The analogies between prototypes of Periodic Schrödinger operators via Bloch-Floquet methods and the Ergodic Laplacian, an ergodic Schrödinger operator

Giovanna Marcelli

SAPIENZA UNIVERSITÀ DI ROMA

Universitá degli studi di Roma, "La Sapienza"

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What is the aim of this talk?

The aim of this talk is to put in evidence the algebraic and hilbertian analogies which emerge from the "diagonalization" via Bloch-Floquet transform of prototypes of **periodic Schrödinger operators** and a particular ergodic random Schrödinger operators, the **ergodic Laplacian**. The analysis of these operators is referred to the determination of their spectrum and spectrum type.
So we will describe the setting and the main results of the **periodic and random spectral problems** of the latter operators separately and at the end we will do a table of the algebraic and hilbertian analogies.

Quantum dynamics in crystalline solids

crystalline solids

Definition

A crystalline solid is a solid in which the fixed positions of the ionic cores are periodic, i.e. are located on a lattice Γ, corresponding to the Bravais lattice in physics,

$$\Gamma := \{\gamma \in \mathbb{R}^d : \gamma = \sum_{i=1}^{d} n_i \gamma_i \text{ for some } n_j \in \mathbb{Z}\},$$

where $\{\gamma_1, \dots, \gamma_d\}$ are fixed linearly independent vectors.

Let $\mathcal{H} := L^2\left(\mathbb{R}^d\right)$. We introduce a unitary representation of Γ, given by

$$T : \Gamma \to \mathcal{U}(\mathcal{H}), \quad \gamma \mapsto T_\gamma,$$

such that $T_\gamma \psi(x) = \psi(x - \gamma)$, $\psi \in \mathcal{H}$.

Quantum dynamics in crystalline solids

Periodic Schrödinger operators

Definition

A periodic Schrödinger operator H_Γ w.r.t. Γ lattice is a selfadjont operator $H_\Gamma : \mathcal{D}(H_\Gamma) \subset \mathcal{H} \to \mathcal{H}$ such that

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

The prototypes of periodic Schrödinger operators are operators in the form

$$H_\Gamma := -\Delta + V_\Gamma, \quad \text{acting in } \mathcal{H}, \tag{1}$$

where the function V_Γ is periodic w.r.t. Bravais lattice $\Gamma \simeq \mathbb{Z}^d$ and Kato-small respect to $-\Delta$,

Quantum dynamics in crystalline solids

Bloch-Floquet transform

Definition

For $\psi \in C_0^\infty(\mathbb{R}^d)$, one defines the (modified) **Bloch-Floquet transform** as

$$
\begin{aligned}
(U_{BF}\psi)(k,y) &:= C_N \sum_{\gamma\in\Gamma} \mathrm{e}^{-\mathrm{i}k\cdot(y-\gamma)}\psi(y-\gamma) \\
&\quad \left[\omega_\gamma := \mathrm{e}^{\mathrm{i}k\cdot\gamma}\right] \\
&= C_N \mathrm{e}^{-\mathrm{i}k\cdot y} \sum_{\gamma\in\Gamma} \omega_\gamma T_\gamma \psi(y), \quad k \in \hat{\mathbb{R}}^d, y \in \mathbb{R}^d.
\end{aligned} \tag{2}
$$

Quantum dynamics in crystalline solids

Bloch-Floquet transform

One immediately reads the periodicity and pseudo-periodicity properties respectively,

1. for any fixed $k \in \hat{\mathbb{R}}^d$, $(U_{BF}\psi)(k,\cdot)$ is a Γ-periodic function and can thus be regarded as an element of $\mathcal{H}_f := L^2\left(\mathbb{T}^d_y\right)$, where $\mathbb{T}^d_y$ the flat torus $\mathbb{R}^d/\Gamma$
2. introducing the dual lattice, w.r.t. the ordinary inner product, is

$$\Gamma^* = \{k \in \hat{\mathbb{R}}^d : k \cdot \gamma \in 2\pi\mathbb{Z}, \text{ for all } \gamma \in \Gamma\}$$

   and defining a unitary representation of the group Γ^* , given by

$$\rho \colon \Gamma^* \to \mathcal{U}(\mathcal{H}_f), \quad \lambda \mapsto \rho(\lambda), \quad (\rho(\lambda)\varphi)(y) = \mathrm{e}^{\mathrm{i}\lambda\cdot y}\varphi(y).$$

   we have the following equation,

$$(U_{BF}\psi)(k-\lambda, y) = \rho(\lambda)(U_{BF}\psi)(k,y) \quad \forall \lambda \in \Gamma^*,$$

   and rename this property ρ-**equivariance**.

Quantum dynamics in crystalline solids

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Quantum dynamics in crystalline solids

Bloch-Floquet transform

It is convenient to introduce the Hilbert space

$$\mathcal{H}_\rho := \left\{ \varphi \in L^2_{loc}(\hat{\mathbb{R}}^d, \mathcal{H}_f) : \varphi(k-\lambda) = \rho(\lambda)\varphi(k) \; \forall \lambda \in \Gamma^*, \text{ q.o. } k \in \hat{\mathbb{R}}^d \right\},$$

Obviously, $\mathcal{H}_\rho \simeq L^2(Y^*, \mathcal{H}_f) = \int_{Y^*}^{\oplus} \mathrm{d}k \, \mathcal{H}_f$.
The map defined by (2) extends to a unitary operator

$$(\tilde{U}_{BF}\psi) \colon \mathcal{H} \to \mathcal{H}_\rho \simeq \int_{Y^*}^{\oplus} \mathrm{d}k \, \mathcal{H}_f, \tag{3}$$

Quantum dynamics in crystalline solids

trasformed the periodic Schrödinger operator via BF

Now we can transform the periodic Schrödinger operator introduced in (1) by unitary operator $\tilde{U}_{BF}$ and obtain

$$\begin{aligned} \tilde{U}_{BF} H_\Gamma \tilde{U}_{BF}^{-1} &= \tilde{U}_{BF} \left(-\Delta + V_\Gamma(x)\right) \tilde{U}_{BF}^{-1} \\ &= \int_{Y^*}^{\oplus} \mathrm{d}k \, H(k), \end{aligned} \tag{4}$$

with fiber operator

$$H(k) = (-\mathrm{i}\nabla_y + k)^2 + V_\Gamma(y), \quad k \in Y^*,$$

acting on the k-independent domain $\mathcal{D}(-\Delta_{per}) := W^{2,2}(\mathbb{T}^d_y)$. Each fiber operator, $H(k)$ is self-adjoint, has compact resolvent and thus pure point spectrum accumulating at infinity. Moreover, $H(k)$ is ρ-**covariant**, i.e.

$$H(k+\lambda) = \rho(\lambda)^{-1} H(k) \rho(\lambda) \quad \text{per ogni } \lambda \in \Gamma^*, \tag{5}$$

thus the eigenvalues of $H(k)$ are Γ^*-periodic.

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Ergodic Laplacian

ergodic group action and stationary function

Let be $(\Omega, \mathcal{F}, \mathbb{P})$ a probability space.
Let be $(\Lambda, +)$ a discrete group of $\mathbb{R}^d$ of maximal dimension, thus $\Lambda \simeq \mathbb{Z}^d$.

Definition

A map $\tau \colon \Lambda \to Aut(\Omega, \mathcal{F}, \mathbb{P})$ is an **ergodic group action** if

1. τ is a group homomorphism;
2. $\tau_\lambda(A) = A$ for all $\lambda \in \Lambda$ for some $A \in \mathcal{F}$ implies that $\mathbb{P}(A) \in \{0, 1\}$.

Definition

A measurable function $f \colon \Omega \times \mathbb{R}^d \to \mathbb{C}$ is called **stationary** if

$$f(\tau_\lambda(\omega), x) = f(\omega, x + \lambda) \quad \text{a.s. in } \omega \text{ and a.e. in } x \quad \text{for all } \lambda \in \Lambda$$

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Ergodic Laplacian

stationary functions spaces

So we introduce stationary function spaces. Let $Q := \left[-\frac{1}{2}, \frac{1}{2}\right)^d \subset \mathbb{R}^d$,

1.
$$L^2_{stat} := \left\{ f \in L^2\left(\Omega, L^2_{loc}\left(\mathbb{R}^d\right)\right) \mid f \text{ is stationary} \right\}, \qquad (6)$$

endowed with the scalar product

$$(f \mid g)_{L^2_{stat}} = \mathbb{E}\left((f \mid g)_{L^2(Q)}\right)$$

2.
$$H^m_{stat} := \left\{ f \in L^2\left(\Omega, H^m_{loc}\left(\mathbb{R}^d\right)\right) \mid f \text{ is stationary} \right\}, \quad 1 \leq m < \infty, \qquad (7)$$

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Ergodic Laplacian

We define an operator which we call the **ergodic Laplacian**, *which is nothing but the usual Laplacian in the x variable acting on $L^2(\Omega \times Q)$, with stationary boundary conditions at the boundary of Q.*
Let $(A_0, \mathcal{D}(A_0))$ be the operator on L^2_{stat} defined by

$$\begin{cases} \mathcal{D}(A_0) = L^2_{stat} \cap L^2(\Omega, C^2(\mathbb{R}^d)) \\ A_0 f(\omega, x) = -\Delta_x f(\omega, x) \text{ a.s. in } \omega \text{ e a.e. in } x, \text{ for } f \in \mathcal{D}(A_0). \end{cases} \tag{8}$$

One checks that,

$$(f \mid A_0 g)_{L^2_{stat}} = \mathbb{E}\left(\int_Q \overline{\nabla f(\cdot, x)} \cdot \nabla g(\cdot, x) \mathrm{d}x\right) = (\nabla f \mid \nabla g)_{(L^2_{stat})^d}$$

Ergodic Laplacian

Thus, A_0 is a symmetric, non-negative operator on L^2_{stat} with dense domain $\mathcal{D}(A_0)$.

We denote by $-\Delta_{erg}$ its Friedrichs extension and call the operator the **ergodic Laplacian**

Proposition

The form domain of $-\Delta_{erg}$

$$\mathcal{Q}\left(-\Delta_{erg}\right) = H^1_{stat}$$

and the domain of $-\Delta_{erg}$

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Ergodic Laplacian

So we can justify the name of **Ergodic Laplacian**.

If an ergodic group action $\tau = \{ \tau_\lambda \}_{\lambda \in \mathbb{Z}^d}$ exists, then $-\Delta_{erg}$ is **ergodic** in the sense that it satisfies the following relation

$$\Delta_{erg}(\tau_\lambda(\omega)) = U_\lambda^{-1} \Delta_{erg}(\omega) U_\lambda \quad \text{for all } \lambda \in \Lambda,$$

where

$$U : \Lambda \to \mathcal{O}\left(L^2_{loc}(\mathbb{R}^d) \right), \quad U_\lambda f(x) = f(x - \lambda) \text{ a.e. } \forall f \in L^2_{loc}(\mathbb{R}^d),\ \forall \lambda \in \Lambda.$$

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Ergodic Laplacian

The features of the Ergodic Laplacian depend on what probability space $(\Omega, \mathcal{F}, \mathbb{P})$ we choose, so we analyze three different cases

(1) if Ω is s.t. $\mathbb{P}(\omega) > 0, \forall \omega \in \Omega$ and $|\Omega| \leq |\mathbb{N}|$, then

$$\begin{cases} \text{If } \Omega = \{\, \omega_1, \ldots, \omega_n \,\}, \\ \text{then } \sigma(-\Delta_{erg}) = \sigma_{disc}(-\Delta_{erg}) = \left\{ \left(\frac{2\pi}{n}\right)^2 |\, j \,|^2, \quad j \in \mathbb{Z}^d \right\}; \\ \text{If } |\Omega| = |\mathbb{N}|, \text{ then there exists no ergodic group action of } \mathbb{Z}^d \text{ on } \Omega. \end{cases}$$

(2) $(\Omega, \mathcal{F}, \mathbb{P}) = ([0,1), \mathcal{B}([0,1)), \lambda)$,
$\tau : \mathbb{Z} \to Aut(\Omega, \mathcal{F}, \mathbb{P})$ s.t. $\lambda \mapsto \tau_\lambda$, is defined as
$\tau_\lambda(\omega) = \omega + \alpha\lambda - [\omega + \alpha\lambda] = mod(\omega + \alpha\lambda, 1)$, with $\alpha \in \mathbb{R}$, then

$$\begin{cases} \text{If } \alpha \text{ is irrational then,} \\ \sigma(-\Delta_{erg}) = \sigma_{ess}(-\Delta_{erg}) = [0, +\infty); \\ \text{If } \alpha \text{ is rational, then there exists no ergodic group action of } \mathbb{Z} \text{ on } \Omega. \end{cases}$$

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Ergodic Laplacian

(3) $(\Omega, \mathcal{F}, \mathbb{P}) = \left(\{-1,1\}^{\mathbb{Z}^d}, \sigma(Y_i, i \in \mathbb{Z}^d), p^{\mathbb{Z}^d}\right)$,
where $Y_i(\omega) = \omega_i$ is a sequence of real valued random variables and $p = p_1\delta_1 + (1-p_1)\delta_{-1}$, with $0 < p_1 < 1$,
$\tau : \mathbb{Z}^d \to Aut(\Omega, \mathcal{F}, \mathbb{P})$ s.t. $\lambda \mapsto \tau_\lambda$, is defined as $\tau_\lambda(\omega) = \omega_{\cdot+\lambda}$, then

$$\sigma(-\Delta_{erg}) = \sigma_{ess}(-\Delta_{erg}) = [0, +\infty).$$

A table of **analogies** between the **periodic Schrödinger operators via B-F** and the **ergodic Laplacian**

periodic Schrödinger operators via B-F	**ergodic Laplacian**
$\mathcal{H}_f := L^2\left(\mathbb{T}^d_y\right)$	there exists no fiber Hilbert space
$V := L^2_{loc}(\hat{\mathbb{R}}^d, \mathcal{H}_f)$	$V := L^2(\Omega, L^2_{loc}(\mathbb{R}^d))$
$\tau\colon \Gamma^* \simeq \mathbb{Z}^d \to Aut(\hat{\mathbb{R}}^d, \hat{\mathcal{L}}, \mathrm{d}k)$ $\lambda \mapsto \tau_\lambda,\ \tau_\lambda(k) = k - \lambda$	$\tau\colon \Lambda \simeq \mathbb{Z}^d \to Aut(\Omega, \mathcal{F}, \mathbb{P})$ $\lambda \mapsto \tau_\lambda,\ \tau$ ergodic group action

A table of **analogies** between the **periodic Schrödinger operators via B-F** and the **ergodic Laplacian**

periodic Schrödinger operators via B-F	**ergodic Laplacian**
Let $\varphi \in V$, it is **ρ-equivariant** if $\varphi(\tau_\lambda(k), y) = \rho(\lambda)\varphi(k, y), \ \forall \lambda \in \Gamma^*$, where $\rho(\lambda) = \mathrm{e}^{\mathrm{i}\lambda \cdot y}$	Let $\varphi \in V$, it is **stationary** if $\varphi(\tau_\lambda(\omega), x) = T(\lambda)\varphi(\omega, x), \ \forall \lambda \in \Lambda$, where $T(\lambda)\varphi(\omega, x) = \varphi(\omega, x + \lambda)$
$\mathcal{H}_\rho := \{ \varphi \in V : \varphi \text{ is } \rho\text{-equivariant} \}$ $\mathcal{H}_\rho \simeq L^2(Q, \mathcal{H}_f) = \int_Q^\oplus \mathrm{d}k \, \mathcal{H}_f$, where $Q = \left[-\frac{1}{2}, \frac{1}{2}\right)^d \subset \hat{\mathbb{R}}^d$	$\mathcal{H}_{stat} := \{ \varphi \in V : \varphi \text{ is stationary} \}$ $\mathcal{H}_{stat} \simeq L^2(\Omega \times Q)$, where $Q = \left[-\frac{1}{2}, \frac{1}{2}\right)^d \subset \mathbb{R}^d$

A table of **analogies** between the **periodic Schrödinger operators via B-F** and the **ergodic Laplacian**

periodic Schrödinger operators via B-F	**ergodic Laplacian**
Let A s-a on $\mathcal{H}_\rho \simeq \int_Q^\oplus \mathrm{d}k\, \mathcal{H}_f$, $A = \int_Q \mathrm{d}k A(k)$, $A(k)$ s-a on $\mathcal{H}_f$ A is **ρ-covariant** if, for all $\lambda \in \Gamma^*$, $A(\tau_\lambda(k)) = \rho(\lambda)A(k)\rho(\lambda)^{-1}$	Let A s-a acting on $\mathcal{H}_{stat}$, A is **ergodic** if, for all $\lambda \in \Lambda$ $A(\tau_\lambda(\omega)) = T(\lambda)A(k)T(\lambda)^{-1}$
$\rho \colon \Gamma^* \simeq \mathbb{Z}^d \to \mathcal{U}(\mathcal{H}_f)$ is a unitary representation $\Rightarrow$ $\int_Q^\oplus \mathrm{d}k \rho \colon \Gamma^* \to \mathcal{U}\left(\int_Q^\oplus \mathrm{d}k \mathcal{H}_f\right)$ is a unitary representation	$T \colon \Lambda \simeq \mathbb{Z}^d \to \mathcal{O}(L^2_{loc}(\mathbb{R}^d))$ $T \colon \Lambda \simeq \mathbb{Z}^d \to \mathcal{U}(\mathcal{H}_{stat})$ is a unitary representation

Main References

- G. Panati, A. Pisante, *Bloch Bundles, Marzari-Vanderbilt Functional and Maximally Localized Wannier Functions*, Commun. Math. Phys 2013.
- S. Lahbabi with supervisors M. Lewin, É. Cancés, *Mathematical study of quantum and classical models for random materials in the atomic scale*, Phd Thesis in Mathematics at University of Cergy-Pontoise 2013.
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