Random Schrödinger Operators arising in the study of aperiodic media

Constandza ROJAS-MOLINA
Heinrich-Heine-Universität Düsseldorf
joint work with P. Müller (LMU)

Konstanz, July 2018
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).

- **Conductor**: Electrons propagate through the material.
- **Insulator**: Electrons do not propagate.

Electric current

Electrons can propagate in space as time evolves

$\sim$ electronic transport
Electronic transport in a material

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

What happens when there are impurities in the crystal?
Electronic transport in a material

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

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

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

spectrum of \( H \)
- real energies
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 \( \omega \) in a probability space \( (\Omega, P) \).

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 \( \omega_j \in \{●, ○\} \) bounded, independent, identically distributed random variables.

For typical \( \omega \), \( \psi_\omega(t, x) \) 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 \( \omega \).
\( H_\omega \) has *pure point spectrum*

Delocalization (conductor)
extended state \( \psi_\omega(t, x) \) propagates in space as time evolves.
*continuous spectrum*
Mathematical theory of random Schrödinger operators

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

- Multiscale Analysis (Fröhlich-Spencer).
- Fractional Moment Method (Aizenman-Molchanov).
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Ergodic properties: consequence of translation invariance on average of $H_\omega$. 

Energy spectrum of $H_\omega$
Mathematical theory of random Schrödinger operators

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Ergodic properties: consequence of translation invariance on average of $H_\omega$.

- The spectrum as a set is independent of the realization $\omega$. 
Localization

We say that the operator $H_\omega$ 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,

i. for $\lambda > 0$ large enough, $H_\omega$ exhibits localization throughout its spectrum.

ii. for fixed $\lambda$, $H_\omega$ exhibits localization in intervals $I$ at spectral edges.
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Proof based on resolvent estimates. Key idea: Suppose $\psi$ satisfies "$H_\omega \psi = E \psi". We split the space into a cube $\Lambda$, its complement $\Lambda^c$, and its boundary $\Gamma_\Lambda$,

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

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

$$\psi(x) = -\left( (H_\omega,\Lambda - E)^{-1} \Gamma_\Lambda \psi \right)(x)$$

$$= -\sum_{(k,m) \in \partial \Lambda, \ k \in \partial - \Lambda, \ m \in \partial - \Lambda} \langle \delta_x, (H_\omega,\Lambda - E)^{-1} \delta_k \rangle \psi(m),$$
Break of lattice structure: aperiodic media


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](image1.png)  ![Penrose tiling](image2.png)  ![lattice](image3.png)

Delone set  Penrose tiling  lattice

Al$_{71}$Ni$_{24}$Fe$_5$
Steinhardt et al. 2015
Electronic Transport in aperiodic media

A Delone set $D$ of parameters $(r, R)$ is a discrete point set in space that is uniformly discrete ($r$) and relatively dense ($R$).

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 $\mathcal{D}$ 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 \textit{localization} for Delone operators?
Is the "geometric diversity" in the space of Delone sets rich enough to produce pure point spectrum? and dynamical localization?
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?

**Theorem (Müller-RM)**

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

1. $D_n$ converges to $D$ in the topology of Delone sets.
2. $H_{D_n}$ converges to $H_D$ in the sense of resolvents.
3. $H_{D_n}$ exhibits localization at the bottom of the spectrum for all $n \in \mathbb{N}$. 
Delone operators as random operators: Bernoulli r.v.

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

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

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

**Theorem (Müller-RM)**

Let $D \in \mathcal{D}$. There exists a set $\hat{\Omega} \subset \Omega$ of full probability measure such that $H_{D^\omega}$, $\omega \in \hat{\Omega}$ exhibits localization at the bottom of the spectrum.
Key ingredient of the proof: a *Quantitative Unique Continuation Principle*.

**Theorem (RM-Veselić’12)**

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

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

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

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

Consequence: $H_{D_\omega}$ restricted to a cube $\Lambda$ 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!