Random Schrödinger Operators arising in the study of aperiodic media

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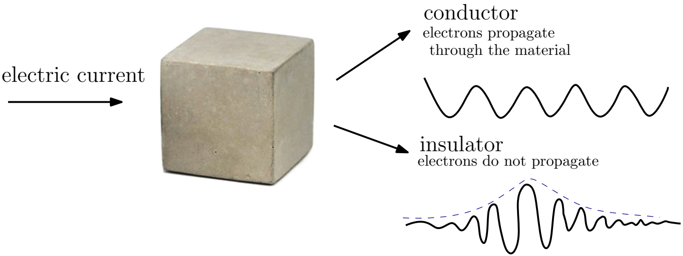
Outline

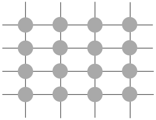
- Introduction
  - Random Schrödinger operators
  - Aperiodic media and Delone operators
- Results
  - Localization for Delone operators

Electronic transport in a material

Electrons in a material, as time evolves, can either propagate or not.



Example : a material with crystalline atomic structure (lattice).



electrons can propagate in space as time evolves
$\sim$ electronic transport

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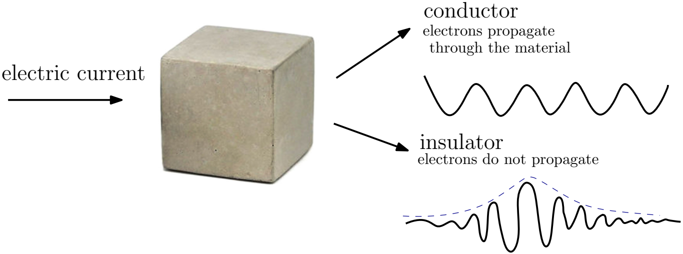
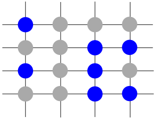


What happens when there are impurities in the crystal ?



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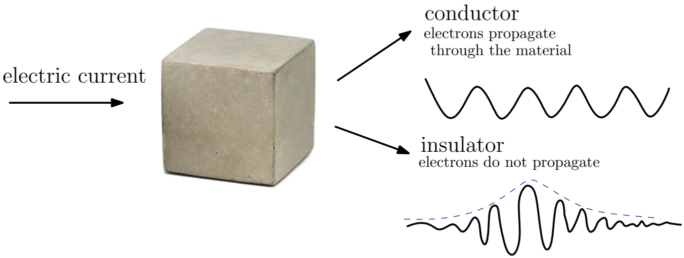
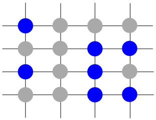


P.W. Anderson discovered in 1958 that disorder in the crystal was enough to suppress the propagation of electrons→ Anderson localization (Nobel 1977)

1958 *"Absence of diffusion in certain random lattices"*, Phys. Rev.



Mathematics of electronic transport in a solid

An electron moving in a material is represented by a wave function $\psi(t,x)$ in a Hilbert space $\mathcal{H}$, where $|\psi(t,x)|^2$ represents the probability of finding the particle in x at time t, therefore $\int |\psi(t,x)|^2 = 1$.

This function solves Schrödinger's equation :

$$\partial_t \psi(t,x) = -iH\psi(t,x),$$

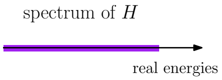
$$\psi(t,x) = e^{-itH}\psi(0,x),$$

where x is in a d-dimensional space and $H = -\Delta + V$ is a one-particle *self-adjoint Schrödinger operator* acting on $\mathcal{H}$.

$$H = -\Delta + V$$

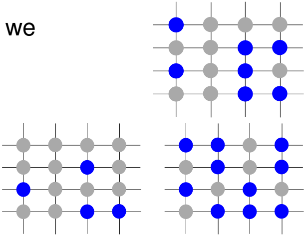
kinetic energy

interaction with the environment



Mathematics of electronic transport in a disordered solid

The Anderson Model : on each point of the lattice we place a potential, which can be • or •.



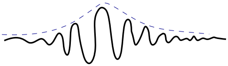
We consider many possible configurations. Every configuration of the potential is a vector ω in a probability space $(\Omega, \mathbb{P})$.

We get a random operator $\omega \mapsto H_\omega = -\Delta + V_\omega$, where

$$V_\omega(x) = \sum_{j \in \mathbb{Z}^d} \omega_j \delta_j(x),$$

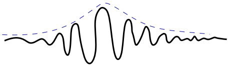
with $\omega_j \in \{\bullet, \bullet\}$ bounded, independent, identically distributed random variables.

For typical ω, $\psi_\omega(t, x)$ does not propagate in space as t grows $\sim$ absence of transport



Mathematical theory of random Schrödinger operators

Localization (insulator)
bound state $\psi_\omega(t,x) = e^{-itH_\omega}\psi(0,x)$ is confined in space for all times, for most ω.
H_ω has *pure point spectrum*



Delocalization (conductor)
extended state $\psi_\omega(t,x)$ propagates in space as time evolves.
continuous spectrum

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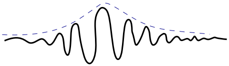

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Methods to prove localization in arbitrary dimension combine functional analysis and probability tools to show *the decay of eigenfunctions*,

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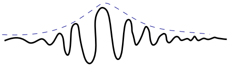

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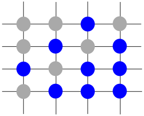
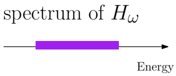
Ergodic properties : consequence of translation invariance on average of H_ω.





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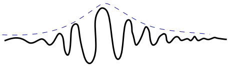

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Ergodic properties : consequence of translation invariance on average of H_ω.

- The spectrum as a set is independent of the realization ω.

Localization

We say that the operator H_ω exhibits (dynamical) localization in an interval I if the following holds for any $\varphi \in \mathcal{H}$ with compact support, and any $p \geq 0$,

$$\mathbb{E}\left(\sup_t \left\| |X|^{p/2} e^{-itH_\omega} \chi_I(H_\omega)\varphi \right\|^2\right) < \infty$$

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Theorem

Consider the operator $H_\omega = -\Delta + \lambda V_\omega$, with $\lambda > 0$. Then,

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Proof based on resolvent estimates. Key idea : Suppose ψ satisfies "$H_\omega\psi = E\psi$". We split the space into a cube Λ, its complement Λ^c, and its boundary Υ_Λ,

$$(H_{\omega,\Lambda} \oplus H_{\omega,\Lambda^c} - E)\psi = -\Upsilon_\Lambda \psi.$$

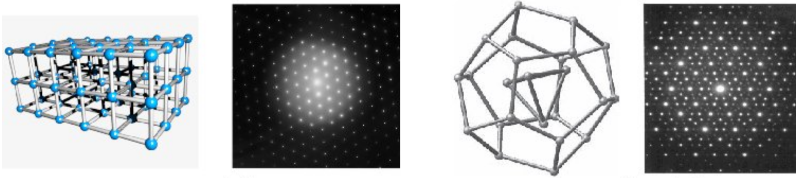
Therefore, for $x \in \Lambda$ we have

$$\begin{aligned} \psi(x) &= -\left((H_{\omega,\Lambda} - E)^{-1}\Upsilon_\Lambda\psi\right)(x) \\ &= -\sum_{\substack{(k,m)\in\partial\Lambda,\\ k\in\partial_-\Lambda,\, m\in\partial_-\Lambda}} \langle \delta_x, (H_{\omega,\Lambda} - E)^{-1}\delta_k\rangle \psi(m), \end{aligned}$$

Break of lattice structure : aperiodic media

1984 ('82) D. Shechtman, I. Blech, D. Gratias, J.W. Cahn, *"Metallic phase with long-range orientational order and no translation symmetry"*, Phys. Rev. Letters. (Schechtman : Nobel 2011).

Diffraction patterns



crystal quasicrystal

A way to model quasicrystals is using a Delone set D of parameters (r, R) : a discrete point set in space that is uniformly discrete (r) and relatively dense (R).

Electronic Transport in aperiodic media

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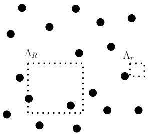
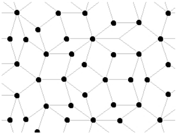
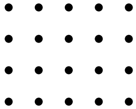


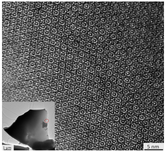
Delone set



Penrose tiling



lattice



$Al_{71}Ni_{24}Fe_5$
Steinhardt et al. 2015

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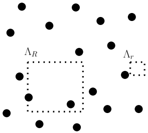

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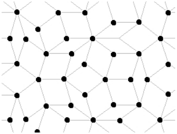

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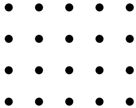

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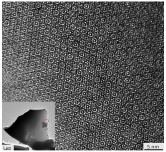

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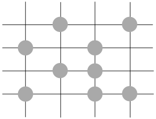
The Delone operator :

models the energy of an electron moving in a material where atoms sit on a Delone set.



$$H_D = -\Delta + V_D, \quad V_D(x) = \sum_{\gamma \in D} \delta_\gamma(x),$$

Let $\mathbb{D}$ be the space of Delone sets and consider $D \mapsto H_D$. The operator has generically singular continuous spectrum (e.g. Lenz-Stollmann'06, and collaborators).

What about *localization* for Delone operators ?

Is the "geometric diversity" in the space of Delone sets rich enough to produce pure point spectrum ? and dynamical localization ?

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Is the "geometric diversity" in the space of Delone sets rich enough to produce pure point spectrum ? and dynamical localization ?

Theorem (Müller-RM)

Given a Delone set D, there exists a family of Delone sets D_n such that

i. *D_n converges to D in the topology of Delone sets.*
ii. *H_{D_n} converges to H_D in the sense of resolvents.*
iii. *H_{D_n} exhibits localization at the bottom of the spectrum for all $n \in \mathbb{N}$.*

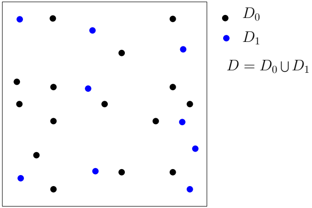
Delone operators as random operators : Bernoulli r.v.

Let $\mathbb{D}$ be the space of all Delone sets.
Take $D \in \mathbb{D}$ and write $D = D_0 \cup D_1$,
with $D_0, D_1 \in \mathbb{D}$.
We define the random potential

$$V_{D_1^\omega}(x) = \sum_{\gamma \in D_1} \omega_\gamma u(x - \gamma)$$

$x \in \mathbb{R}^d$, with $\omega_\gamma \in \{0, 1\}$, and
consider the operator

$$H_{D^\omega} = -\Delta + V_{D_0} + V_{D_1^\omega} \quad \text{on } L^2(\mathbb{R}^d)$$



Theorem (Müller-RM)

Let $D \in \mathbb{D}$. There exists a set $\hat{\Omega} \subset \Omega$ of full probability measure such that H_{D^ω}, $\omega \in \hat{\Omega}$ exhibits localization at the bottom of the spectrum.

Key ingredient of the proof : a *Quantitative Unique Continuation Principle*.

Theorem (RM-Veselić'12)

For ψ *eigenfunction of* H_Λ *and D a Delone set of parameters (r',R') and* $B(\gamma,\delta)$ *a ball around the point* γ*. There exists a constant* $C_{UCP} > 0$*, depending on* R' *but independent of* Λ*, such that,*

$$\sum_{\gamma \in D \cap \Lambda} \|\psi\|_{B(\gamma,\delta)} \geq C_{UCP} \|\psi\|_\Lambda .$$

With large probability, $V_{\omega,\Lambda} \geq V_\Lambda$, V_Λ a Delone potential. Then, the effect of adding a Delone potential to $-\Delta + V_{D_0}$ is

$$\inf \sigma((-\Delta + V_0)_\Lambda + V_\Lambda) \geq \inf \sigma(-\Delta + V_0) + C_{UCP} \cdot C_u .$$

Consequence : H_{D^ω} restricted to a cube Λ with Dirichlet b.c. has a spectral gap above E_0, *with good probability*
$\Rightarrow$ Decay of the resolvent by the Combes-Thomas estimate
$\Rightarrow$ localization via the multiscale analysis.

Thank you !