l'École Normale Supérieure 12: 47 - 88.
- George William Hill (1886), *On the part of the motion of the lunar perigee which is a function of the mean motions of the sun and moon*. Acta Math. 8: 136.
- Alexander Mihailovich Lyapunov (1892), *The General Problem of the Stability of Motion*. London: Taylor and Francis. Translated by A. T. Fuller from Edouard Davaux's French translation (1907) of the original Russian dissertation (1892).
- Felix Bloch (1928), *Über die Quantenmechanik der Elektronen in Kristallgittern*. Z. Phys. 52: 555 - 600.

Textbook References:

- P.A. Kuchment, *Floquet theory for partial differential equations*, Operator Theory: Advances and Applications, 60, Birkhäuser, Basel, 1993.

Complete \mathbb{R}^d -invariance.

- being abelian, all its unitary irreducible representations are of dimension 1, i.e. acting on \mathbb{C} considered as 1-dimensional complex linear space
Commutation of our operator with all translations just means that it reduces on each irreducible representation to multiplication by a complex number and thus, on functions on the Pontriaghin dual group, that is isomorphic to \mathbb{R}^d itself, it is represented by multiplication with a function.
- in this case $L : BC^\infty(\mathcal{X}) \rightarrow BC^\infty(\mathcal{X})$ is a differential operator with constant coefficients: $L_0(\nabla) = \sum_{|\alpha| \leq p} a_\alpha \partial^\alpha$.

- the Fourier transform

$$(\mathcal{F}\phi)(\xi) := \int_{\mathbb{R}^d} dx e^{-2\pi i \langle \xi, x \rangle} \phi(x) \quad (1.2)$$

defines a bijection between the spaces of tempered distributions.

- $\hat{L}_0 := \mathcal{F}L_0\mathcal{F}^{-1}$ is just multiplication with the polynomial $\hat{L}_0(\xi) := \sum_{|\alpha| \leq p} a_\alpha \xi^\alpha$.

Considering now invariance only by translations with elements from $\mathbb{Z}^d \subset \mathbb{R}^d$ we must notice that we start with a unitary representation of \mathbb{R}^d that is a direct integral of irreducible 1-dimensional representations and we have to restrict this direct integral to the discrete subgroup $\mathbb{Z}^d \subset \mathbb{R}^d$. Thus we are reduced to study the topological and Hilbertian structure of this direct sum of restrictions.

For any abelian locally compact group G let us denote by G° the abelian group of its characters (i.e. its Pontriaghin dual). We shall denote by $\Gamma_* \subset \mathcal{X}^*$ the dual lattice of $\Gamma \subset \mathcal{X}$:

$$\Gamma_* := \left\{ \gamma^* \in \mathcal{X}^* , \langle \gamma^*, \gamma \rangle \in \mathbb{Z}, \forall \gamma \in \Gamma \right\} \quad (1.3)$$

More precisely, we start with an operator acting in $L^2(\mathbb{R}^d)$ that is the natural unitary representation by translations of \mathbb{R}^d on itself that we denote by

$$\rho : \mathbb{R}^d \rightarrow \mathbb{U}(L^2(\mathbb{R}^d)), \quad (\rho(x)u)(y) := u(\tau_x(y)) = u(x+y). \quad (1.4)$$

The Fourier theory tells us that this representations is unitarily equivalent with a direct integral¹ of irreducible (1-dimensional) unitary representations:

$$\hat{\rho} := \mathcal{F}\rho\mathcal{F}^{-1} : \mathbb{R}^d \rightarrow \mathbb{U}(L^2([\mathbb{R}^d]^\circ)), \quad (1.5)$$

$$\hat{\rho} = \int_{[\mathbb{R}^d]^\circ}^\oplus d\xi \epsilon_\xi, \quad \epsilon_\xi : \mathbb{R}^d \rightarrow \mathbb{U}(\mathbb{C}) = \mathbb{S}, \quad \epsilon_\xi(x) := e^{2\pi i \langle \xi, x \rangle}. \quad (1.6)$$

We have thus

$$\hat{\rho}|_{\mathbb{Z}^d} = \int_{[\mathbb{R}^d]^\circ}^\oplus d\xi \epsilon_\xi|_{\mathbb{Z}^d}. \quad (1.7)$$

At this point we have to notice that

$$\epsilon_\xi(\gamma) = \epsilon_\eta(\gamma), \quad \forall \gamma \in \mathbb{Z}^d \iff \xi - \eta = \gamma^* \in \mathbb{Z}_*^d \subset [\mathbb{R}^d]^\circ \quad (1.8)$$

so that we have to restrict our direct integral to the quotient space $[\mathbb{R}^d]^\circ / \mathbb{Z}_*^d = [\mathbb{R}^d]^\circ / [\mathbb{S}^d]^\circ = [\mathbb{Z}^d]^\circ \stackrel{\text{d}}{=} \mathbb{S}_*^d$. Moreover, we notice that for any $\gamma^* \in \mathbb{Z}_*^d$ the character ϵ_{γ^*} are Γ -periodic functions on \mathbb{R}^d .

Thus, let us consider the short exact sequence of dual groups

$$\begin{array}{ccccccc} 0 & \hookrightarrow & [\mathbb{S}^d]^\circ & \hookrightarrow & [\mathbb{R}^d]^\circ & \twoheadrightarrow & [\mathbb{Z}^d]^\circ \twoheadrightarrow \mathbf{1} \\ & & \downarrow \cong & & \downarrow \cong & & \downarrow \cong \\ & & \mathbb{Z}_*^d & & \mathcal{X}^* & & \mathbb{S}_*^d \end{array}$$

and define a representation of our operator as a function of the variable in $[\mathbb{Z}^d]^\circ \cong \mathbb{S}^d$ with operator values acting on a space of functions on $[\mathbb{S}^d]^\circ \cong \mathbb{Z}^d$. Unfortunately, the relation between the

¹Definition 3.1 in ch. II §1 of J. Dixmier *Les algèbres d'opérateurs dans l'espaces Hilbertien*

standard representation by translations of \mathbb{R}^d on itself and its restriction to the discrete subgroup \mathbb{Z}^d is more complicated due to the topological and algebraic structure of the short exact sequence

$$0 \hookrightarrow \mathbb{Z}^d \hookrightarrow \mathbb{R}^d \twoheadrightarrow \mathbb{S}^d \twoheadrightarrow 1 \quad (1.9)$$

that does not split. The main point is that while the quotient $\mathbb{R}^d/\mathbb{Z}^d \cong \mathbb{S}^d$ has a group structure, the topological group \mathbb{R}^d is not the product (neither topologically nor as algebraic structures) of the two groups \mathbb{Z}^d and \mathbb{S}^d

1.1 The discrete Fourier transform.

We recall that \mathbb{Z}^d being a discrete abelian group all its irreducible unitary representations are 1-dimensional and form a compact abelian group isomorphic to the d -dimensional torus \mathbb{S}^d considered as subgroup of the multiplicative group $[\mathbb{C} \setminus \{0\}]^d$ with componentwise multiplication.

More precisely we have the isomorphism:

$$\mathbb{S}^d \ni \mathbf{z} = (\zeta_1, \dots, \zeta_d) \xrightarrow{\sim} \Theta_{\mathbf{z}} \in \widehat{\mathbb{Z}^d}, \quad \Theta_{\mathbf{z}}(\gamma) := \mathbf{z}^\gamma := \prod_{1 \leq j \leq d} \zeta_j^{\gamma_j}. \quad (1.10)$$

We have the imaginary exponential representation:

$$\mathbb{S}^d \ni \mathbf{z} = (e^{-2\pi i \theta_1}, \dots, e^{-2\pi i \theta_d}), \quad (\theta_1, \dots, \theta_d) \in [-1/2, 1/2]^d.$$

Some spaces of complex sequences. Let us consider the following complex linear spaces:

$$\mathfrak{c}(\mathbb{Z}^d) := \{ \underline{s} : \mathbb{Z}^d \rightarrow \mathbb{C}, \exists N(\underline{s}) \in \mathbb{N}, |\gamma| \geq N(\underline{s}) \Rightarrow \underline{s}_\gamma = 0 \}, \quad (1.11)$$

$$\mathfrak{c}_0(\mathbb{Z}^d) := \{ \underline{s} : \mathbb{Z}^d \rightarrow \mathbb{C}, \lim_{|\gamma| \nearrow \infty} \underline{s}_\gamma = 0 \}, \quad (1.12)$$

$$\mathfrak{o}(\mathbb{Z}^d) := \{ \underline{s} : \mathbb{Z}^d \rightarrow \mathbb{C}, \forall N \in \mathbb{N}, \lim_{|\gamma| \nearrow \infty} \langle \gamma \rangle^N \underline{s}_\gamma = 0 \}, \quad (1.13)$$

$$\ell^p(\mathbb{Z}^d) := \{ \underline{s} : \mathbb{Z}^d \rightarrow \mathbb{C}, \sum_{\gamma \in \mathbb{Z}^d} |\underline{s}_\gamma|^p < \infty \}, \quad 1 \leq p < \infty, \quad (1.14)$$

$$\ell^\infty(\mathbb{Z}^d) := \{ \underline{s} : \mathbb{Z}^d \rightarrow \mathbb{C}, \sup_{\gamma \in \mathbb{Z}^d} |\underline{s}_\gamma| < \infty \}. \quad (1.15)$$

Let us define *the discrete Fourier transform*:

$$\mathring{\mathcal{F}} : \mathfrak{c} \rightarrow C(\mathbb{S}^d), \quad (\mathring{\mathcal{F}}(\underline{s}))(\mathbf{z}) := \sum_{\gamma \in \mathbb{Z}^d} \underline{s}_\gamma \mathbf{z}^\gamma, \quad (1.16)$$

$$(\mathring{\mathcal{F}}(\underline{s}))(\theta) = \sum_{\gamma \in \mathbb{Z}^d} \underline{s}_\gamma e^{-2\pi i \langle \theta, \gamma \rangle} \quad (1.17)$$

We recall the following well known results:

$$\mathring{\mathcal{F}}[\ell^1(\mathbb{Z}^d)] \subset C(\mathbb{S}^d), \quad (1.18)$$

$$\mathring{\mathcal{F}}[\ell^2(\mathbb{Z}^d)] = L^2(\mathbb{S}^d), \quad (1.19)$$

$$\mathring{\mathcal{F}}[\mathfrak{o}(\mathbb{Z}^d)] = C^\infty(\mathbb{S}^d) \quad (1.20)$$

and the fact that $\mathring{\mathcal{F}} : \ell^2(\mathbb{Z}^d) \xrightarrow{\sim} L^2(\mathbb{S}^d)$ is a unitary transformation.

Finally let us recall the Poisson formula² that we shall use several times. We have the following equality, as distributions in $\mathcal{S}'(\mathcal{X})$ with series converging in the weak sense (as tempered distributions):

$$\text{(Poisson Formula)} \quad \sum_{\gamma \in \Gamma} \delta_\gamma = \sum_{\gamma^* \in \Gamma^*} \epsilon_{\gamma^*}. \quad (1.21)$$

Here δ_γ is the Dirac measure in $\gamma \in \mathcal{X}$ and $\epsilon_{\gamma^*}(x) := e^{-2\pi i \langle \gamma^*, x \rangle}$.

1.2 The short exact sequence of topological groups.

$$0 \hookrightarrow \mathbb{Z}^d \hookrightarrow \mathbb{R}^d \twoheadrightarrow \mathbb{S}^d \twoheadrightarrow 1$$

The Borelian section:

- We shall consider the borelian decomposition $\mathbb{R}^d = \mathbb{Z}^d \times J^d$ with $J := [-1/2, 1/2)$
- using the usual *entire part function*:

$$[\cdot] : \mathbb{R} \rightarrow \mathbb{Z}, \quad [t] := \max \{ k \in \mathbb{Z}, k \leq t \} \in \mathbb{Z}, \quad \forall t \in \mathbb{R}, \quad (1.22)$$

- and defining

$$\mathbb{R} \ni t \mapsto ([t]_2, \{t\}_2) \in \mathbb{Z} \times [-1/2, 1/2) \quad : \quad [t]_2 := [t + 1/2] \quad (1.23)$$

$$\{t\}_2 := t - [t]_2. \quad (1.24)$$

We obtain a bijective application $\mathbf{t}_2 : \mathbb{R}^d \ni x \mapsto ([x]_2, \{x\}_2) \in \mathbb{Z}^d \times J^d$.

- We use the notations $\tilde{x}, \tilde{y}, \dots$ for the points of J^d .

Group structure on \mathbb{S}^d : On the quotient space $\mathbb{S}^d \cong \mathbb{R}^d / \mathbb{Z}^d$ we can define the following abelian group structure:

$$\tilde{x} \hat{+} \tilde{y} := \{\tilde{x} + \tilde{y}\}_2. \quad (1.25)$$

It only depends on the classes of \tilde{x} and \tilde{y} in the quotient space $\mathbb{R}^d / \mathbb{Z}^d$.

The cocycle: Let us notice that

$$\mathbf{t}_2(\mathbf{t}_2^{-1}(\alpha, \tilde{x}) + \mathbf{t}_2^{-1}(\beta, \tilde{y})) = (\alpha + \beta + \nu(\tilde{x}, \tilde{y}), \tilde{x} \hat{+} \tilde{y}) \quad (1.26)$$

where

$$\nu : \mathbb{S}^d \times \mathbb{S}^d \rightarrow \mathbb{Z}^d, \quad \nu(\tilde{x}, \tilde{y}) := ([\tilde{x}_1 + \tilde{y}_1]_2, \dots, [\tilde{x}_d + \tilde{y}_d]_2) \quad (1.27)$$

is a 2-cocycle for the translations that is the origin of the twist of the decomposition of the representations.

²§7.2 in Lars Hörmander *The Analysis of Linear Partial Differential Operators, I*. 2-nd edition, Springer-Verlag, 1990.

The projection: We have the following explicit model for the quotient group $\mathbb{R}^d/\mathbb{Z}^d$:

$$\mathbb{R}^d/\mathbb{Z}^d \simeq \mathbb{S}^d := \{\mathbf{z} = (\check{z}_1, \dots, \check{z}_d) \in \mathbb{C}^d, |\check{z}_1| = \dots = |\check{z}_d| = 1\} \subset \mathbb{C}^d \quad (1.28)$$

with the projection defined by the imaginary exponential:

$$\mathfrak{e}^d : \mathbb{R}^d \ni x \mapsto \mathfrak{e}^d(x) := (e^{-2\pi i x_1}, \dots, e^{-2\pi i x_d}) \in \mathbb{S}^d \quad (1.29)$$

and the group structure induced from $(\mathbb{C} \setminus \{0\})^d$ considered as direct product of d copies of the multiplicative group $\mathbb{C} \setminus \{0\}$.

The Borelian section: We notice that the function

$$\mathfrak{s}^d : \mathbb{S}^d \ni \mathbf{z} = (\check{z}_1, \dots, \check{z}_d) \mapsto ((1/2\pi i) \ln \check{z}_1, \dots, (1/2\pi i) \ln \check{z}_d) \in J^d \quad (1.30)$$

with \ln the principal determination of the logarithm on \mathbb{C} , defines a section for \mathfrak{e}^d over \mathbb{S}^d .

(We have here a very well-known aspect of a rather deep result ³.)

³Theorem 5.11 in V.S. Varadarajan, *Geometry of Quantum Theory*, 2-nd edition, Springer 2007

2 The Bloch-Floquet-Zak transform.

Due to the commutation of our periodic differential operator with the \mathbb{Z}^d -translations, **it will leave invariant all the unitary irreducible representations of \mathbb{Z}^d .**

These representations are in bijective correspondence with the classes of characters in the dual $[\mathbb{R}^d]^\circ$ of \mathbb{R}^d modulo their action on $[\mathbb{S}^d]^\circ \cong \mathbb{Z}^d_*$, i.e. with the classes of characters in $[\mathbb{R}^d]^\circ/[\mathbb{S}^d]^\circ \cong [\mathbb{Z}^d]^\circ \cong \mathbb{S}^d_*$.

A. Let us start with the Fourier transform

$$\mathcal{F} : L^2(\mathcal{X}) \xrightarrow{\sim} L^2(\mathcal{X}^*), \quad (\mathcal{F}f)(\xi) := \int_{\mathcal{X}} dx e^{-2\pi i \langle \xi, x \rangle} f(x) \quad (2.31)$$

taking the canonical unitary representation of \mathbb{R}^d by translations into the direct integral of unitary irreducible representations.

- Decompose $L^2(\mathcal{X}^*) \simeq L^2([\mathbb{S}^d]^\circ) \otimes L^2([\mathbb{Z}^d]^\circ) \cong L^2(\mathbb{S}^d_*; \ell^2(\mathbb{Z}^d_*))$.
- Thus our initial representation of \mathbb{Z}^d on $L^2(\mathcal{X})$ becomes a direct integral over $[\mathbb{Z}^d]^\circ \cong \mathbb{S}^d_*$ of unitary reducible representations given by scalar multiples of the identity on the Hilbert space $L^2([\mathbb{S}^d]^\circ) \cong \ell^2(\mathbb{Z}^d_*)$. Then, our Γ -translation invariant operator will become a *direct integral over $[\mathbb{Z}^d]^\circ \cong \mathbb{S}^d_*$ of operators acting in $L^2([\mathbb{S}^d]^\circ) \cong \ell^2(\mathbb{Z}^d_*)$.*

In fact, we can go further and obtain some more interesting structure to be used in our analysis. In fact, going back to (1.1) and considering the case $N = 1$ we notice that we have in fact *two types of 'elementary operators' involved*:

- multiplication with functions $a \in BC^\infty(\mathcal{X})$:

$$BC^\infty(\mathcal{X}) \ni f \mapsto af \in BC^\infty(\mathcal{X})$$

- differential operators that can be considered as products of the generators of the unitary translations on \mathcal{X} .

In conclusion we shall be interested also in the Fourier transform of operators of multiplication with smooth functions on \mathcal{X} and these are easy to be described using the \mathbb{R}^d -translations on \mathcal{X}^* :

$$\mathcal{F}(af) = (\mathcal{F}a) * (\mathcal{F}f), \quad \forall (a, f) \in BC^\infty(\mathcal{X}^*) \times C_0^\infty(\mathcal{X}^*) \quad (2.32)$$

with $*$ the usual convolution: $(\phi * \psi)(\xi) := \int_{\mathcal{X}^*} d\eta \phi(\xi - \eta)\psi(\eta)$. Thus, denoting by $a(Q)$ the operator of multiplication with the C_0^∞ function a on $L^2(\mathcal{X}^*)$ and by $\hat{U} : \mathbb{R}^d \rightarrow \mathbb{U}(L^2(\mathcal{X}^*))$ the natural representation by translations, we can write (in the weak operator topology):

$$\mathcal{F}a(Q)\mathcal{F}^{-1} = \int_{\mathcal{X}^*} d\xi (\mathcal{F}a)(\xi)\hat{U}(\xi). \quad (2.33)$$

Thus, working with functions $a \in BC^\infty$ will imply having integrands $(\mathcal{F}a) \in \mathcal{S}'(\mathcal{X}^*)$ and thus will oblige us to impose some regularity conditions on the functions in $L^2(\mathcal{X}^*)$ (at least continuity!). But the existence of the cocycle $\nu : \mathbb{S}^d \times \mathbb{S}^d \rightarrow \mathbb{Z}^d$ and the discontinuity of the section $\mathfrak{s}^d : \mathbb{S}^d \rightarrow \mathbb{R}^d$ imply a complicated form for the representation of $\hat{U} : \mathbb{R}^d \rightarrow \mathbb{U}(L^2(\mathcal{X}^*))$ with respect to the tensor decomposition introduced above. In fact, the canonical action of \mathbb{R}^d on itself by translations is

different of the direct product of the canonical actions by translations of the two groups \mathbb{Z}^d and \mathbb{S}^d (see (1.25)). Taking into account the cocycle (1.27) comes to consider the projection $\mathbb{R}^d \rightarrow \mathbb{S}^d$ as a *principal bundle with group \mathbb{Z}^d* ; we shall analyse this structure further.

For the moment let us consider this 'continuity problem' in a different way:

- Consider on $\mathfrak{l}^2(\mathbb{Z}^d_*)$ the restriction of the Γ_* -translations:

$$\hat{U}^\dagger : \mathbb{Z}^d_* \rightarrow \mathcal{U}(\mathfrak{l}^2(\mathbb{Z}^d_*)), \quad (\hat{U}^\dagger(\gamma^*)\underline{s})(\alpha^*) := \underline{s}(\alpha^* + \gamma^*). \quad (2.34)$$

- Define

$$\mathcal{L} := \{F \in C(\mathcal{X}^*; \mathfrak{c}(\mathbb{Z}^d_*)), (\mathcal{F}^*(\gamma^*)F)(\xi) = \hat{U}^\dagger(\gamma^*)F(\xi), \forall(\gamma^*, \xi) \in \Gamma_* \times \mathcal{X}^*\}, \quad (2.35)$$

$$\|F\|_{\mathcal{L}}^2 := \int_{E_*} d\tilde{\xi} \|F(\tilde{\xi})\|_{\mathfrak{l}^2(\Gamma_*)}^2 \quad (2.36)$$

and the completion \mathcal{L} that is a Hilbert space.

B. Let us apply a *dual discrete Fourier transform* in order to come back to the \mathcal{X} -representation only for the variables 'modulo Γ ', i.e.:

$$\mathring{\mathcal{F}}_* : \mathfrak{l}^2(\Gamma_*) \xrightarrow{\sim} L^2(\mathbb{S}^d), \quad (\mathring{\mathcal{F}}_*\underline{s})(\tau) := \sum_{\gamma^* \in \Gamma_*} e^{2\pi i \langle \gamma^*, \tau \rangle} \underline{s}_{\gamma^*}. \quad (2.37)$$

Definition 2.1.

$$U^\dagger := \mathring{\mathcal{F}}_* \hat{U}^\dagger (\mathring{\mathcal{F}}_*^{-1}) : \mathbb{Z}^d_* \rightarrow \mathcal{U}(L^2(\mathbb{S}^d)), \quad (U^\dagger(\gamma^*)\phi)(\tau) = e^{-2\pi i \langle \gamma^*, \tau \rangle} \phi(\tau), \quad (2.38)$$

$$\mathring{\mathcal{G}} := (\mathring{\mathcal{F}}_* \otimes \mathbf{1}) \mathcal{L} \subset \{F \in C(\mathcal{X}^*; C(\mathbb{S}^d)), (\mathcal{F}^*(\gamma^*)F)(\xi) = U^\dagger(\gamma^*)F(\xi), \forall(\gamma^*, \xi) \in \Gamma_* \times \mathcal{X}^*\}$$

$$\|F\|_{\mathring{\mathcal{G}}}^2 := \int_{E_*} d\tilde{\xi} \|F(\tilde{\xi})\|_{L^2(\mathbb{S}^d)}^2 \quad (2.39)$$

and the completion $\mathring{\mathcal{G}}$ that is a Hilbert space.

Definition 2.2. We define the following uniray operator

$$\mathcal{U}_\Gamma^\dagger : L^2(\mathcal{X}^*) \ni \hat{f} \mapsto \tilde{f} \in \mathring{\mathcal{G}}, \quad \tilde{f}(\mathbf{z}, \tilde{\xi}) := \sum_{\gamma^* \in \Gamma_*} e^{2\pi i \langle \gamma^*, \mathbf{s}^d(\mathbf{z}) \rangle} \hat{f}(\tilde{\xi} + \gamma^*). \quad (2.40)$$

C. We define finally the *Bloch-Floquet-Zak transform*⁴ as the composition of the two unitaries $\mathcal{U}_\Gamma^\dagger$ and \mathcal{F} :

$$\tilde{\mathcal{U}}_\Gamma := \mathcal{U}_\Gamma^\dagger \circ \mathcal{F} : L^2(\mathcal{X}^*) \xrightarrow{\sim} \mathring{\mathcal{G}} \quad (2.41)$$

$$\tilde{f}(\xi, \tau) := \sum_{\gamma^* \in \Gamma_*} e^{2\pi i \langle \gamma^*, \tau \rangle} \hat{f}(\xi + \gamma^*) = \sum_{\gamma^* \in \Gamma_*} e^{2\pi i \langle \gamma^*, \tau \rangle} \int_{\mathcal{X}} dx e^{-2\pi i \langle \xi + \gamma^*, x \rangle} f(x) = \quad (2.42)$$

$$= \int_{\mathcal{X}} dx \left(\sum_{\gamma^* \in \Gamma_*} e^{2\pi i \langle \gamma^*, \tau - x \rangle} \right) e^{-2\pi i \langle \xi, x \rangle} f(x) = \sum_{\gamma \in \Gamma} e^{-2\pi i \langle \xi, \gamma + \tau \rangle} f(\gamma + \tau). \quad (2.43)$$

⁴

- G De Nittis, M Lein: *Applications of magnetic DO techniques to SAPT* Reviews in Mathematical Physics 23 (03), 233-260
- J. Zak: *Dynamics of electrons in solids in external fields*, Phys. Rev. 168(3) (1968) 686695.

2.1 The Bloch-Floquet Hilbert bundle.

2.1.1 The principal bundle $\mathbb{R}^d \mapsto \mathbb{S}^d$ with fiber group \mathbb{Z}^d :

The manifold structure on \mathbb{S}^1 .

- **Charts:** $\mathbb{S}^1 \subset V_0 \cup V_1$,

$$V_0 := \{ \zeta = e^{-2\pi i \tau}, \tau \in (-3/8, 3/8) \subset \mathbb{R} \} \subset \mathbb{S},$$

$$\phi_0 : V_0 \ni \zeta \mapsto (1/2\pi i) \ln \zeta \in I := (-3/8, 3/8) \subset \mathbb{R},$$

$$V_1 := \{ \zeta = e^{-2\pi i \tau}, \tau \in (1/8, 7/8) \subset \mathbb{R} \} \subset \mathbb{S},$$

$$\phi_1 : V_1 \ni \zeta \mapsto (1/2\pi i) \ln(-\zeta) = ((1/2\pi i) \ln \zeta - 1/2) \in I := (-3/8, 3/8) \subset \mathbb{R}.$$

- **Chart intersections:** $V_0 \cap V_1 = W = W_0 \sqcup W_1$,

$$W_0 := \{ \zeta = e^{-2\pi i \tau}, \tau \in (-3/8, -1/8) \subset \mathbb{R} \}$$

$$= \{ \zeta = e^{-2\pi i \tau}, \tau \in (5/8, 7/8) \subset \mathbb{R} \} \subset \mathbb{S},$$

$$\phi_0[W_0] = I_0 := (-3/8, -1/8) \subset I \subset \mathbb{R},$$

$$\phi_1[W_0] = I_1 := (5/8 - 1/2, 7/8 - 1/2) = (1/8, 3/8) \subset I \subset \mathbb{R},$$

$$W_1 := \{ \zeta = e^{-2\pi i \tau}, \tau \in (1/8, 3/8) \subset \mathbb{R} \} \subset \mathbb{S},$$

$$\phi_0[W_1] = (1/8, 3/8) = I_1 \subset I \subset \mathbb{R},$$

$$\phi_1[W_1] = (1/8 - 1/2, 3/8 - 1/2) = (-3/8, -1/8) = I_0 \subset I \subset \mathbb{R},$$

- **Coordinate change:**

$$\psi := \phi_1 \circ \phi_0^{-1} : I_0 \sqcup I_1 \rightarrow I_0 \sqcup I_1.$$

$$\psi|_{I_j} =: \psi_j \ (j \in \{0, 1\}) \begin{cases} \psi_0(t) = t + 1/2 \in I_1 \\ \psi_1(t) = t - 1/2 \in I_0 \end{cases}$$

The manifold structure on \mathbb{S}^d . Let $\mathbb{I} := \{0, 1\}^d$.

- **Charts:** $\mathbb{S}^d \subset \bigcup_{\mathbf{a} \in \mathbb{I}} V_{\mathbf{a}}^d$,

$$V_{\mathbf{a}}^d := \bigtimes_{1 \leq j \leq d} V_{\mathbf{a}_j}, \quad \phi_{\mathbf{a}}^d := \bigtimes_{1 \leq j \leq d} \phi_{\mathbf{a}_j} : V_{\mathbf{a}}^d \rightarrow I^d \subset \mathbb{R}^d.$$

- **Chart intersections:** $W_{\mathbf{a}, \mathbf{b}}^d = \bigtimes_{1 \leq j \leq d} (V_{\mathbf{a}_j} \cap V_{\mathbf{b}_j}) = \bigtimes_{1 \leq j \leq d} W_{\mathbf{a}, \mathbf{b}}^d(j)$ where

$$W_{\mathbf{a}, \mathbf{b}}^d(j) := \begin{cases} = V_{\mathbf{a}_j}, & \text{for } \mathbf{a}_j = \mathbf{b}_j \\ = W, & \text{for } \mathbf{a}_j \neq \mathbf{b}_j \end{cases}.$$

We notice that for $\mathbf{a} \neq \mathbf{b}$, the intersection $W_{\mathbf{a}, \mathbf{b}}^d$ are disjoint unions of elements of the form $\bigtimes_{1 \leq j \leq d} \mathcal{V}(\kappa_j)$ for any $\kappa \in \{0, 1, 2, 3\}^d$ and $\mathcal{V}(j) := V_j$ for $j = 0, 1$ and $\mathcal{V}(j) := W_{j-2}$ for $j = 2, 3$.

- **Coordinate change:**

$$\psi^d \Big|_{\bigtimes_{1 \leq j \leq d} \mathcal{V}(\kappa_j)} = \bigtimes_{1 \leq j \leq d} \psi_{\kappa_j - 2}$$

where we define $\psi_{-2} = \psi_{-1} = \text{Id}$.

The principal bundle structure on $\epsilon : \mathbb{R} \rightarrow \mathbb{S}$.

- **Local trivialisations:**

1. $\epsilon^{-1}[V_0] \ni t \mapsto \Phi_0(t) = (\phi_0(\epsilon(t)), [t]_2) \in I \times \mathbb{Z}$.

2. $\epsilon^{-1}[V_1] \ni t \mapsto \Phi_1(t) = (\phi_1(\epsilon(t)), [t]) = (\phi_1(\epsilon(t)), [t - 1/2]_2) \in I \times \mathbb{Z}$.

- **Transition functions:** $\Psi := \Phi_1 \circ \Phi_0^{-1} = (\psi(\tau), F_\tau(k)) : (I_0 \cup I_1) \times \mathbb{Z} \rightarrow (I_0 \cup I_1) \times \mathbb{Z}$ with $F_\tau(k+p) = F_\tau(k) + p$ for any $\tau \in I_0 \cup I_1$ and $(k, p) \in \mathbb{Z}^2$. Thus $F_\tau(k) = F_\tau(0) + k$ and $F_\tau(0) \in \mathbb{Z}$ is constant on any connex domain.

1. For $(\tau, k) \in I_0 \times \mathbb{Z} = (-3/8, -1/8) \times \mathbb{Z}$ we have $\psi(\tau) = \tau + 1/2$ and $F_\tau(0) = \Phi_1(\Phi_0^{-1}(\tau, 0)) = \Phi_1(\tau) = -1$.

2. For $(\tau, k) \in I_1 \times \mathbb{Z} = (1/8, 3/8) \times \mathbb{Z}$ we have $\psi(\tau) = \tau - 1/2$ and $F_\tau(0) = \Phi_1(\Phi_0^{-1}(\tau, 0)) = \Phi_1(\tau) = 0$.

Thus: $F_\tau(0) = \begin{cases} = -1, & \forall \tau \in I_0, \\ = 0, & \forall \tau \in I_1. \end{cases}$

The principal bundle structure on $\epsilon^d : \mathbb{R}^d \rightarrow \mathbb{S}^d$.

Transition functions: $\Psi_{a,b}(\theta, \gamma) = (\psi_{a,b}(\theta), F_{a,b,\theta}(\gamma))$ with $F_{a,b,\theta}(\gamma) = F_{a,b,\theta}(0) + \gamma$ on $W_{a,b}^d$.

With the above results we obtain a family $\{\rho_\kappa = \prod_{1 \leq j \leq d} \rho_{\kappa_j}\}_{\kappa \in \{0,1,2,3\}^d} \subset \mathbb{Z}^d$

where $\rho_0 = \rho_1 = \rho_3 = 0$ and $\rho_2 = -1$

such that the transition functions on $\prod_{1 \leq j \leq d} \mathcal{V}_{\kappa_j}$ is $\rho_\kappa \in \mathbb{Z}^d$.

Remark 2.3. The fiber associated to the structure group \mathbb{Z}^d being discrete we also have a canonical connection with holonomy $\mathcal{Hol}_x^o(\mathbb{R}^d; \mathbb{S}^d) \cong \{0\}$ and $\mathcal{Hol}_x(\mathbb{R}^d; \mathbb{S}^d) \cong \mathbb{Z}^d$ for any $x \in \mathbb{R}^d$.

2.1.2 The associated bundle defined by U^\dagger .

Having the principal bundle $\epsilon^d : \mathbb{R}^d \rightarrow \mathbb{S}^d$ with fibres free transitive \mathbb{Z}^d -spaces and the representation $U^\dagger : \mathbb{Z}_*^d \rightarrow \mathcal{U}(L^2(\mathbb{S}^d))$ we can construct a vector bundle $p : \mathcal{E}^* \rightarrow \mathbb{S}_*^d$ with fibres Hilbert spaces unitary equivalent with $L^2(\mathbb{S}^d)$ through the following canonical procedure.

- **The direct product:** $\mathbb{E}_* := \mathcal{X}^* \times L^2(\mathbb{S}^d)$

- **The orbits of the \mathbb{Z}_*^d -action:**

$$(\xi, f) \bowtie (\eta, g) \Leftrightarrow \exists \gamma^* \in \mathbb{Z}_*^d, \eta = \xi + \gamma^*, g = [U^\dagger]^{-1}(\gamma^*)f. \quad (2.44)$$

For $(\xi, f) \in \mathcal{X}^* \times L^2(\mathbb{S}^d)$ the equivalence class $[(\xi, f)]_\bowtie$ may be identified with the point $(\epsilon^d(\xi), U^\dagger([\xi]_2)f) \in \mathbb{S}_*^d \times L^2(\mathbb{S}^d)$;

Thus we shall simply denote $[(\xi, f)]_\bowtie =: e(\epsilon^d(\xi), U^\dagger([\xi]_2)f)$.

- **The associated bundle:**

$$\mathcal{E}^* := (\mathcal{X}^* \times L^2(\mathbb{S}^d)) / \bowtie, \quad (2.45)$$

$$p([\xi, f]_\bowtie) := \epsilon^d(\xi). \quad (2.46)$$

- **The fiber** over $\mathbf{z}_* \in \mathbb{S}_*^d$

$$\rho^{-1}(\mathbf{z}_*) = \{e(\mathbf{z}_*, f)\}_{f \in L^2(\mathbb{S}^d)} \simeq L^2(\mathbb{S}^d). \quad (2.47)$$

- **The local trivializations:**

$$\tilde{\Phi}_a := (\phi_a \circ \rho, \tilde{F}_a \circ (\rho, \text{Id})) : \rho^{-1}[V_a] \rightarrow I^d \times L^2(\mathbb{S}^d) \text{ where}$$

$$\tilde{F}_a(\rho(e(\mathbf{z}, f)), (e(\mathbf{z}, f))) := U^\dagger(F_{a,\mathbf{z}}(e(\mathbf{z}, f)))f$$

$$\tilde{\Psi}_\kappa := (\psi_\kappa, \tilde{F}_\kappa) : I_\kappa \times L^2(\mathbb{S}^d) \rightarrow I_\kappa \times L^2(\mathbb{S}^d) \text{ where } \tilde{F}_\kappa := U^\dagger(\rho_\kappa) \text{ with } \rho_\kappa \in \mathbb{Z}^d \text{ defined at the end of the last subsection.}$$

Remark 2.4. Let us notice that each element $x \in \mathbb{R}^d$ defines an identification

$$\mathfrak{q}(x) : L^2(\mathbb{S}^d) \xrightarrow{\sim} \mathcal{E}_{\rho(x)}^* \quad (2.48)$$

given by the following relation: $\mathfrak{q}(x)f := [(x, f)]_{\boxtimes}$.

The canonical lift of basic curves. Suppose given a continuous curve $[0, 1] \ni \tau \mapsto \mathbf{z}_*(\tau) \in \mathbb{S}_*^d$ and let us fix some point $e_0 \in \rho^{-1}(\mathbf{z}_*(0))$. Now, let $[0, 1] \ni \tau \mapsto \xi(\tau) \in \mathbb{R}^d$ be the unique lift of $\{\mathbf{z}_*(\tau)\}_{\tau \in [0,1]} \subset \mathbb{S}^d$ to \mathbb{R}^d through $\xi(0) = \mathfrak{s}^d(\mathbf{z}_*(0))$ given by Remark 2.3. Then there exists a unique $f_0 \in L^2(\mathbb{S}_*^d)$ such that $e_0 = e(\mathbf{z}_*(0), f_0)$. One can easily verify that the lifted curve is then given by

$$[0, 1] \ni \tau \mapsto [(\xi(\tau), f_0)]_{\boxtimes} \in \mathcal{E}^*. \quad (2.49)$$

This is the linear connection associated to the canonical connection in Remark 2.3 and allows us to identify from now on the tangent space to \mathbb{S}_*^d at any point $\mathbf{z}_* \in \mathbb{S}_*^d$, that is isomorphic to \mathbb{R}^d , with the horizontal tangent space to \mathcal{E}^* at any point $e \in \mathcal{E}^*$ with $\rho(e) = \mathbf{z}_*$.

The canonical action of \mathbb{R}^d : $\tilde{\mathcal{T}} : \mathbb{R}^d \rightarrow \text{Aut}\mathcal{E}^*$:

$$\forall \zeta \in \mathbb{R}^d, \quad \tilde{\mathcal{T}}(\zeta)[(\xi, f)]_{\boxtimes} := [(\mathcal{T}(\zeta)\xi, f)]_{\boxtimes}. \quad (2.50)$$

2.1.3 The sections in $\rho : \mathcal{E}^* \rightarrow \mathbb{S}_*^d$.

Noticing that $C(\mathbb{S}^d) \subset L^2(\mathbb{S}^d)$ is a dense subspace, we can consider a subbundle of $\rho : \mathcal{E}^* \rightarrow \mathbb{S}_*^d$ associated to it.

- The equivalence relation \boxtimes on \mathbb{E}^* can be restricted to $\mathbb{E}_\circ^* := \mathcal{X}^* \times C(\mathbb{S}^d)$ because the representation $U^\dagger : \mathbb{Z}_*^d \rightarrow \mathcal{U}(L^2(\mathbb{S}^d))$ leaves the subspace $C(\mathbb{S}^d) \subset L^2(\mathbb{S}^d)$ invariant.
- Thus we can define $\mathcal{E}_\circ^* := \mathbb{E}_\circ^* / \boxtimes$ and $\rho_\circ := \rho|_{\mathcal{E}_\circ^*} : \mathcal{E}_\circ^* \rightarrow \mathbb{S}_*^d$ as subbundle of \mathcal{E}^* .

The space of regular sections: Let us define $\mathcal{C}(\mathcal{E}_\circ^*; \mathbb{S}_*^d)$ as the linear space of continuous sections $s : \mathbb{S}_*^d \rightarrow \mathcal{E}_\circ^* \subset \mathcal{E}^*$.

A standard argument allows us to prove that $\mathcal{C}(\mathcal{E}_\circ^*; \mathbb{S}_*^d)$ is dense in $L^2(\mathcal{E}_\circ^*; \mathbb{S}_*^d)$ (the space of L^2 -sections in $\rho : \mathcal{E}^* \rightarrow \mathbb{S}_*^d$), for the L^2 -norm. The action induced by (2.50) on $L^2(\mathcal{E}_\circ^*; \mathbb{S}_*^d)$ is simply the canonical action by translations on \mathcal{G} .

2.1.4 The induced representation.

Definition 2.5. Let us define $\mathring{C}(\mathcal{X}^*; C(\mathbb{S}^d))$ as the linear subspace of continuous functions $F : \mathcal{X}^* \rightarrow C(\mathbb{S}^d)$ that verify the *covariance condition*

$$(\mathcal{J}^*(\gamma^*)F)(\xi) = U^\dagger(\gamma^*)(F(\xi)), \quad \forall \xi \in \mathcal{X}^*, \forall \gamma^* \in \Gamma_*. \quad (2.51)$$

Proposition 2.6. *There is a canonical identification $\mathcal{I}_o : \mathcal{C}(\mathcal{E}_o^*; \mathbb{S}_*^d) \xrightarrow{\sim} \mathring{C}(\mathcal{X}^*; C(\mathbb{S}^d))$.*

Proof.

- Let $\tilde{F} \in \mathring{C}(\mathcal{X}^*; C(\mathbb{S}^d))$ and let us define

$$F : \mathbb{S}_*^d \rightarrow \mathcal{E}_o^*, \quad F(\mathbf{z}_*) := [(\xi, \tilde{F}(\xi))]_{\boxtimes}, \quad \forall \xi \in (\mathbf{e}^d)^{-1}(\mathbf{z}_*). \quad (2.52)$$

It defines a section of the fiber bundle $p_o : \mathcal{E}_o^* \rightarrow \mathbb{S}_*^d$ that is continuous (see the definition).

- Let $F \in \mathcal{C}(\mathcal{E}_o^*; \mathbb{S}_*^d)$ and let us fix some $\xi \in \mathcal{X}^*$ and look at the fiber $p_o^{-1}(\mathbf{e}^d(\xi))$ and at the image $F(\mathbf{e}^d(\xi)) \in p_o^{-1}(\mathbf{e}^d(\xi))$.

By construction there exists a unique element $f \in C(\mathbb{S}^d)$ such that

$$[(\xi, f)]_{\boxtimes} = F(\mathbf{e}^d(\xi)) \in p_o^{-1}(\mathbf{e}^d(\xi)). \quad (2.53)$$

We define then $\tilde{F}(\xi) := f \in C(\mathbb{S}^d)$ with the unique choice explained above.

□

Remarks:

- $\mathring{C}(\mathcal{X}^*; C(\mathbb{S}^d))$ is a subspace of $L_{\text{loc}}^2(\mathcal{X}^*; L^2(\mathbb{S}^d))$,
- given a function $\tilde{F} \in \mathring{C}(\mathcal{X}^*; C(\mathbb{S}^d))$ its restriction $\tilde{F}_E := \tilde{F}|_E$ to the unit cell completely defines the entire function $\tilde{F} \in \mathring{C}(\mathcal{X}^*; C(\mathbb{S}^d))$,
- the closure of $\mathring{C}(\mathcal{X}^*; C(\mathbb{S}^d))$ for the Hilbertian norm

$$\|F\|_{E,2} := \int_E d\xi \|F(\xi)\|_{L^2(\mathbb{S}^d)}^2 \quad (2.54)$$

is a Hilbert space containing $\mathring{C}(\mathcal{X}^*; C(\mathbb{S}^d))$ as dense linear subspace. An easy argument proves that this Hilbert space coincides with the Hilbert space \mathcal{G} from Definition 2.1.

2.1.5 Conclusion

Then we obtain a simplified version of Theorem 2.2.3 in P.A. Kuchement (one can obtain the complete version with some work in the fiber bundle formulation):

$$\left(\mathcal{F}_\Gamma L(Q, \nabla) u \right) (\xi, \tau) = \sum_{\gamma \in \Gamma} e^{-2\pi i \langle \xi, \gamma + \tau \rangle} \sum_{|\alpha| \leq p} a(\tau) (\partial^\alpha u)(\gamma + \tau) \quad (2.55)$$

$$= \sum_{|\alpha| \leq p} a(\tau) ((\tilde{\partial} + 2\pi i \{\xi\})^\alpha \tilde{u})(\xi, \tau) \quad (2.56)$$

$$= \left[\left(\mathbf{1} \otimes \tilde{L}(Q, \nabla + 2\pi i \{\xi\}) \right) \tilde{u} \right] (\xi, \tau) \quad (2.57)$$

2.2 The Floquet representation.

Let us recall the discontinuous section $\mathfrak{s}^d : \mathbb{S}_*^d \rightarrow \mathcal{X}^*$ and define the function $\Upsilon : \mathbb{S}_*^d \times \mathcal{X} \rightarrow \mathbb{S}^1 \subset \mathbb{C}$ by $\Upsilon(\mathbf{z}_*, x) := e^{2\pi i \langle \mathfrak{s}^d(\mathbf{z}_*), x \rangle}$ such that for any function $F \in \mathcal{G}$, its restriction to $E_* \subset \mathcal{X}^*$ multiplied with Υ becomes a periodic function on \mathbb{S}_*^d . The problem is that now the fiber is no longer constant. If we denote by $\Upsilon_{\mathbf{z}_*}$ the operator of multiplication with the function $\Upsilon(\mathbf{z}_*, \mathfrak{s}^d(\cdot))$ on $L^2(\mathbb{S}^d)$ and define Hilbert spaces $\mathfrak{F}_{\mathbf{z}_*} := \Upsilon_{\mathbf{z}_*} \mathcal{E}_{\mathbf{z}_*}^* = \Upsilon_{\mathbf{z}_*} L^2(\mathbb{S}^d)$ we can easily verify that the family

$$\{\Upsilon_{\mathbf{z}_*} u, u \in L^2(\mathbb{S}^d)\}_{\mathbf{z}_* \in \mathbb{S}_*^d} \subset \prod_{\mathbf{z}_* \in \mathbb{S}_*^d} \mathfrak{F}_{\mathbf{z}_*} \quad (2.58)$$

defines a measurable (and even smooth) "field of vectors" in the sense of ⁽⁵⁾ and we can associate to it a direct integral

$$\mathfrak{F} := \int_{\mathbb{S}_*^d}^{\oplus} dz_* \mathfrak{F}_{\mathbf{z}_*} \quad (2.59)$$

that is unitarily equivalent with our Hilbert space $\mathcal{G} \cong L^2(\mathcal{E}^*; \mathbb{S}_*^d)$; let us denote by $\mathcal{F}^\dagger : \mathcal{G} \rightarrow \mathfrak{F}$ this unitary (i.e. the operator of multiplication with the function Υ) and by $\mathcal{F}_\Gamma := \mathcal{F}^\dagger \circ \mathcal{U}_\gamma^\dagger$. Explicitely we have that for any $f \in L^2(\mathcal{X})$

$$(\mathcal{F}_\Gamma f)(x, \theta) = \sum_{\gamma \in \mathbb{Z}^d} f(\gamma + x) e^{-2\pi i \langle \theta, \gamma \rangle} \quad (2.60)$$

⁵J. Dixmier ("Les algèbres d'opérateurs dans l'espaces Hilbertien" Definition 3.1 in ch. II §1)

3 The periodic Schrödinger Hamiltonian.⁶

We shall look at the above problem having in mind one of its very important and intensively studied application in the mathematical description of periodic quantum Hamiltonians. Without trying to make a real introduction into the foundations of the mathematical description of physical systems let us very briefly try to formulate the problem of mathematical physics that we have in view.

3.1 Mathematical description of physical observables.

- *systems of particles evolving in a 3-dimensional real affine space with the time considered as a real parameter.*
- their *state* is characterised by two families of real vectorial observables: *the position* associated with the 3-dimensional real affine space \mathcal{X} where we observe the particles moving and *the momentum* that the mathematical description associates with the dual \mathcal{X}^* .
This feature is in some sense the manifestation of the "law of movement" being a second order differential equation.
- **Fixing a frame:** $\mathfrak{F}_0 := \{x^\circ, \mathcal{T}(e^1)x^\circ, \dots, \mathcal{T}(e^d)x^\circ\} \subset \mathcal{X}$ with $x^\circ \in \mathcal{X}$ and $\{e^j\}_{1 \leq j \leq d} \subset \mathbb{R}^d$ the canonical linear basis of \mathbb{R}^d , we can identify $\mathcal{X} \equiv \mathbb{R}^d$. Then $\mathcal{X}^* \cong \mathbb{R}^d$ is its dual with $\langle \cdot, \cdot \rangle: \mathcal{X}^* \times \mathcal{X} \rightarrow \mathbb{R}$ the duality map.
- its *physical observables* are described by functions of the 'state' observables position and momentum.
- One of these observables, the one measuring the energy, called the Hamiltonian of the system is also the *generator of the time evolution*.
- **For the classical theory** the states are points of a finite dimensional real symplectic space $\Xi := \mathcal{X} \times \mathcal{X}^*$ with symplectic form $\sigma((x, \xi), (y, \eta)) := \langle \xi, y \rangle - \langle \eta, x \rangle$, with the evolution defined by the flow of the vector field associated to the Hamiltonian function by the symplectic form σ .
- **For the quantum theory,**
 - the states are points of the projective space of an infinite dimensional complex Hilbert space \mathcal{H}
 - the physical observables are self-adjoint operators on the given Hilbert space \mathcal{H} .
 - the basic *interpretation rule* is
the mean value of the observable associated to the operator T in the state described by the 1-dimensional projection $q \in \mathbb{P}(\mathcal{H})$ is given by $\text{Tr}(qT) \in \mathbb{R}$.

⁶Michael Reed, Barry Simon, *Analysis of Operators, Vol. IV*. Academic Press 1978.

3.1.1 Self-adjoint operators.

In fact there are 4 main aspects concerning self-adjoint operators in complex Hilbert spaces that are of importance for considering them as *mathematical objects associated to physical measurable observables*:

- Given a self-adjoint operator $T : \mathcal{D}(T) \rightarrow \mathcal{H}$ in the Hilbert space \mathcal{H} :
 - for any measurable function $F : \mathbb{R} \rightarrow \mathbb{C}$ we have a uniquely defined normal operator $F(T) : \mathcal{D}(F(T)) \rightarrow \mathcal{H}$;
 - the subset $\mathfrak{sp}(T) \subset \mathbb{R}$ gives the subset of *possible measured values* of the observable it represents.
 - there exists a spectral measure $E_T : \beta(\mathbb{R}) \rightarrow \mathcal{P}(\mathcal{H})$ such that $T = \int_{\mathfrak{sp}(T)} E_T(dt)$.
- The Stone Theorem states that there exists a bijective correspondence between self-adjoint operators T in \mathcal{H} and 1-parameter unitary, strongly continuous groups $\mathbb{R} \ni t \mapsto U_T(t) \in \mathcal{U}(\mathcal{H})$ on \mathcal{H} given explicitly by

$$U_T(t) = \exp \{-itT\}.$$

The time evolution. Finally, given the Hamiltonian self-adjoint operator $H : \mathcal{D}(H) \rightarrow \mathcal{H}$ representing *the energy* of the system, the time evolution is given by the unitary strongly continuous 1-parameter group $U_H(t) = e^{-itH}$ in the sense that $U_H(t)qU_H(t)^* \in \mathbb{P}(\mathcal{H})$ is the state at time $t \in \mathbb{R}$ corresponding to the state $q \in \mathbb{P}(\mathcal{H})$ at time 0.

Fundamental self-adjointness criterion. Suppose given a symmetric operator

$$T : \mathcal{D}(T) \rightarrow \mathcal{H}.$$

Then it is self-adjoint if and only if $(T \pm i\mathbf{1})\mathcal{D}(T) = \mathcal{H}$.

Remark 3.7. Clearly, if $T : \mathcal{D}(T) \rightarrow \mathcal{H}$ is a self-adjoint linear operator and $a \in \mathbb{R}$, then $T + a\mathbf{1} : \mathcal{D}(T) \rightarrow \mathcal{H}$ is self-adjoint.

In fact we have

$$\mathcal{D}((T + a\mathbf{1})^*) = \{f \in \mathcal{H}, \exists g \in \mathcal{H}, \langle f, (T + a\mathbf{1})h \rangle_{\mathcal{H}} = \langle g, h \rangle_{\mathcal{H}}\} \quad (3.61)$$

$$= \{f \in \mathcal{H}, \exists g \in \mathcal{H}, \langle f, Th \rangle_{\mathcal{H}} = \langle g - af, h \rangle_{\mathcal{H}}\} \quad (3.62)$$

$$= \mathcal{D}(T^*) = \mathcal{D}(T). \quad (3.63)$$

3.1.2 The Weyl system.

In the quantum theory the relation between states and observables is more subtle and we can no longer interpret the main observables defining a classical state: the position and the momentum observables as some kind of 'coordinates of the state'(!). Instead we can still view the rest of the observables as '*functions*' of these basic observables for a non-commutative calculus: *the Weyl calculus*.

- In fact we can consider a *Weyl system*, as a strongly continuous application

$$W : \Xi \ni X \mapsto W(X) \in \mathcal{U}(\mathcal{H})$$

that verifies the identity: $W(X)W(Y) = e^{(i/2)\sigma(X,Y)}W(X+Y)$.

- Taking into account that $\Xi = \mathcal{X} \times \mathcal{X}^*$ we shall emphasize the existence of the following unitary strongly continuous representation of $\mathcal{X} \cong \mathbb{R}^d$:

$$\mathcal{X} \ni x \mapsto U(x) := W((x, 0)) \in \mathcal{U}(\mathcal{H}). \quad (3.64)$$

- Then the space $\mathcal{S} \subset \mathcal{H}$ of smooth vectors for the 1-parameter unitary strongly continuous groups

$$\mathbb{R} \ni t \mapsto W_X(t) := W(tX) \in \mathcal{U}(\mathcal{H})$$

indexed by $X \in \Xi$ defines a canonical Fréchet space associated to the Weyl system, continuously embedded in \mathcal{H} . Let \mathcal{S}' be its dual with the dual continuous embedding $\mathcal{H} \rightarrow \mathcal{S}'$.

- Some technical arguments allow to define for any $F \in \mathcal{S}'(\Xi)$ the following integrals

$$\mathfrak{Op}(F) := (2\pi)^{-d} \int_{\Xi} dZ \left(\int_{\Xi} dX e^{i\sigma(X,Z)} F(X) \right) W(Z)$$

considered as oscillatory integrals of sesqui-linear forms on \mathcal{H} . One can prove that we obtain a topological and linear isomorphism

$$\mathfrak{Op} : \mathcal{S}'(\Xi) \xrightarrow{\sim} \mathcal{L}(\mathcal{S}; \mathcal{S}')$$

with $\mathcal{L}(\mathcal{V}_1; \mathcal{V}_2)$ the linear space of continuous operators from the locally convex space \mathcal{V}_1 to the locally convex space \mathcal{V}_2 .

We shall be interested by the movement of a quantum particle in the real affine space of dimension $d = 1, 2, 3$ in the presence of a *regular lattice of fixed atoms*, representing a first approximation for the movement of electrons in solids, a system of enormous theoretical and practical interest.

3.2 The problem.

1. We start with a d -dimensional real affine space \mathcal{X} in which we suppose embedded a regular lattice $\Gamma \subset \mathcal{X}$; we shall be mainly interested in the case $d = 1, 2, 3$.
2. Suppose that the lattice Γ is generated by the d linearly independent vectors $\{e_j\}_{1 \leq j \leq d}$ starting from a point $x^0 \in \Gamma \subset \mathcal{X}$. Modulo a *change of basis matrix* we may suppose that the above frame $\{x^0, e_1, \dots, e_d\}$ also gives the identification $\mathcal{X} \equiv \mathbb{R}^d$ i.e. the configuration space with the Lie group acting on it freely and transitively. Then we identify also $\Gamma \equiv \mathbb{Z}^d$ as normal discrete subgroup of \mathbb{R}^d .

Many times we shall 'tacitly' identify $\mathcal{X} \equiv \mathbb{R}^d$ and $\Gamma \equiv \mathbb{Z}^d$.

We shall denote by $E \subset \mathcal{X}$ the *unit cell* of $\Gamma \subset \mathcal{X}$ defined as the image of the Borel section. We shall also denote by $E_* \subset \mathcal{X}^*$ the unit cell of the dual space.

3. We fix some function $V \in L^2_{\text{loc}}(\mathcal{X}; \mathbb{R})$ that is Γ -periodic, i.e. $V(x + \gamma) = V(x)$ for any $\gamma \in \Gamma$ and a.e. in $x \in \mathcal{X}$. We conclude that $V \in L^2_{\text{loc,unif}}(\mathcal{X}; \mathbb{R})$.
4. We consider the linear differential operator $-\Delta : BC^\infty(\mathcal{X}) \rightarrow BC^\infty(\mathcal{X})$ given by

$$-\Delta := \sum_{1 \leq j \leq d} (-i\partial_{x_j})^2 \equiv \sum_{1 \leq j \leq d} D_j^2. \quad (3.65)$$

We consider its restriction

$$-\Delta|_{C_0^\infty(\mathcal{X})} : C_0^\infty(\mathcal{X}) \rightarrow C_0^\infty(\mathcal{X}) \quad (3.66)$$

and the operator sum

$$-\Delta|_{C_0^\infty(\mathcal{X})} + V(Q) : C_0^\infty(\mathcal{X}) \rightarrow C_0^\infty(\mathcal{X}). \quad (3.67)$$

3.3 The periodic Hamiltonian.

We are working on the Hilbert space $L^2(\mathcal{X})$ considered as the natural representation of \mathbb{R}^d by translations on itself (see (3.64)).

\mathbf{H}_0 :

- We know that the differential operator $-\Delta|_{C_0^\infty(\mathcal{X})} : C_0^\infty(\mathcal{X}) \rightarrow C_0^\infty(\mathcal{X}) \subset L^2(\mathcal{X})$ **has a self-adjoint extension H_0 with domain**

$$\mathcal{D}(H_0) := \mathcal{F}^{-1} \left\{ f \in L^2(\mathcal{X}^*), (1 + |\cdot|^2)f \in L^2(\mathcal{X}^*) \right\} = \quad (3.68)$$

$$= \left\{ f \in L^2(\mathcal{X}^*), (1 - \Delta)f \in L^2(\mathcal{X}^*) \right\} \equiv \mathcal{H}^2(\mathbb{R}^d). \quad (3.69)$$

where $(1 - \Delta)f$ is considered in the sense of tempered distributions.

Using the derivatives in the sense of distributions: H_0 **is the closure of** $-\Delta|_{C_0^\infty(\mathcal{X})}$.

- For any $a \geq 0$ the operator $(H_0 + a\mathbf{1} \pm i\mathbf{1}) = \mathcal{F}^{-1}(|\cdot|^2 + a \pm i)\mathcal{F}$ is invertible (the function $|\xi|^2 + a \pm i$ being invertible) and has the inverse $\mathcal{F}^{-1}(|\cdot|^2 + a \pm i)^{-1}\mathcal{F}$.
- Given $f \in L^2(\mathcal{X})$ and $p \geq 2$ (we can also take $p = \infty$), we have

$$\|(H_0 + (a \pm i)\mathbf{1})^{-1}f\|_p = \left\| \mathcal{F}^{-1}(Q_*^2 + a \pm i)^{-1}\hat{f} \right\|_p \leq \left\| (Q_*^2 + a \pm i)^{-1}\hat{f} \right\|_{p'} \quad (3.70)$$

$$\leq \left(\int_{\mathbb{R}} dt (t^2 + a)^{-q} t^{d-1} \right)^{1/q} \|f\|_2 \quad (3.71)$$

using the inequalities Hausdorff-Young and Hölder with $p' = p(p-1)^{-1}$ and $q = 2p'(2-p')^{-1}$. For $q > d/2$ the integral above is finite and we have the estimation

$$\left(\int_{\mathbb{R}} dt (t^2 + a)^{-q} t^{d-1} \right)^{1/q} = C(d, q) a^{d/2q-1} \leq C(d, q) a^s, \quad \text{with } s < 0. \quad (3.72)$$

- We conclude that for $f \in L^2(\mathcal{X})$ and $p > 2$, for any $\epsilon > 0$ there exists some constant $C(d, p) > 0$ depending only on the dimension and on the exponent $p > 2$ such that

$$\|(H_0 + (a \pm i)\mathbf{1})^{-1}f\|_p \leq C(d, p)\epsilon \|f\|_{L^2(\mathcal{X})}. \quad (3.73)$$

- Equivalently, for any $p > 2$ and any $\epsilon > 0$ there exists some finite constant $C(d, p, \epsilon) > 0$ such that for any $f \in \mathcal{H}^2(\mathcal{X})$ we have that

$$\|f\|_p \leq \epsilon \|H_0 f\|_{L^2(\mathcal{X})} + C(d, p, \epsilon) \|f\|_{L^2(\mathcal{X})}. \quad (3.74)$$

\mathbf{V} :

- We can consider the linear operator of multiplication with V defined above

$$C_0^\infty(\mathcal{X}) \ni \phi \mapsto V\phi \in L^2(\mathcal{X}) \quad (3.75)$$

and the unbounded self-adjoint operator it induces in $L^2(\mathcal{X})$

$$V : \mathcal{D}(V) := \{f \in L^2(\mathcal{X}), Vf \in L^2(\mathcal{X})\} \rightarrow L^2(\mathcal{X}). \quad (3.76)$$

H₀ + V :

- $C_0^\infty(\mathcal{X}) \subset \mathcal{D}(H_0) \cap \mathcal{D}(V) \in L^2(\mathcal{X})$, thus $H_0\phi + V\phi$ for any $\phi \in C_0^\infty(\mathcal{X})$.
- For any $a \geq 0$ we can write

$$(H_0 + V + a\mathbf{1} \pm i\mathbf{1}) = \left[\mathbf{1} + V(H_0 + a\mathbf{1} \pm i\mathbf{1})^{-1} \right] (H_0 + a\mathbf{1} \pm i\mathbf{1}) \quad (3.77)$$

- **The partition of unity:**

- let us choose a function $\chi \in C_0^\infty(2E; [0, 1])$ with $\chi|_E = 1$ (where $2E := \{2x, x \in E\}$).
- For any $\gamma \in \Gamma$ we consider the translate $\mathcal{J}(\gamma)\chi$ (i.e. $(\mathcal{J}(\gamma)\chi)(x) := \chi(x + \gamma)$).
- any point $x \in \mathcal{X}$ belongs to the supports of at most 2^d functions in $\{\mathcal{J}(\gamma)\chi\}_{\gamma \in \Gamma}$.
- the following series is well defined, invariant for translations by $\gamma \in \Gamma$ and:

$$1 \leq \sum_{\gamma \in \Gamma} (\mathcal{J}(\gamma)\chi(x)) \leq 2^d, \quad \forall x \in \mathcal{X}, \quad (3.78)$$

- Let $\tilde{\chi}(x) := \chi(x) \left(\sum_{\gamma \in \Gamma} \mathcal{J}(\gamma)\chi(x) \right)^{-1}$ and define $\varphi_\gamma := \mathcal{J}(\gamma)\tilde{\chi}$ for any $\gamma \in \Gamma$.

- they take values in $[0, 1]$, have supports in $\mathcal{J}(\gamma)(2E)$ for each $\gamma \in \Gamma$ and satisfy:

$$\sum_{\gamma \in \Gamma} \varphi_\gamma(x) = 1, \quad \forall x \in \mathcal{X}. \quad (3.79)$$

- Moreover we can find a second function $\dot{\chi} \in C_0^\infty(3E; [0, 1])$ with $\chi|_{2E} = 1$ such that:

$$1 \leq \sum_{\gamma \in \Gamma} (\mathcal{J}(\gamma)\dot{\chi}(x)) \leq C, \quad \forall x \in \mathcal{X}, \quad (3.80)$$

$$\partial^\alpha \tilde{\chi} = \dot{\chi}(\partial^\alpha \tilde{\chi}), \quad \forall \alpha \in \mathbb{N}^d. \quad (3.81)$$

We shall use the notation $\dot{\varphi}_\gamma := \mathcal{J}(\gamma)\dot{\chi}$.

- for any $f \in \mathcal{H}^2(\mathcal{X})$ we can write:

$$\begin{aligned} (Vf)(x) &= \sum_{\gamma \in \Gamma} \varphi_\gamma(x) V(x) f(x) \\ |(Vf)(x)|^2 &\leq C(d) \sum_{\gamma \in \Gamma} \varphi_\gamma(x)^2 V(x)^2 |f(x)|^2 \\ \|Vf\|_{L^2(x)}^2 &\leq C(d) \left(\sup_{\gamma \in \Gamma} \|\varphi_\gamma V\|_{L^2(x)}^2 \right) \sum_{\gamma \in \Gamma} \|\varphi_\gamma f\|_\infty^2 \\ &\leq C(d) \left(\sup_{\gamma \in \Gamma} \|\varphi_\gamma V\|_{L^2(x)}^2 \right) \sum_{\gamma \in \Gamma} \left(\epsilon \|H_0 \varphi_\gamma f\|_2^2 + C(d, \epsilon) \|\varphi_\gamma f\|_2^2 \right) \end{aligned} \quad (3.82)$$

using (3.74) at point (4.) above.

- Let us compute

$$H_0\varphi_\gamma f = \sum_{1 \leq j \leq d} (-i\partial_j)^2(\varphi_\gamma f) \quad (3.83)$$

$$= \sum_{1 \leq j \leq d} \left[\varphi_\gamma((-i\partial_j)^2 f) + 2((-i\partial_j)\varphi_\gamma)((-i\partial_j)f) + f((-i\partial_j)^2\varphi_\gamma) \right] \quad (3.84)$$

and using

$$\|((-i\partial_j)\varphi_\gamma)((-i\partial_j)f)\|_2^2 = \langle((-i\partial_j)\varphi_\gamma)((-i\partial_j)f), ((-i\partial_j)\varphi_\gamma)((-i\partial_j)f)\rangle_2 \quad (3.85)$$

$$= 2\langle(\partial_j\varphi_\gamma)(\partial_j^2\varphi_\gamma)(\partial_j f), f\rangle_2 + \langle(\partial_j\varphi_\gamma)^2(\partial_j^2 f), f\rangle_2 \\ \leq C\left[\|\dot{\varphi}_\gamma H_0 f\|_2^2 + \|\dot{\varphi}_\gamma f\|_2^2\right] \quad (3.86)$$

we obtain

$$\sum_{\gamma \in \Gamma} \|H_0\varphi_\gamma f\|_2^2 \leq C \sum_{\gamma \in \Gamma} \left[\|\dot{\varphi}_\gamma H_0 f\|_2^2 + \|\dot{\varphi}_\gamma f\|_2^2 \right] \leq C' \left[\|H_0 f\|_2^2 + \|f\|_2^2 \right]. \quad (3.87)$$

- Coming back to (3.82) we conclude that

$$\|Vf\|_{L^2(\mathcal{X})}^2 \leq C(d) \left[\epsilon \|H_0 f\|_2^2 + C(\epsilon) \|f\|_2^2 \right] \quad (3.88)$$

or equivalently that for any $\epsilon > 0$ there is some $a_\epsilon \geq 0$ such that

$$\left(V(H_0 + a_\epsilon \mathbf{1} \pm i\mathbf{1})^{-1} \right)(x) \leq \epsilon. \quad (3.89)$$

- It follows that the operator $\left[\mathbf{1} + V(H_0 + a_\epsilon \mathbf{1} \pm i\mathbf{1})^{-1} \right]$ is invertible in $L^2(\mathcal{X})$ and thus it is surjective. From (3.77), using also the surjectivity of $(H_0 + a_\epsilon \mathbf{1} \pm i\mathbf{1})$ and the Fundamental self-adjointness criterium, we obtain the self-adjointness of the operator $(H_0 + V + a_\epsilon \mathbf{1})$ for $\epsilon \in (0, 1)$ on the domain $\mathcal{H}^2(\mathcal{X})$ of H_0 .

Proposition 3.8. *The operator $H_V := H_0 + V : \mathcal{H}^2(\mathcal{X}) \rightarrow L^2(\mathcal{X})$ is well defined and self-adjoint.*

We evidently have invariance for any translations with elements in Γ :

$$\mathcal{T}^*(\gamma)\mathcal{H}^2(\mathcal{X}) = \mathcal{H}^2(\mathcal{X}); \quad \mathcal{T}^*(\gamma)^{-1}H_V\mathcal{T}^*(\gamma) = H_V, \quad \forall \gamma \in \Gamma. \quad (3.90)$$

3.4 The Bloch-Floquet-Zak representation of the Hamiltonian.

Let us consider now the Bloch-Floquet-Zak transform of the Hamiltonian $H_V : \mathcal{H}^2(\mathcal{X}) \rightarrow L^2(\mathcal{X})$.

$$\left(\widetilde{\mathcal{U}}_\Gamma(\partial_{x_j} f)\right)(\mathbf{z}, \tilde{\xi}) = 2\pi i \left(\mathcal{U}^\dagger(Q_{*,j} \hat{f})\right)(\mathbf{z}, \tilde{\xi}) = 2\pi i \sum_{\gamma^* \in \Gamma_*} e^{2\pi i \langle \gamma^*, \mathbf{s}^d(\mathbf{z}) \rangle} (\tilde{\xi}_j + \gamma_j^*) \hat{f}(\tilde{\xi} + \gamma^*) \quad (3.91)$$

$$= \left((2\pi i \tilde{\xi}_j + \tilde{\partial}_j) \tilde{f}\right)(\mathbf{z}, \tilde{\xi}) = \left((2\pi i(\mathbf{1} \otimes Q_{*,j}) + (\tilde{\partial}_j \otimes \mathbf{1})) \tilde{f}\right)(\mathbf{z}, \tilde{\xi}) \quad (3.92)$$

where $\tilde{\partial}_j$ is the derivative with respect to the coordinate on the j -th factor of the direct product \mathbb{S}^d ; more precisely we have $\tilde{\partial}_j = \mathbf{e}_*^d \partial_{x_j}$ as tangent fields.

$$\left(\widetilde{\mathcal{U}}_\Gamma(-\Delta f)\right)(\mathbf{z}, \tilde{\xi}) = \left(\left(\sum_{1 \leq j \leq d} (2\pi i \tilde{\xi}_j + \tilde{\partial}_j)^2\right) \tilde{f}\right)(\mathbf{z}, \tilde{\xi}). \quad (3.93)$$

- Thus: $\widetilde{\mathcal{U}}_\Gamma \mathcal{H}^2(\mathcal{X}) =: \mathcal{G}_2$ is the Hilbert space obtained by completion of the space

$$\mathcal{G}_\infty := \left\{ F \in C^\infty(\mathcal{X}^*; C^\infty(\mathbb{S}^d)), (\mathcal{J}(\gamma^*)F)(\xi) = U^\dagger(\gamma^*)F(\xi), \forall (\gamma^*, \xi) \in \Gamma_* \times \mathcal{X}^* \right\} \quad (3.94)$$

for the Hilbertian norm

$$\|F\|_{\mathcal{G}_2}^2 := \int_{E_*} d\tilde{\xi} \|F(\tilde{\xi})\|_{\mathcal{H}^2(\mathbb{S}^d)}^2. \quad (3.95)$$

- For the *position operator*:

$$\left(\widetilde{\mathcal{U}}_\Gamma(Q_j f)\right)(\mathbf{z}, \tilde{\xi}) = -\frac{i}{2\pi} \left(\mathcal{U}^\dagger(\partial_{\xi_j} \hat{f})\right)(\mathbf{z}, \tilde{\xi}) = -\frac{i}{2\pi} \sum_{\gamma^* \in \Gamma_*} e^{2\pi i \langle \gamma^*, \mathbf{s}^d(\mathbf{z}) \rangle} (\partial_{\xi_j} \hat{f})(\tilde{\xi} + \gamma^*) \quad (3.96)$$

$$\forall W \in C(\mathbb{S}^d) \implies \left(\widetilde{\mathcal{U}}_\Gamma W(\mathbf{e}^d(Q))f\right)(\mathbf{z}, \tilde{\xi}) = W(\mathbf{z}) \tilde{f}(\mathbf{z}, \tilde{\xi}). \quad (3.97)$$

- In conclusion

$$\left(\widetilde{\mathcal{U}}_\Gamma(H_V f)\right)(\mathbf{z}, \tilde{\xi}) = \left(\left(\sum_{1 \leq j \leq d} (2\pi i \tilde{\xi}_j + \tilde{\partial}_j)^2 + V(\mathbf{z})\right) \tilde{f}\right)(\mathbf{z}, \tilde{\xi}). \quad (3.98)$$

All our operators act in \mathcal{G} and thus have a continuation for $(\mathbf{z}, \xi) \in \mathbb{S}^d \times \mathcal{X}^*$ that leaves invariant the condition

$$(\mathcal{J}(\gamma^*)F)(\xi) = U^\dagger(\gamma^*)F(\xi), \quad \forall (\gamma^*, \xi) \in \Gamma_* \times \mathcal{X}^* \quad (3.99)$$

We conclude that

$$\mathcal{J}(\gamma^*) \widetilde{\mathcal{U}}_\Gamma T \widetilde{\mathcal{U}}_\Gamma^{-1} \mathcal{J}(\gamma^*)^{-1} = U^\dagger(\gamma^*) \widetilde{\mathcal{U}}_\Gamma T \widetilde{\mathcal{U}}_\Gamma^{-1} U^\dagger(\gamma^*)^{-1}, \quad \forall \gamma^* \in \Gamma_*. \quad (3.100)$$

Conclusion 3.9. *Thus, in the BFZ representation, the Hamiltonian H_V has the domain*

$$\mathcal{G}^2 = \left\{ F \in L_{\text{loc}}^2(\mathcal{X}^*; \mathcal{H}^2(\mathbb{S}^d)), (\mathcal{J}(\gamma^*)F)(\xi) = \epsilon_{-\gamma^*} F(\xi), \forall \gamma^* \in \Gamma_* \right\}$$

and is given by a family of differential operators

$$\left\{ \tilde{H}_{V,\xi} : \mathcal{H}^2(\mathbb{S}^d) \rightarrow L^2(\mathbb{S}^d), \tilde{H}_{V,\xi} := U^\dagger([\xi]_2) \left[(2\pi i \{\xi\}_2 + \tilde{\nabla})^2 + V(Q) \right] U([\xi]_2)^{-1} \right\}_{\xi \in \mathcal{X}^*}$$

so that

$$\left(\widetilde{\mathcal{U}}_\Gamma(H_V)(\widetilde{\mathcal{U}}_\Gamma^{-1}F)\right)(\mathbf{z}, \xi) = \left(\tilde{H}_{V,\xi}F(\xi)\right)(\mathbf{z}).$$

3.5 Properties of the Bloch-Floquet-Zak Hamiltonians.

1. Making a discrete Fourier transform it is rather evident that for any $\tilde{\xi} \in E_*$ the differential operator

$$\tilde{H}_{0,\tilde{\xi}} := (2\pi i\tilde{\xi} + \tilde{\nabla})^2 : \mathcal{H}^2(\mathbb{S}^d) \rightarrow L^2(\mathbb{S}^d) \quad (3.101)$$

is self-adjoint and positive definite.

2. Thus, for any $\tilde{\xi} \in E_*$, the resolvent set of $\tilde{H}_{0,\tilde{\xi}}$ contains $\mathbb{R} \setminus [0, \infty)$ and $\mathbb{C} \setminus \mathbb{R}$. Let us consider some $a > 0$, so that $-a \in \rho(\tilde{H}_{0,\tilde{\xi}})$, and the associated resolvent $(\tilde{H}_{0,\tilde{\xi}} + a\mathbf{1})^{-1}$. We notice that

$$(\mathcal{F}^{-1}(\tilde{H}_{0,\tilde{\xi}} + a\mathbf{1})^{-1}\hat{\phi})_{\gamma^*} = (4\pi^2(\tilde{\xi} + \gamma^*)^2 + a)^{-1}\hat{\phi}_{\gamma^*} \quad (3.102)$$

admits each vector \mathbf{v}_{γ^*} of the canonical orthonormal basis of $\mathfrak{l}^2(\Gamma^*)$ as eigenvector with eigenvalue $(4\pi^2(\tilde{\xi} + \gamma^*)^2 + a)^{-1} \in \mathbb{R}_+$. But $\lim_{|\gamma^*| \nearrow \infty} (4\pi^2(\tilde{\xi} + \gamma^*)^2 + a)^{-1} = 0$. Thus **the resolvent** $(\tilde{H}_{0,\tilde{\xi}} - \delta\mathbf{1})^{-1}$ **is compact** for any $\tilde{\xi} \in E_*$ and any $\delta \in \rho(\tilde{H}_{0,\tilde{\xi}})$.

3. Repeating the arguments in paragraph 3.2.(4) we obtain (3.74) also for functions defined on \mathbb{S}^d with the natural measure and with H_0 replaced by the Laplace operator on the d -dimensional torus denoted by $-\tilde{\Delta}$. Thus, taking $p = \infty$ we notice that for any $f \in \mathcal{H}^2(\mathbb{S}^d)$

$$\boxed{\|Vf\|_2 \leq \|V\|_2 \|f\|_\infty \leq \|V\|_2 [\epsilon \|-\tilde{\Delta}f\|_2 + C(\epsilon)\|f\|_2].} \quad (3.103)$$

Using this estimation we notice further that for any $a > 0$ we can write:

$$\left\| V \left((2\pi i\tilde{\xi} + \tilde{\nabla})^2 + (a \pm i)\mathbf{1} \right)^{-1} \phi \right\|_{L^2(\mathbb{S}^d)}^2 \quad (3.104)$$

$$\begin{aligned} &\leq C(d) \|V\|_{L^2(\mathbb{S}^d)}^2 \left[\epsilon \left\| (-\tilde{\Delta}) \left((2\pi i\tilde{\xi} + \tilde{\nabla})^2 + (a \pm i)\mathbf{1} \right)^{-1} \phi \right\|_{L^2(\mathbb{S}^d)}^2 \right. \\ &\quad \left. + C(\epsilon) \left\| \left((2\pi i\tilde{\xi} + \tilde{\nabla})^2 + (a \pm i)\mathbf{1} \right)^{-1} \phi \right\|_{L^2(\mathbb{S}^d)}^2 \right] \quad (3.105) \end{aligned}$$

$$\begin{aligned} &\leq C(d) \|V\|_{L^2(\mathbb{S}^d)}^2 \sum_{\gamma^* \in \Gamma^*} [\epsilon |\gamma^*|^2 + C(\epsilon)] \left| 4\pi^2(\tilde{\xi} + \gamma^*)^2 + (a \pm i) \right|^{-2} |\hat{\phi}_{\gamma^*}|^2 \\ &\leq C(d) (\epsilon + C(\epsilon)a^{-2}) \|V\|_{L^2(\mathbb{S}^d)}^2 \|\phi\|_{L^2(\mathbb{S}^d)}^2 < \underline{C'(\epsilon + C(\epsilon)a^{-2})} \|\phi\|_{L^2(\mathbb{S}^d)}^2 \quad (3.106) \end{aligned}$$

for $\epsilon > 0$ small enough and $a > 0$ large enough.

We conclude that the operator $\tilde{H}_{V,\tilde{\xi}} : \mathcal{H}^2(\mathbb{S}^d) \rightarrow L^2(\mathbb{S}^d)$ **is self-adjoint** for any $\tilde{\xi} \in E_*$.

4. Let us also notice that our above result implies that for any $\phi \in \mathcal{H}^2(\mathbb{S}^d)$ we can write

$$\|V\phi\|_2 \leq \epsilon \|H_0\phi\|_2 + C(\epsilon)\|\phi\|_2 \leq \epsilon \|H_V\phi\|_2 + \epsilon \|V\phi\|_2 + C(\epsilon)\|\phi\|_2 \quad (3.107)$$

and conclude that

$$\|V\phi\|_2 \leq \frac{\epsilon}{1-\epsilon} \|H_V\phi\|_2 + \frac{C(\epsilon)}{1-\epsilon} \|\phi\|_2. \quad (3.108)$$

5. Moreover, we can use the above estimation in order to prove that $\tilde{H}_{V,\tilde{\xi}} : \mathcal{H}^2(\mathbb{S}^d) \rightarrow L^2(\mathbb{S}^d)$ **is bounded from below**:

$$\forall \phi \in \mathcal{H}^2(\mathbb{S}^d) : \quad \langle \phi, (H_0 + V + a\mathbf{1})\phi \rangle_2 > (a - C)\|\phi\|_2^2. \quad (3.109)$$

6. Further let us notice that we can write for any $\tilde{\xi} \in E_*$:

$$(\tilde{H}_{V,\tilde{\xi}} - \mathfrak{z}\mathbf{1})^{-1} = (\tilde{H}_{0,\tilde{\xi}} - \mathfrak{z}\mathbf{1})^{-1} - (\tilde{H}_{V,\tilde{\xi}} - \mathfrak{z}\mathbf{1})^{-1}V(\tilde{H}_{0,\tilde{\xi}} - \mathfrak{z}\mathbf{1})^{-1} \quad (3.110)$$

and deduce that

$$\|(\tilde{H}_{V,\tilde{\xi}} + a\mathbf{1})^{-1} - (\tilde{H}_{0,\tilde{\xi}} + a\mathbf{1})^{-1}\|_{\mathbb{B}(L^2(\mathbb{S}^d))} \leq \quad (3.111)$$

$$\leq \|(\tilde{H}_{V,\tilde{\xi}} + a\mathbf{1})^{-1}\|_{\mathbb{B}(L^2(\mathbb{S}^d))} \|V(\tilde{H}_{0,\tilde{\xi}} + a\mathbf{1})^{-1}\|_{\mathbb{B}(L^2(\mathbb{S}^d))} \quad (3.112)$$

$$< \frac{C(\epsilon + C(\epsilon)a^{-2})}{a - C} \quad (3.113)$$

and thus **can be made arbitrarily small** for $\epsilon > 0$ small enough and $a > C > 0$ large enough. We may conclude that for $a > 0$ large enough, the resolvent $(\tilde{H}_{V,\tilde{\xi}} + a\mathbf{1})^{-1}$ is in the closure of the ideal of compact operators and thus it is compact. But for any $\mathfrak{z} \in \rho(\tilde{H}_{V,\tilde{\xi}})$ we can write

$$(\tilde{H}_{V,\tilde{\xi}} - \mathfrak{z}\mathbf{1})^{-1} = (\tilde{H}_{V,\tilde{\xi}} + a\mathbf{1})^{-1} - (a + \mathfrak{z})(\tilde{H}_{V,\tilde{\xi}} + a\mathbf{1})^{-1}(\tilde{H}_{V,\tilde{\xi}} - \mathfrak{z}\mathbf{1})^{-1} \quad (3.114)$$

and thus $(\tilde{H}_{V,\tilde{\xi}} - \mathfrak{z}\mathbf{1})^{-1}$ **is also compact** due to the ideal property of the subalgebra of compact operators.

7. Let us consider now the variation of the operators $\tilde{H}_{V,\tilde{\xi}} : \mathcal{H}^2(\mathbb{S}^d) \rightarrow L^2(\mathbb{S}^d)$ when we vary $\tilde{\xi} \in E_*$. First we notice that they have all of them the same domain $\mathcal{H}^2(\mathbb{S}^d)$. Then let us consider $\tilde{\xi}$ in the interior \mathring{E}_* of E_* . Thus for any such $\tilde{\xi}$ there exists a small neighbourhood of it $W_{\tilde{\xi}}$ such that $\tilde{\xi} \in W_{\tilde{\xi}} \subset E_*$. For any $\tilde{\eta} \in W_{\tilde{\xi}}$ we can write

$$\begin{aligned} (\tilde{H}_{V,\tilde{\xi}} - \mathfrak{z}\mathbf{1})^{-1} - (\tilde{H}_{V,\tilde{\eta}} - \mathfrak{z}\mathbf{1})^{-1} &= (\tilde{H}_{V,\tilde{\xi}} - \mathfrak{z}\mathbf{1})^{-1} \left[\tilde{H}_{0,\tilde{\eta}} - \tilde{H}_{0,\tilde{\xi}} \right] (\tilde{H}_{V,\tilde{\eta}} - \mathfrak{z}\mathbf{1})^{-1} \\ &= 2\pi i (\tilde{H}_{V,\tilde{\xi}} - \mathfrak{z}\mathbf{1})^{-1} (\tilde{\eta} - \tilde{\xi}) (2\pi i (\tilde{\xi} + \tilde{\eta}) + \tilde{\nabla}) (\tilde{H}_{V,\tilde{\eta}} - \mathfrak{z}\mathbf{1})^{-1}. \end{aligned} \quad (3.115)$$

If we notice that for any $\phi \in L^2(\mathbb{S}^d)$ we can write

$$\tilde{\partial}_j (\tilde{H}_{V,\tilde{\eta}} - \mathfrak{z}\mathbf{1})^{-1} \phi = \tilde{\partial}_j (\tilde{H}_{0,\tilde{\eta}} - \mathfrak{z}\mathbf{1})^{-1} (\tilde{H}_{0,\tilde{\eta}} - \mathfrak{z}\mathbf{1}) (\tilde{H}_{V,\tilde{\eta}} - \mathfrak{z}\mathbf{1})^{-1} \phi \quad (3.116)$$

$$= \left[\tilde{\partial}_j (\tilde{H}_{0,\tilde{\eta}} - \mathfrak{z}\mathbf{1})^{-1} \right] \left[\mathbf{1} - V(\tilde{H}_{V,\tilde{\eta}} - \mathfrak{z}\mathbf{1})^{-1} \right] \phi \quad (3.117)$$

$$= \left[\mathring{\mathcal{F}}^{-1} \frac{2\pi i Q_{*,j}}{4\pi^2 |\tilde{\eta} + Q_*|^2 - \mathfrak{z}} \mathring{\mathcal{F}} \right] \left[\mathbf{1} - V(\tilde{H}_{V,\tilde{\eta}} - \mathfrak{z}\mathbf{1})^{-1} \right] \phi \quad (3.118)$$

and we conclude that the operator $\tilde{\partial}_j (\tilde{H}_{V,\tilde{\eta}} - \mathfrak{z}\mathbf{1})^{-1} \phi$ is bounded in $L^2(\mathbb{S}^d)$

and thus that the application: $\mathring{E}_* \ni \tilde{\xi} \mapsto (\tilde{H}_{V,\tilde{\eta}} - \mathfrak{z}\mathbf{1})^{-1} \in \mathbb{B}(L^2(\mathbb{S}^d))$ **is analytic.**

8. Let us **consider now some point** $\tilde{\xi} \in \partial E_*$ and a small neighborhood of it $W \subset \mathcal{X}^*$ diffeomorphic to a d -dimensional disc. For any $\eta \in W$, using Conclusion 3.9 we can write:

$$\tilde{H}_{0,\eta} - \tilde{H}_{0,\tilde{\xi}} = U^\dagger([\eta]_2)\tilde{H}_{0,\{\eta\}_2}U^\dagger([\eta]_2)^{-1} - \tilde{H}_{0,\tilde{\xi}} \quad (3.119)$$

$$= \sum_{1 \leq j \leq d} \left[U^\dagger([\eta]_2)(2\pi i\{\eta_j\}_2 + \tilde{\partial}_j)^2 U^\dagger([\eta]_2)^{-1} - (2\pi i\tilde{\xi}_j + \tilde{\partial}_j)^2 \right] \quad (3.120)$$

$$= \sum_{1 \leq j \leq d} \left[(2\pi i\{\eta_j\}_2 + \partial_j + 2\pi i[\eta]_2)^2 - (2\pi i\tilde{\xi}_j + \partial_j)^2 \right] \quad (3.121)$$

and we recuperate the difference $\eta - \tilde{\xi}$ and thus the derivability of the norm of the resolvent with respect to the variable $\eta \in \mathcal{X}^*$.

3.6 Conclusion.

1. We have put into evidence a unitary transformation

$$\tilde{\mathcal{U}}_\Gamma : L^2(\mathcal{X}) \xrightarrow{\sim} \mathcal{G} := \{F \in L^2_{\text{loc}}(\mathcal{X}^*; L^2(\mathbb{S}^d)), (\mathcal{J}(\gamma^*)F)(\xi) = U^\dagger(\gamma^*)F(\xi), \forall (\gamma^*, \xi) \in \Gamma_* \times \mathcal{X}^*\}$$

where

$$(U^\dagger(\gamma^*)\phi)(\omega) := e^{-2\pi i \langle \gamma^*, \omega \rangle} \phi(\omega).$$

2. The space \mathcal{G} is canonically identified with the space of L^2 sections in the vector bundle $\rho : \mathcal{E}^* \rightarrow \mathbb{S}^d_*$ associated to the principal bundle $\mathfrak{e}^d : \mathbb{R}^d \rightarrow \mathbb{S}^d$ by the canonical diagonal representation $U^\dagger : \mathbb{Z}^d_* \rightarrow \mathcal{U}(L^2(\mathbb{S}^d))$. The transformed Hamiltonian is an analytic section in the vector bundle $\mathcal{L}(\mathcal{E}^*) \rightarrow \mathbb{S}^d$ associated to the principal bundle $\mathfrak{e}^d : \mathbb{R}^d \rightarrow \mathbb{S}^d$ by the canonical conjugate representation $\mathcal{L}(U^\dagger) : \mathbb{Z}^d \rightarrow \mathcal{H}om(\mathbb{B}(\mathcal{H}^2(\mathbb{S}^d); L^2(\mathbb{S}^d)))$.
3. The transformed Hamiltonian associated to H_V is given by multiplication (in the variable $\xi \in \mathcal{X}^*$) with an analytic family in the sense of Kato, of differential operators with compact resolvent:

$$\{\tilde{H}_{V,\xi} : \mathcal{H}^2(\mathbb{S}^d) \rightarrow L^2(\mathbb{S}^d), \tilde{H}_{V,\xi} := U^\dagger([\xi]_2)[(2\pi i\{\xi\}_2 + \tilde{\nabla})^2 + V(Q)]U^\dagger([\xi]_2)^{-1}\}_{\xi \in \mathcal{X}^*}.$$

4. Having compact resolvent, the spectrum of each Hamiltonian $\tilde{H}_{V,\xi} : \mathcal{H}^2(\mathbb{S}^d) \rightarrow L^2(\mathbb{S}^d)$, for any $\xi \in \mathcal{X}^*$, is a countable sequence of eigenvalues of finite multiplicity, diverging to $+\infty$:

$$\mathfrak{sp}(\tilde{H}_{V,\xi}) = \{\lambda_n(\xi)\}_{n \in \mathbb{N}}, \quad \lambda_n(\xi) < \lambda_{n+1}(\xi) \quad \forall n \in \mathbb{N}, \quad \lim_{m \nearrow \infty} \lambda_m(\xi) = +\infty \quad \forall \xi \in \mathcal{X}^*. \quad (3.122)$$

5. Suppose fixed some $\xi \in \mathcal{X}^*$ and some $\lambda_n(\xi) \in \mathfrak{sp}(\tilde{H}_{V,\xi})$. Then $\text{d}(\lambda_n(\xi), \mathfrak{sp}(\tilde{H}_{V,\xi}) \setminus \{\lambda_n(\xi)\}) > 0$ and we can find a circle $\mathcal{C}_n(\xi) \subset \mathbb{C} \setminus \mathfrak{sp}(\tilde{H}_{V,\xi})$ of radius $r > 0$ and center $\lambda_n(\xi)$ such that $\text{d}(\mathcal{C}_n(\xi), \mathfrak{sp}(\tilde{H}_{V,\xi})) \geq r > 0$ and its interior domain $\mathcal{D}_n(\xi) \subset \mathbb{C}$ satisfies $\mathcal{D}_n(\xi) \cap \mathfrak{sp}(\tilde{H}_{V,\xi}) = \{\lambda_n(\xi)\}$. Let us denote by $\mathfrak{p}_n(\xi) \in \mathbb{B}(L^2(\mathbb{S}^d))$ the eigenprojection corresponding to the eigenvalue $\lambda_n(\xi)$, i.e.:

$$\mathfrak{p}_n(\xi)\tilde{H}_{V,\xi}\mathfrak{p}_n(\xi) = \lambda_n(\xi)\mathfrak{p}_n(\xi) \quad (3.123)$$

Using the Riesz-Dunford calculus for the spectral region $\{\lambda_n(\xi)\}$ we obtain that

$$(a) \quad \mathfrak{p}_n(\xi) = -\frac{1}{2\pi i} \oint_{\mathcal{C}_n(\xi)} d\zeta (\tilde{H}_{V,\xi} - \zeta \mathbf{1})^{-1},$$

$$(b) \lambda_n(\xi) = -\frac{1}{2\pi i} \oint_{\mathcal{C}_n(\xi)} d\tilde{z} \tilde{z} (\tilde{H}_{V,\xi} - \tilde{z} \mathbf{1})^{-1}.$$

(c) Let $\mathbf{n}_n(\xi) := \dim(\mathbf{p}_n(\xi) \tilde{H}_{V,\xi}) \in \mathbb{N}$ be the multiplicity of the eigenvalue $\lambda_n(\xi)$.

6. The fact that the family $\{\tilde{H}_{V,\xi}\}_{\xi \in \mathcal{X}^*}$ is an analytic family in the sense of Kato, means that:

(a) the resolvent set $\rho(\tilde{H}_{V,\xi}) \subset \mathbb{C}$ is continuous with respect to the variables $\xi \in \mathcal{X}^*$, i.e. given any $\xi \in \mathcal{X}^*$, for any $\tilde{z} \in \rho(\tilde{H}_{V,\xi})$ there exists some $\delta > 0$ depending on ξ and \tilde{z} such that $|\eta - \xi| < \delta$ implies that $\tilde{z} \in \rho(\tilde{H}_{V,\eta})$,

(b) the resolvents $(\tilde{H}_{V,\xi} - \tilde{z} \mathbf{1})^{-1}$ appearing in the above Riesz-Dunford integrals are analytic functions of $\xi \in \mathcal{X}^*$ on some open domain depending on $\tilde{z} \in \mathbb{C}$.

7. Thus we can find a small neighborhood $W_\xi \subset \mathcal{X}^*$ of $\xi \in \mathcal{X}^*$ such that $d(\mathcal{C}_n(\xi), \mathbf{sp}(\tilde{H}_{V,\eta})) \geq r/2 > 0$ for any $\eta \in W_\xi$. Then

(a) if there exists some neighborhood W_ξ° of ξ such that $W_\xi^\circ \subset W_\xi$ and $\mathbf{n}_n(\eta) = p \in \mathbb{N}$ is constant for $\eta \in W_\xi^\circ$, then the eigenvalue $\lambda_n(\eta)$ has constant multiplicity p on W_ξ° and the application $W_\xi^\circ \ni \eta \mapsto \lambda_n(\eta) \in \mathbb{R}$ is real analytic; then also the application $\mathbf{p}_n : W_\xi^\circ \rightarrow \mathbb{B}(L^2(\mathbb{S}^d))$ is analytic (as vector valued function with values in a Banach space).

(b) if for any neighborhood W'_ξ of ξ such that $W'_\xi \subset W_\xi$ there exists some $\eta \in W'_\xi$ such that $\mathcal{D}_n(\xi) \cap \mathbf{sp}(\tilde{H}_{V,\eta})$ has at least two points, then there exists a neighborhood W_ξ° of ξ such that $W_\xi^\circ \subset W_\xi$ and $k \leq p$ continuous functions $\mu_j : W_\xi^\circ \rightarrow \mathbb{R}$ such that

- i. $\mu_j(\xi) = \lambda_n(\xi)$, for any $j \in \{1, \dots, k\}$ and
- ii. $\mathcal{D}_n(\xi) \cap \mathbf{sp}(\tilde{H}_{V,\eta}) = \bigcup_{1 \leq j \leq k} \{\mu_j(\eta)\}$ for any $\eta \in W_\xi^\circ$,

and p continuous functions $\mathbf{q}_j : W_\xi^\circ \rightarrow \mathbb{B}(L^2(\mathbb{S}^d))$ such that

- i. $\mathbf{q}_j(\eta) \tilde{H}_{V,\xi} \mathbf{q}_j(\eta) = \mu_j(\eta) \mathbf{q}_j(\eta)$ for any $j \in \{1, \dots, k\}$ and $\eta \in W_\xi^\circ$, and
- ii. $-\frac{1}{2\pi i} \oint_{\mathcal{C}_n(\xi)} d\tilde{z} (\tilde{H}_{V,\eta} - \tilde{z} \mathbf{1})^{-1} = \bigoplus_{1 \leq j \leq k} \mathbf{q}_j(\eta)$ for any $\eta \in W_\xi^\circ$.

8. We recall the U^\dagger -covariance of the vectors in \mathcal{G} and of the operator valued section

$$\mathcal{X}^* \ni \xi \mapsto \tilde{H}_{V,\xi} \in \mathbb{B}(\mathcal{H}^2(\mathbb{S}^d); L^2(\mathbb{S}^d)), \quad (3.124)$$

that meaning that $\tilde{H}_{V,\xi} = U^\dagger([\xi]_2) \tilde{H}_{V,\{\xi\}_2} [U^\dagger([\xi]_2)]^{-1}$. We conclude that the Hamiltonians $\tilde{H}_{V,\xi}$ and $\tilde{H}_{V,\{\xi\}_2}$ are unitarily equivalent for any $[\xi]_2 \in \mathbb{Z}^d$ and thus the functions $\lambda_n : \mathcal{X}^* \rightarrow \mathbb{R}$ are Γ_* -periodic and continuous for any $n \in \mathbb{N}$. Moreover they are analytic in all points $\xi \in \mathcal{X}^*$ with the exception of the points where they may intersect.

9. The projection valued functions $\mathbf{p}_n : \mathcal{X}^* \rightarrow \mathbb{B}(L^2(\mathbb{S}^d))$ satisfy the U^\dagger -covariance condition

$$\mathbf{p}_n(\xi + \gamma^*) = U^\dagger(\gamma^*) \mathbf{p}_n(\xi) [U^\dagger(\gamma^*)]^{-1}. \quad (3.125)$$

10. Let us consider some point $\xi \in \mathcal{X}^*$ and an eigenvector $\phi_n(\xi) \in \mathcal{H}^2(\mathbb{S}^d)$ verifying the equation:

$$\tilde{H}_{V,\xi} \phi_n(\xi) = \lambda_n(\xi) \phi_n(\xi), \text{ i.e. } \left[\sum_{1 \leq j \leq d} (-i\tilde{\partial}_j + \xi_j)^2 + V \right] \phi_n(\xi) = \lambda_n(\xi) \phi_n(\xi)(\xi). \quad (3.126)$$

Then

$$(-\tilde{\Delta} + 1)^{-1} \left[\sum_{1 \leq j \leq d} (-i\tilde{\partial}_j + \xi_j)^2 + V \right] \phi_n(\xi) = \lambda_n(\xi) (-\tilde{\Delta} + 1)^{-1} \phi_n(\xi) \quad (3.127)$$

$$\phi_n(\xi) + (-\tilde{\Delta} + 1)^{-1} (-i\xi \cdot \tilde{\nabla} + |\xi|^2 - \mathbf{1} + V) \phi_n(\xi) = \lambda_n(\xi) (-\tilde{\Delta} + 1)^{-1} \phi_n(\xi). \quad (3.128)$$

Thus we get that

$$\phi_n(\xi) = (-\tilde{\Delta} + 1)^{-1} (i\xi \cdot \tilde{\nabla} + |\xi|^2 + \mathbf{1} - V + \lambda_n(\xi)) \phi_n(\xi) \quad (3.129)$$

and

$$(i\xi \cdot \tilde{\nabla} + |\xi|^2 + \mathbf{1} - V + \lambda_n(\xi)) \phi_n(\xi) \in \mathcal{H}^1(L^2(\mathbb{S}^d)) \quad (3.130)$$

in order to conclude that in fact $\phi_n(\xi) \in \mathcal{H}^3(\mathbb{S}^d)$ for any $n \in \mathbb{N}$ and any $\xi \in \mathcal{X}^*$. Iterating this argument we obtain that $\phi_n(\xi) \in C^\infty(\mathbb{S}^d)$ for any $n \in \mathbb{N}$ and any $\xi \in \mathcal{X}^*$.

3.7 The Floquet representation.

In this new representation we can prove by repeating the arguments above, that

- The operator $\mathcal{F}_\Gamma V \mathcal{F}_\Gamma^{-1}$ becomes multiplication with the Γ -periodic function $V : \mathcal{X} \rightarrow \mathbb{R}$ on each $\mathfrak{F}_{\mathbf{z}_*} \simeq \Upsilon_{\mathbf{z}_*} L^2(\mathbb{S}^d)$ that it leaves invariant.
- The operator $\mathcal{F}_\Gamma H \mathcal{F}_\Gamma^{-1}$, we notice that if we define

$$\mathfrak{H}_{\mathbf{z}_*} := \{u \in \mathcal{H}_{\text{loc}}^2(\mathbb{R}^d), \mathcal{F}(\gamma)u = e^{2\pi i \langle s^d(\mathbf{z}_*), \gamma \rangle} u, \forall \gamma \in \mathbb{Z}^d\} \quad (3.131)$$

- the Hilbert space \mathfrak{H}_1 may be identified with the order 2 Sobolev space on the d-dimensional torus $\mathcal{H}^2(\mathbb{S}^d)$,
- for each $\mathbf{z}_* \in \mathbb{S}_*^d$ the space $\mathfrak{H}_{\mathbf{z}_*} \subset \mathfrak{F}_{\mathbf{z}_*}$ is unitarily equivalent with $\Upsilon_{\mathbf{z}_*} \mathcal{H}^2(\mathbb{S}^d)$,
- the family $\{\Upsilon_{\mathbf{z}_*} u, u \in \mathcal{H}^2(\mathbb{S}^d)\}_{\mathbf{z}_* \in \mathbb{S}_*^d} \subset \prod_{\mathbf{z}_* \in \mathbb{S}_*^d} \mathfrak{H}_{\mathbf{z}_*}$, defines a measurable (and even smooth) "field of vectors" in the sense of J. Dixmier ("Les algèbres d'opérateurs dans l'espaces Hilbertien" Definition 3.1 in ch. II §1) and we can define the direct integral

$$\mathfrak{H} := \int_{\mathbb{S}_*^d}^{\oplus} dz_* \mathfrak{H}_{\mathbf{z}_*}. \quad (3.132)$$

We conclude that the operator $\mathcal{F}_\Gamma H \mathcal{F}_\Gamma^{-1}$ decomposes into a family of differential operators

$$\mathcal{F}_\Gamma H \mathcal{F}_\Gamma^{-1} = \int_{\mathbb{S}_*^d}^{\oplus} dz_* H_{\mathbf{z}_*} : \int_{\mathbb{S}_*^d}^{\oplus} dz \mathfrak{H}_{\mathbf{z}_*} \rightarrow \int_{\mathbb{S}_*^d}^{\oplus} dz_* \mathfrak{F}_{\mathbf{z}_*} \quad (3.133)$$

with $H_{\mathbf{z}_*} = -\Delta|_{\mathfrak{H}_{\mathbf{z}_*}}$ for any $\mathbf{z}_* \in \mathbb{S}_*^d \setminus \{1\}$.

Then let us notice that if $\phi \in \mathcal{S}(\mathbb{R}^d)$, then each term in the series in the right member of (2.60) is differentiable (of any order) and the series is convergent due to the fast decay condition in

$\mathcal{S}(\mathbb{R}^d)$. Thus $(\mathcal{F}_\Gamma \phi)(x, \theta)$ is of class $C^\infty(\mathbb{R}^d; C^\infty(\mathbb{S}^d))$. Moreover it is clear that all the derivatives of $\mathcal{F}_\Gamma \phi$ also belongs to $\Upsilon\mathcal{G}$. We have the relation

$$\mathcal{F}_\Gamma \partial_x^\alpha f = (\partial_x^\alpha \otimes \mathbf{1})(\mathcal{F}_\Gamma f), \quad \forall \alpha \in \mathbb{N}^d. \quad (3.134)$$

Let us take $f \in \mathcal{H}^2(\mathcal{X})$ i.e. $\partial^\alpha f \in L^2(\mathcal{X})$ for $|\alpha| \leq 2$. Thus, for $|\alpha| \leq 2$, we conclude that $\mathcal{F}_\Gamma \partial^\alpha f \in L_E^2(\mathbb{R}^d; L^2(\mathbb{S}^d))$ and

$$\mathcal{F}_\Gamma \partial^\alpha f = (\partial_x^\alpha \otimes \mathbf{1}) \mathcal{F}_\Gamma f, \quad \forall \alpha \in \mathbb{Z}^d, \quad (3.135)$$

$$\mathcal{J}(\gamma)(\mathcal{F}_\Gamma \partial^\alpha f) = \hat{U}_\circ(\gamma)(\mathcal{F}_\Gamma \partial^\alpha f), \quad \forall \gamma \in \mathbb{Z}^d. \quad (3.136)$$

We can denote this space $\mathcal{H}_E^2(\mathbb{R}^d; L^2(\mathbb{S}^d))$ and notice that it is a Hilbert space for the scalar product induced from $\mathcal{H}^2(\mathcal{X})$.

4 Isolated Bloch bands

Definition 4.10. Suppose that there exist two natural numbers $(k, N) \in \mathbb{N}^2$ such that:

$$d(\lambda_{k-1}(\tilde{\xi}); \lambda_k(\tilde{\xi})) = d_0(\tilde{\xi}) \geq d_0 > 0, \quad \forall \tilde{\xi} \in E_*; \quad (\text{the condition is void for } k = 0). \quad (4.137)$$

$$d(\lambda_{k+N}(\tilde{\xi}); \lambda_{k+N+1}(\tilde{\xi})) = d_1(\tilde{\xi}) \geq d_1 > 0, \quad \forall \tilde{\xi} \in E_*. \quad (4.138)$$

Then we call the set $\{\lambda_k(\xi), \dots, \lambda_{k+N}(\xi)\}_{\xi \in \mathcal{X}^*}$ an *isolated Bloch band*.

Definition 4.11. Suppose that there exist two natural numbers $(k, N) \in \mathbb{N}^2$ such that:

$$d\left(\inf_{\xi \in E_*} \lambda_k(\xi), \sup_{\xi \in E_*} \lambda_{k-1}(\xi)\right) = d_0 > 0; \quad (\text{the condition is void for } k = 0). \quad (4.139)$$

$$d\left(\inf_{\xi \in E_*} \lambda_{k+N+1}(\xi), \sup_{\xi \in E_*} \lambda_{k+N}(\xi)\right) = d_1 > 0. \quad (4.140)$$

Then we call the set $\{\lambda_k(\xi), \dots, \lambda_{k+N}(\xi)\}_{\xi \in \mathcal{X}^*}$ a *strictly isolated Bloch band*.

The Bloch bundles. Given an isolated Bloch band $\Lambda := \{\lambda_k(\xi), \dots, \lambda_{k+N}(\xi)\}_{\xi \in \mathcal{X}^*}$ we define its associated *Bloch bundle* as the subbundle

$$\mathcal{E}_\Lambda^* \xrightarrow{\varepsilon^d} \mathbb{S}^d, \quad \mathcal{E}_{\Lambda, \mathbf{z}_*}^* := \bigoplus_{k \leq j \leq k+N} \mathfrak{p}_j(\mathfrak{s}^d(\mathbf{z}_*)) \mathcal{E}_{\mathbf{z}_*}, \quad \forall \mathbf{z}_* \in \mathbb{S}^d_*. \quad (4.141)$$

We shall use the notation

$$\mathfrak{P}_\Lambda(\xi) := \bigoplus_{k \leq j \leq k+N} \mathfrak{p}_j(\xi), \quad \forall \xi \in \mathcal{X}^* \quad (4.142)$$

verifying evidently the relation:

$$\mathfrak{P}_\Lambda(\xi + \gamma^*) = U^\dagger(\gamma^*) \mathfrak{P}_\Lambda(\xi) U^\dagger(\gamma^*)^{-1}, \quad \forall \xi \in \mathcal{X}^*, \quad \forall \gamma^* \in \Gamma_*. \quad (4.143)$$

The Berry parallel transport. Given two points $(\xi, \eta) \in \mathcal{X}^* \times \mathcal{X}^*$ and the oriented line segment from $\xi \in \mathcal{X}^*$ to $\eta \in \mathcal{X}^*$:

$$[0, 1] \ni \tau \mapsto \zeta(\tau) := \xi + \tau(\eta - \xi) \in \mathcal{X}^* \quad (4.144)$$

we want to define a strongly-differentiable function

$$[0, 1] \ni \tau \mapsto \mathfrak{T}_{\xi \rightarrow \eta}(\tau) \in \mathbb{U}(L^2(\mathbb{S}^d)) \quad (4.145)$$

satisfying the intertwining property

$$\mathfrak{T}_{\xi \rightarrow \eta}(\tau) \mathfrak{P}_\Lambda(\xi) = \mathfrak{P}_\Lambda(\zeta(\tau)) \mathfrak{T}_{\xi \rightarrow \eta}(\tau), \quad \forall \tau \in [0, 1]. \quad (4.146)$$

Let us differentiate with respect to $\tau \in (0, 1)$ in order to obtain the equation:

$$\frac{\partial}{\partial \tau} \mathfrak{T}_{\xi \rightarrow \eta}^{-1}(\tau) \mathfrak{P}_\Lambda(\zeta(\tau)) \mathfrak{T}_{\xi \rightarrow \eta}(\tau) = 0, \quad \forall \tau \in (0, 1). \quad (4.147)$$

$$0 = -\mathfrak{T}_{\xi \rightarrow \eta}^{-1}(\tau) \left(\partial_\tau \mathfrak{T}_{\xi \rightarrow \eta} \right) (\tau) \mathfrak{T}_{\xi \rightarrow \eta}^{-1}(\tau) \mathfrak{P}_\Lambda(\zeta(\tau)) \mathfrak{T}_{\xi \rightarrow \eta}(\tau) + \quad (4.148)$$

$$+ \mathfrak{T}_{\xi \rightarrow \eta}^{-1}(\tau) \left(\partial_\tau \mathfrak{P}_\Lambda(\zeta(\tau)) \right) \mathfrak{T}_{\xi \rightarrow \eta}(\tau) + \mathfrak{T}_{\xi \rightarrow \eta}^{-1}(\tau) \mathfrak{P}_\Lambda(\zeta(\tau)) \left(\partial_\tau \mathfrak{T}_{\xi \rightarrow \eta} \right) (\tau) \quad (4.149)$$

$$\left(\partial_\tau \mathfrak{T}_{\xi \rightarrow \eta}\right)(\tau) \mathfrak{T}_{\xi \rightarrow \eta}^{-1}(\tau) \mathfrak{P}_\Lambda(\zeta(\tau)) \mathfrak{T}_{\xi \rightarrow \eta}(\tau) = \quad (4.150)$$

$$= \left(\partial_\tau \mathfrak{P}_\Lambda(\zeta(\tau))\right) \mathfrak{T}_{\xi \rightarrow \eta}(\tau) + \mathfrak{P}_\Lambda(\zeta(\tau)) \left(\partial_\tau \mathfrak{T}_{\xi \rightarrow \eta}\right)(\tau) \quad (4.151)$$

$$\left(\partial_\tau \mathfrak{T}_{\xi \rightarrow \eta}\right)(\tau) \mathfrak{T}_{\xi \rightarrow \eta}^{-1}(\tau) \mathfrak{P}_\Lambda(\zeta(\tau)) \mathfrak{T}_{\xi \rightarrow \eta}(\tau) = \quad (4.152)$$

$$= \left\langle d\mathfrak{P}_\Lambda(\zeta(\tau)), (\eta - \xi) \right\rangle \mathfrak{T}_{\xi \rightarrow \eta}(\tau) + \mathfrak{P}_\Lambda(\zeta(\tau)) \left(\partial_\tau \mathfrak{T}_{\xi \rightarrow \eta}\right)(\tau) \quad (4.153)$$

$$\left(\partial_\tau \mathfrak{T}_{\xi \rightarrow \eta}\right)(\tau) \mathfrak{T}_{\xi \rightarrow \eta}^{-1}(\tau) \mathfrak{P}_\Lambda(\zeta(\tau)) - \mathfrak{P}_\Lambda(\zeta(\tau)) \left(\partial_\tau \mathfrak{T}_{\xi \rightarrow \eta}\right)(\tau) \mathfrak{T}_{\xi \rightarrow \eta}^{-1}(\tau) = \quad (4.154)$$

$$= \left\langle d\mathfrak{P}_\Lambda(\zeta(\tau)), (\eta - \xi) \right\rangle \quad (4.155)$$

One can easily verify that the above equation is implied by

$$\left(\partial_\tau \mathfrak{T}_{\xi \rightarrow \eta}\right)(\tau) \mathfrak{T}_{\xi \rightarrow \eta}^{-1}(\tau) = \left\langle d\mathfrak{P}_\Lambda(\zeta(\tau)), (\eta - \xi) \right\rangle \mathfrak{P}_\Lambda(\zeta(\tau)) - \mathfrak{P}_\Lambda(\zeta(\tau)) \left\langle d\mathfrak{P}_\Lambda(\zeta(\tau)), (\eta - \xi) \right\rangle. \quad (4.156)$$

Let us denote by

$$(D_{\xi \rightarrow \eta} \mathfrak{P}_\Lambda)(\zeta) := \left\langle d\mathfrak{P}_\Lambda(\zeta), (\eta - \xi) \right\rangle. \quad (4.157)$$

In conclusion, the parallel transport is given by the unique solution of the following Cauchy problem:

$$\begin{aligned} \left(\partial_\tau \mathfrak{T}_{\xi \rightarrow \eta}\right)(\tau) &= \left[(D_{\xi \rightarrow \eta} \mathfrak{P}_\Lambda), \mathfrak{P}_\Lambda \right](\zeta(\tau)) \mathfrak{T}_{\xi \rightarrow \eta}(\tau), \\ \mathfrak{T}_{\xi \rightarrow \eta}(0) &= \mathbf{1} \in \mathbb{B}(L^2(\mathbb{S}^d)). \end{aligned} \quad (4.158)$$

Our arguments above have shown that the solution $\mathfrak{T}_{\xi \rightarrow \eta}(\tau)$ of this Cauchy problem satisfies the identity (4.146) for any $\tau \in [0, 1]$ and thus we have

$$\mathfrak{T}_{\xi \rightarrow \eta}(1) \mathfrak{P}_\Lambda(\xi) = \mathfrak{P}_\Lambda(\eta) \mathfrak{T}_{\xi \rightarrow \eta}(1) \quad (4.159)$$

so that $\mathfrak{U}(\eta, \xi) := \mathfrak{T}_{\xi \rightarrow \eta}(1)$ is a intertwining operator between $\mathfrak{P}_\Lambda(\xi)$ and $\mathfrak{P}_\Lambda(\eta)$.

Proposition 4.12. *For any $(\xi, \eta) \in \mathcal{X}^* \times \mathcal{X}^*$ the operator $\mathfrak{U}(\eta, \xi)$ is a unitary operator on the Hilbert space $L^2(\mathbb{S}^d)$ and verifies the covariance property:*

$$\mathfrak{U}(\eta + \gamma^*, \xi + \gamma^*) = U^\dagger(\gamma^*) \mathfrak{U}(\eta, \xi) U^\dagger(\gamma^*)^{-1}$$

Proof. The unitarity follows easily from the fact that the bounded operator $i \left[(D_{\xi \rightarrow \eta} \mathfrak{P}_\Lambda), \mathfrak{P}_\Lambda \right]$ in the Cauchy problem (4.158) is hermitian.

Let us recall the property (3.125) of the projections $\{\mathfrak{P}_\Lambda(\xi)\}_{\xi \in \mathcal{X}^*}$. Then we can write for any $\gamma^* \in \mathbb{Z}^d_*$

$$(D_{\xi + \gamma^* \rightarrow \eta + \gamma^*} \mathfrak{P}_\Lambda)(\zeta + \gamma^*) := \left\langle d_{\mathcal{X}^*} \mathfrak{P}_\Lambda(\zeta + \gamma^*), (\eta - \xi) \right\rangle = \quad (4.160)$$

$$= \left\langle d_{\mathcal{X}^*} \left(U^\dagger(\gamma^*) \mathfrak{P}_\Lambda(\zeta) U^\dagger(\gamma^*)^{-1} \right), (\eta - \xi) \right\rangle =$$

$$= \left\langle \left(U^\dagger(\gamma^*) (d_{\mathcal{X}^*} \mathfrak{P}_\Lambda(\zeta)) U^\dagger(\gamma^*)^{-1} \right), (\eta - \xi) \right\rangle =$$

$$= U^\dagger(\gamma^*) \left\langle \left(d_{\mathcal{X}^*} \mathfrak{P}_\Lambda(\zeta) \right), (\eta - \xi) \right\rangle U^\dagger(\gamma^*)^{-1} =$$

$$= U^\dagger(\gamma^*) (D_{\xi \rightarrow \eta} \mathfrak{P}_\Lambda)(\zeta) U^\dagger(\gamma^*)^{-1}. \quad (4.161)$$

We may conclude that $\mathfrak{T}_{\xi+\gamma^* \rightarrow \eta+\gamma^*}(\tau)$ is the unique solution of the Cauchy problem:

$$\begin{aligned} \left(\partial_\tau \tilde{\mathfrak{T}}_{\xi \rightarrow \eta}\right)(\tau) &= \left[(D_{\xi+\gamma^* \rightarrow \eta+\gamma^*} \mathfrak{P}_\Lambda), \mathfrak{P}_\Lambda \right] (\zeta(\tau) + \gamma^*) \tilde{\mathfrak{T}}_{\xi \rightarrow \eta}(\tau) = \\ &= U^\dagger(\gamma^*) \left[(D_{\xi \rightarrow \eta} \mathfrak{P}_\Lambda), \mathfrak{P}_\Lambda \right] (\zeta(\tau)) U^\dagger(\gamma^*)^{-1} \tilde{\mathfrak{T}}_{\xi \rightarrow \eta}(\tau), \\ \tilde{\mathfrak{T}}_{\xi \rightarrow \eta}(0) &= \mathbf{1} \in \mathbb{B}(L^2(\mathbb{S}^d)). \end{aligned} \quad (4.162)$$

and thus we must have the equality:

$$\mathfrak{T}_{\xi+\gamma^* \rightarrow \eta+\gamma^*}(\tau) = U^\dagger(\gamma^*) \mathfrak{T}_{\xi \rightarrow \eta}(\tau) U^\dagger(\gamma^*)^{-1}. \quad (4.163)$$

From this we evidently obtain

$$\mathfrak{U}(\eta + \gamma^*, \xi + \gamma^*) = U^\dagger(\gamma^*) \mathfrak{U}(\eta, \xi) U^\dagger(\gamma^*)^{-1}. \quad (4.164)$$

□

The Berry connection. We can associate the above parallel transport defined by the Bloch projections with a covariant derivative: *the Berry covariant derivative*. Given $\xi \in \mathcal{X}^*$, a tangent vector $v \in \mathbb{T}_\xi \mathcal{X}^*$ and a smooth curve $[-1, 1] \ni \tau \mapsto \zeta(\tau) \in \mathcal{X}^*$ with $\zeta(0) = \xi$ and $(\partial_\tau \zeta)(0) = v$, for any $F \in \mathcal{G}$ we can define

$$(\nabla_v^\Lambda F)(\xi) := \lim_{\tau \rightarrow 0} (1/\tau) \left((\mathfrak{T}_{\xi \rightarrow \eta}^{-1})(\tau) F(\zeta(\tau)) - F(\xi) \right) = \quad (4.165)$$

$$= (\partial_\tau \mathfrak{T}_{\xi \rightarrow \eta}^{-1})(0) (F(\xi)) + (\nabla_v F)(\xi) = \quad (4.166)$$

$$= - \left[(D_v \mathfrak{P}_\Lambda), \mathfrak{P}_\Lambda \right] (F(\xi)) + (\nabla_v F)(\xi) \quad (4.167)$$

with $D_v \mathfrak{P}_\Lambda := \langle d\mathfrak{P}_\Lambda(\zeta(\tau)), v \rangle$.