Spectral properties of materials cut in half

David Gontier

CEREMADE, Université Paris-Dauphine & DMA, École Normale Supérieure de Paris

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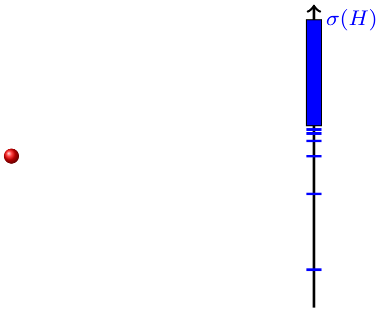
Mathematical results of many-body quantum systems
Herrsching (online).

Goal of the talk

- Make a connection between spectral properties of materials, and electronic transport
- The case of periodic materials.
- The case of periodic materials, cut in half.

Start with a single atom in $\mathbb{R}^d$. We study the spectrum of the Schrödinger operator

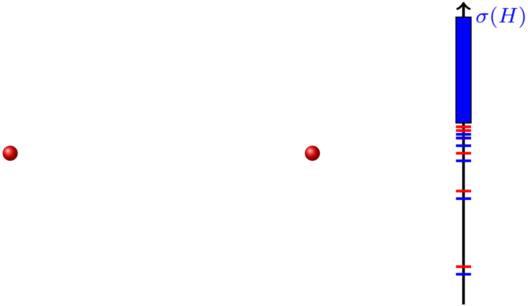
$$H = -\Delta + V(\mathbf{x}), \quad \text{e.g.} \quad V(\mathbf{x}) = \frac{-Z}{|\mathbf{x}|}.$$



- Discrete spectrum (= eigenvalues), and continuous/essential spectrum.
- lowest part of the spectrum = ground state energy, then excited state energy.
- An electron needs energy to *jump* from one level to the next (*quantum*).

Then take two atoms in $\mathbb{R}^d$.

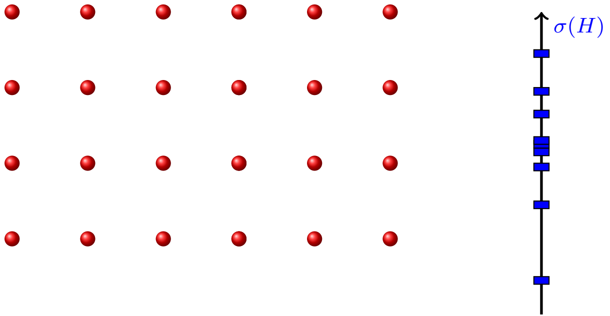
$$H = -\Delta + V\left(\mathbf{x} - \frac{R}{2}\right) + V\left(\mathbf{x} + \frac{R}{2}\right).$$



- When $R = \infty$, the spectrum is copied twice (each eigenvalue doubles its multiplicity);
- When $R \gg 1$, *tunnelling* effect = interaction of eigenvectors $\implies$ splitting of the eigenvalues;
- The eigenvectors are delocalized between the two atoms;

Now take an infinity of atoms in $\mathbb{R}^d$, located along a lattice (= material)

$$H = -\Delta + \sum_{\mathbf{v} \in R\mathbb{Z}^d} V(\mathbf{x} - \mathbf{v})$$



- When $R = \infty$, each eigenvalue is of infinite multiplicity;
- When $R \gg 1$, each eigenvalue becomes a **band of essential spectrum**;
- Each band represents «*one electron per unit cell* »;
- When R decreases, the bands may overlap.

The spectrum of $-\Delta + V$ with V-periodic has a band-gap structure!

Usual proof with the *Bloch transform* ($\sim$ discrete version of the Fourier transform).

Motivation: Spectral pollution

Let's compute numerically the spectrum of the (simple, one-dimensional) operator

$$H := -\partial_{xx}^2 + V(x), \quad \text{with} \quad V(x) = 50 \cdot \cos(2\pi x) + 10 \cdot \cos(4\pi x).$$

The potential V is 1-periodic. We expect a band-gap structure for the spectrum.
We study H in a box $[t, t+L]$ with Dirichlet boundary conditions, and with finite difference.

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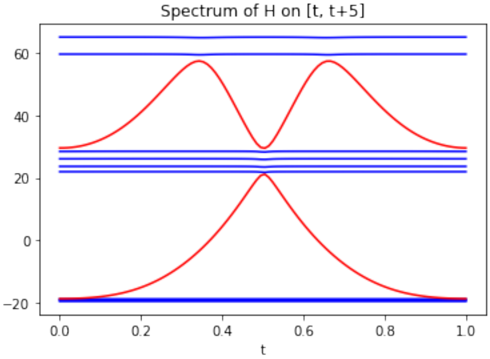


Depending on where we fix the origin t, the spectrum differs...
There are branches of spurious eigenvalues = spectral pollution (they appear for all L).
The corresponding eigenvectors are edge modes: they are localized near the boundaries.

In this talk: understand why edge modes *must* appear.

Setting

Let V be a 1-periodic potential, and consider the cut (one-dimensional) Hamiltonian

$$H_t^\sharp = -\partial_{xx}^2 + V(x-t) \quad \text{on} \quad L^2(\mathbb{R}^+),$$

with Dirichlet boundary conditions, that is with domain $H^2(\mathbb{R}^+) \cap H_0^1(\mathbb{R}^+)$.
Since V is 1-periodic, the map $t \mapsto H_t^\sharp$ is also 1-periodic.

Theorem (Korotyaev 2000, Hempel Kohlmann 2011, DG 2020)

In the n-th essential gap, there is a flow of n eigenvalues going downwards as t goes from 0 to 1.
In addition, these eigenvalues are simple, and their associated eigenvectors are exponentially localised.

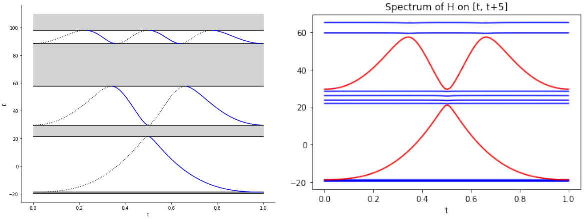


Figure: (left) Spectrum of $H^\sharp(t)$ for $t \in [0, 1]$. (right) Spectrum of the operator on $[t, t + L]$.

E. Korotyaev, Commun. Math. Phys., 213(2):471–489, 2000.
R. Hempel and M. Kohlmann, J. Math. Anal. Appl., 381(1):166–178, 2011.
D. Gontier, J. Math. Phys. 61, 2020.

Idea of the proof

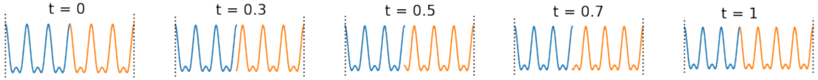
Step 1. Prove the result for *dislocations* (following *Hempel and Kohlmann*).
Introduce the dislocated operator

$$H_t^{\text{disloc}} := -\partial_{xx}^2 + \left[V(x) \mathbb{1}(x < 0) + V(x-t) \mathbb{1}(x > 0) \right], \quad \text{on} \quad L^2(\mathbb{R}).$$

Let $L \in \mathbb{N}$ be a (large) integer. Consider the periodic dislocated operator

$$H_{L,t}^{\text{disloc}} := -\partial_{xx}^2 + \left[V(x) \mathbb{1}(x < 0) + V(x-t) \mathbb{1}(x > 0) \right], \quad \text{on} \quad L^2([-\tfrac{1}{2}L, \tfrac{1}{2}L + t])$$

with periodic boundary conditions.



Remarks

- The branches of eigenvalues of $t \mapsto H_{L,t}^{\text{disloc}}$ are continuous;
- At $t = 0$, the system is 1-periodic, on a box of size L. Each «band» contributes to L eigenvalues;
- At $t = 1$, the system is 1-periodic, on a box of size $L + 1$. Each «band» contributes to $L + 1$ eigenvalues.

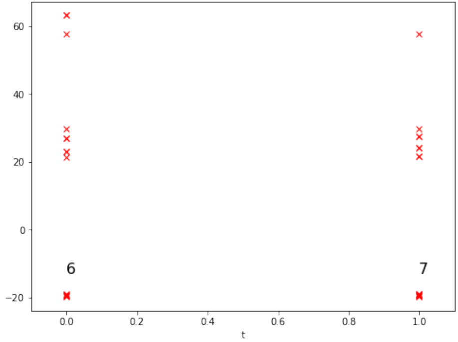


Figure: Spectrum of $H^{\text{disloc}}_{L,t}$ for $L = 6$ at $t = 0$ (6 cells) and $t = 1$ (7 cells).

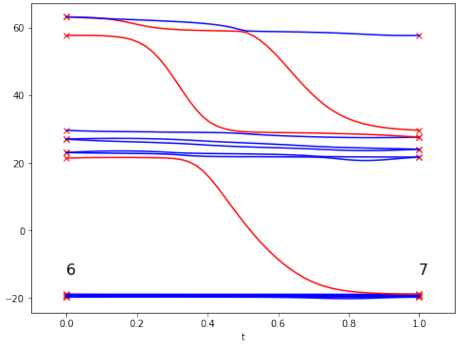


Figure: Spectrum of $H_{L,t}^{\text{disloc}}$ for all $t \in [0, 1]$.

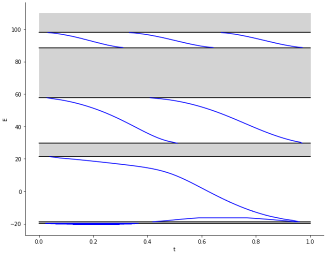
The presence and the number of the red lines are independent of $L \in \mathbb{N}$.
They survive in the limit $L \to \infty$.

This implies that there the result holds for the family of dislocated operators $t \mapsto H_t^{\text{disloc}}$.

The Spectral flow

If $t \mapsto A_t$ is a 1-periodic and *continuous* family of self-adjoint operators, and if $E \notin \sigma_{\text{ess}}(A_t)$ for all t, we can define its Spectral flow as

$$\text{Sf}\,(A_t, E) := \text{number of eigenvalues going } \textbf{downwards} \text{ in the essential gap where } E \text{ lies.}$$



The previous result can be formulated as:

$$\text{Sf}\left(H_t^{\text{disloc}}, E\right) = \mathcal{N}(E), \quad \mathcal{N}(E) := \text{number of bands below } E.$$

Facts :

- If $t \mapsto K_t$ is a 1-periodic continuous family of **compact** operators, then

$$\text{Sf}\,(A_t, E) = \text{Sf}\,(A_t + K_t, E)\,.$$

- If $f : \mathbb{R} \to \mathbb{R}$ is strictly increasing, then

$$\text{Sf}\,(f\,(A_t)\,, f(E)) = \text{Sf}\,(A_t, E)\,.$$

Step 2. From the dislocated case to the Dirichlet case.

Recall that the dislocated operator is

$$H_t^{\text{disloc}} := -\partial_{xx}^2 + [V(x)\mathbb{1}(x<0) + V(x-t)\mathbb{1}(x>0)] \quad \text{on} \quad L^2(\mathbb{R}).$$

Consider the cut Hamiltonian

$$H_t^{\text{cut}} := -\partial_{xx}^2 + [V(x)\mathbb{1}(x<0) + V(x-t)\mathbb{1}(x>0)] \quad \text{on} \quad L^2(\mathbb{R}) = L^2(\mathbb{R}^-) \cup L^2(\mathbb{R}^+),$$

and with Dirichlet boundary conditions at $x=0$.

Fact: For any Σ negative enough (below the essential spectra of all operators), we have

$$K_t := \left(\Sigma - H_t^{\text{cut}}\right)^{-1} - \left(\Sigma - H_t^{\text{disloc}}\right)^{-1} \quad \text{is compact (here, it is finite rank).}$$

So

$$\mathrm{Sf}\left(\left(\Sigma - H_t^{\text{disloc}}\right)^{-1}, (\Sigma - E)^{-1}\right) = \mathrm{Sf}\left(\left(\Sigma - H_t^{\text{cut}}\right)^{-1}, (\Sigma - E)^{-1}\right).$$

Since $f(x) := (\Sigma - x)^{-1}$ is strictly increasing on $x > \Sigma$, we have

$$\mathcal{N}(E) = \mathrm{Sf}\left(H_t^{\text{disloc}}, E\right) = \mathrm{Sf}\left(H_t^{\text{cut}}, E\right) = \mathrm{Sf}\left(H_t^{\sharp,+}, E\right). \quad \square$$

A «fun» analogy

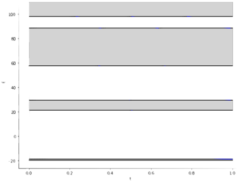
The *«Grand Hilbert Hotel»*
An infinity of floors, an infinity of rooms in each floor.

Idea: each period represents 1 room (per floor), each spectral band represents one floor.

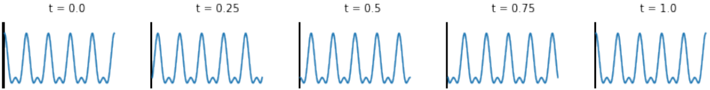
… Floor 3.

… Floor 2.

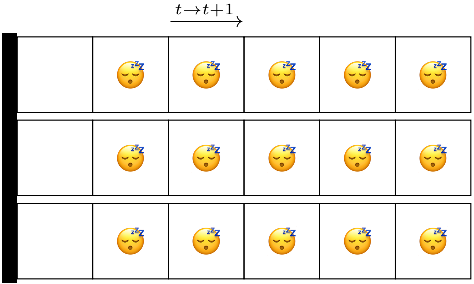
… Floor 1.



As t moves from 0 to 1...



... a new room is created on each floor!



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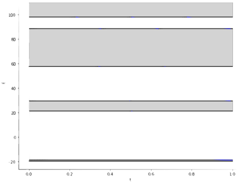

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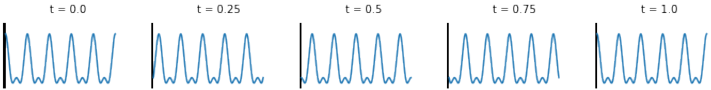

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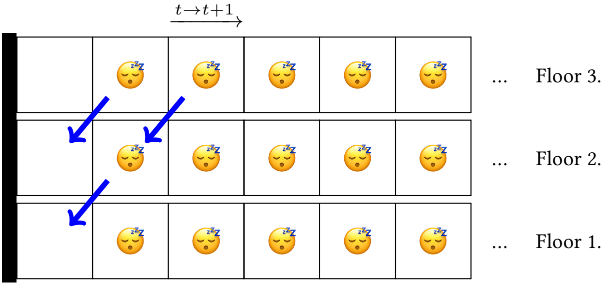

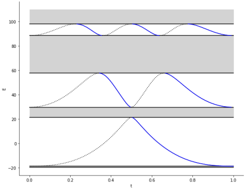

In order to fill the new rooms,

- 1 person from floor 2 must come down to floor 1;
- 2 persons from floor 3 must come down to floor 2;
- and so on.

This phenomenon is sometimes called «charge pumping».

The case of junctions

Take two 1-periodic potentials

$$V_L(x) = 50\cos(2\pi x) + 10\cos(4\pi x), \qquad V_R(x) = 10\cos(2\pi x) + 50\cos(4\pi x)$$

Consider the **junction** Hamiltonian

$$H_t^{\text{junct}} := -\partial_{xx}^2 + \left(V_L(x)\mathbb{1}(x<0) + V_R(x-t)\mathbb{1}(x>0)\right) \quad \text{on} \quad L^2(\mathbb{R}).$$

Reasoning as before (using a cut as a compact perturbation), one can prove that $\mathrm{Sf}\left(H_t^{\text{junct}}, E\right) = \mathcal{N}_R(E)$.

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$$V_L(x) = 50\cos(2\pi x) + 10\cos(4\pi x), \qquad V_R(x) = 10\cos(2\pi x) + 50\cos(4\pi x)$$

Consider the **junction** Hamiltonian

$$H_t^{\rm junct} := -\partial_{xx}^2 + (V_L(x)\mathbb{1}(x<0) + V_R(x-t)\mathbb{1}(x>0)) \quad \text{on} \quad L^2(\mathbb{R}).$$

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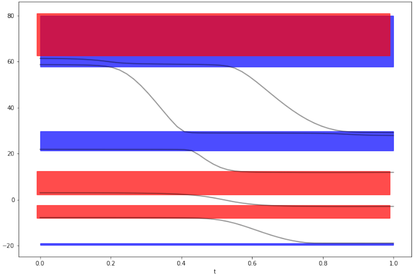


Figure: Spectrum of $H_t^{\rm junc}$ as a function of t.

A typical spectrum contains:

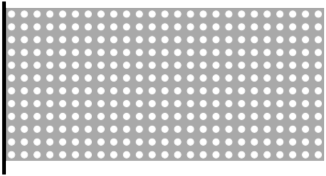
- The essential spectrum of the left and right side.
- Additional edge mode at the junction

Remark. This works for any junction, say of the form $V_L\chi + V_R(1-\chi)$, with χ a switch function.

The two-dimensional case

Let V be a $\mathbb{Z}^2$-periodic potential, and we study the edge operator

$$H^\sharp(t) = -\Delta + V(x-t, y), \quad \text{on} \quad L^2(\mathbb{R}_+ \times \mathbb{R}), \quad \text{with Dirichlet boundary conditions.}$$



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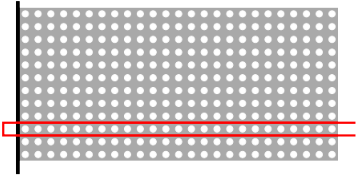


After a Bloch transform in the y-direction, we need to study the **family** of operators

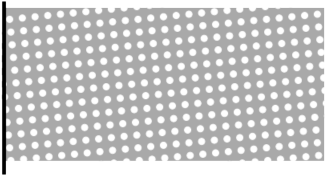
$$H_k^\sharp(t) = -\partial_{xx}^2 + (-\mathrm{i}\partial_y + k)^2 + V(x-t, y), \quad \text{on the } \textbf{tube} \quad L^2(\mathbb{R}_+ \times [0,1]).$$

- Consider again the **«Grand Hilbert Hotel»** (= on a tube).
- For each k, as t moves from 0 to 1, a new room is created on each floor $\implies$ spectral flow.
- As k varies, each branch of eigenvalue becomes of branch of essential spectrum.

There is a «spectral flow» of **essential spectrum** appearing in each gap.
The corresponding modes can only propagate along the boundary.

The two-dimensional twisted case.

We rotate V by θ.



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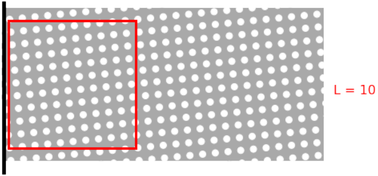


Commensurate case ($\tan\theta = \frac{p}{q}$)

Considering a **Supercell** of size $L = \sqrt{p^2+q^2}$, we recover a $L\mathbb{Z}^2$-periodic potential.
On the tube $\mathbb{R}^+ \times [0, L]$ (at the k-Bloch point $k = 0$ for instance),

« As t moves from 0 to L, L^2 new rooms are created»

Key remark:

- The map $t \mapsto H_\theta^\sharp(t)$ is now $1/L$-periodic (up to some x_2 shifts)
- So the map $t \mapsto \sigma(H_\theta^\sharp(t))$ is $1/L$ periodic.

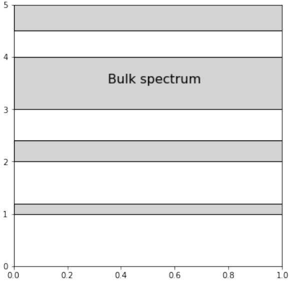
«As t moves from 0 to $\frac{1}{L}$, 1 new room is created»

In-commensurate case ($\tan\theta \notin \mathbb{Q}$, corresponds to $L \to \infty$)

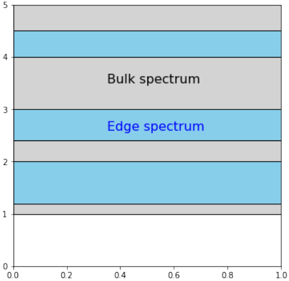
- The spectrum of $H^\sharp(t)$ is independent of t (ergodicity);
- All bulk gaps are filled with edge spectrum!

Theorem (DG, Comptes Rendus. Mathématique, Tome 359 (2021))

If $\tan\theta \notin \mathbb{Q}$, the spectrum of $H^\sharp_\theta$ is of the form $[\Sigma, \infty)$.



(a) Uncut two-dimensional material



(b) Two-dimensional material with **incommensurate** cut

Idea of the proof

Remark: The map $\theta \mapsto H_\theta$ is not *norm-resolvent* continuous.
The convergence of the spectrum is not guaranteed, and we need to prove it.

Limiting procedure

Consider a sequence $\theta_n \to \theta$, with $\tan(\theta_n) = \frac{p_n}{q_n} \in \mathbb{Q}$, and set $L_n := \sqrt{p_n^2 + q_n^2}$.
By the commensurate case result, there is $t_n \in [0, \frac{1}{L_n}]$ and $\phi_n \in L^2_{\text{per}}(\mathbb{R}^+ \times [0, L_n])$ so that

$$(-\Delta + V_{\theta_n}(t - t_n) - E)\phi_n = 0, \qquad \int_{\mathbb{R}^+ \times [0, L_n]} |\phi_n|^2 = 1.$$

It is tempting to extract a weak-limit of ϕ_n, but this will fail (we would get $\phi_* = 0$ at the end).

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It is tempting to extract a weak-limit of ϕ_n, but this will fail (we would get $\phi_* = 0$ at the end).

Idea: Normalize the functions in L^∞
Consider the functions

$$\Psi_n := \frac{\phi_n}{\|\phi_n\|_{L^\infty}}, \quad \text{so that} \quad (-\Delta + V_{\theta_n}(t - t_n) - E)\Psi_n = 0, \quad \|\Psi_n\|_{L^\infty} = 1.$$

(the parameter L_n is no longer here).

$$(-\Delta + V_{\theta_n}(t - t_n) - E)\Psi_n = 0, \quad \|\Psi_n\|_{L^\infty} = 1.$$

Step 1: Control the mass

Consider $x_n \in \mathbb{R}^2$ so that $\Psi_n(x_n) > \frac{1}{2}$.

- Upon shifting the whole system in the x_2-direction (which effectively corresponds to changing t_n), we may assume $x_{n,2} = 0$.
- Since $E \notin \sigma_{\text{ess}}(H)$, the function Ψ_n is exponentially decaying away from the boundary (the bulk is an insulator). So there is $C > 0$ independent of n so that $0 < x_{n,1} < C$ (the full proof uses Combes-Thomas estimates).

Step 2: Regularity and taking the limit

- Since $\|(-\Delta\Psi_n)\| \leq C$, there is $\delta > 0$ so that $\Psi_n(x) > \frac{1}{4}$ for all $x \in \mathcal{B}(x_n, \delta)$.
- Take the limit $n \to \infty$, and sub-sequences. $\Psi_n \to \Psi_*$ weakly-* in L^∞.
- We have, in the distributional sense

$$(-\Delta + V_\theta(x - t^*) - E)\Psi_* = 0.$$

- We have $\|\Psi_*\|_\infty \leq 1$, and since $\int_{\mathcal{B}(0,\delta)} \Psi_* \neq 0$, $\Psi_* \neq 0$.
- This implies that $E \in \sigma(H_\theta)$.

$$(-\Delta + V_{\theta_n}(t - t_n) - E)\Psi_n = 0, \quad \|\Psi_n\|_{L^\infty} = 1.$$

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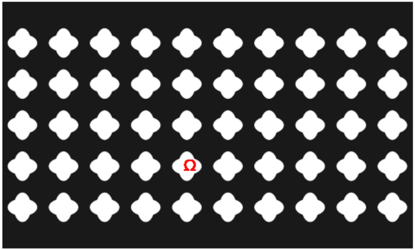
Open question

Is the spectrum pure point ($\sim$ Anderson localization), or absolutely continuous (travelling waves)?

A degenerate case

Consider $\Omega \subset \mathbb{R}^2$, and repeat it on a $\mathbb{Z}^2$ grid.
Consider $H = -\Delta$ on $L^2(\mathbb{R}^2)$, with Dirichlet boundary conditions «everywhere».



In the un-cut situation, the spectrum equals $\sigma\left(-\Delta|_\Omega\right)$, and each eigenvalue is of infinite multiplicities.

A degenerate case

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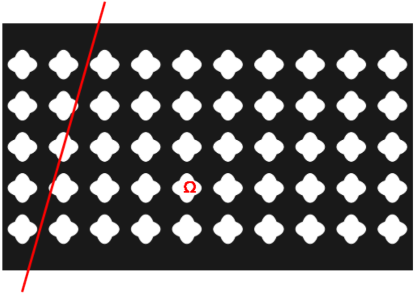

In the un-cut situation, the spectrum equals $\sigma\left(-\Delta|_\Omega\right)$, and each eigenvalue is of infinite multiplicities.
In the cut situation:

- If $\tan\theta \in \mathbb{Q}$, a finite number of new motifs appear
  $\Longrightarrow$ finite number of new eigenvalues appear in each gap (all of infinite multiplicities)
- If $\tan\theta \notin \mathbb{Q}$, an infinite (countable) number of new motifs appear
  $\Longrightarrow$ pure-point spectrum everywhere.

Bonus: «Quantum Hall Effect»

Consider a $2d$ electron gas, under a constant magnetic field B orthogonal to the plane.
We choose the gauge

$$\mathbf{A} = \mathbf{A}(x,y) = \begin{pmatrix} 0 \\ Bx \end{pmatrix}.$$

We obtain the **Landau** Hamiltonian

$$H_B = -\partial_{xx}^2 + (-\mathrm{i}\partial_y + Bx)^2.$$

After a Fourier transform in y, we get

$$H_{B,k_y} = -\partial_{xx}^2 + (k_y + Bx)^2 = -\partial_{xx}^2 + B^2(x-t)^2, \quad \text{with} \quad t = \frac{-k_y}{B}.$$

The Bloch momentum k_y plays the role of the pump.

Lemma

If $B \neq 0$, the bulk Hamiltonian has discrete spectrum. $\sigma(H_B) = |B|(2\mathbb{N}+1)$. (Landau operator).
The edge Hamiltonian $H_{B,t}^\sharp$ has flows of eigenvalues between the Landau levels.
In particular $\sigma(H_B^\sharp) = [|B|, \infty)$.

Consider a $2d$ electron gas, under a constant magnetic field B orthogonal to the plane.
We choose the gauge

$$\mathbf{A} = \mathbf{A}(x,y) = \begin{pmatrix} 0 \\ Bx \end{pmatrix}.$$

We obtain the **Landau** Hamiltonian

$$H_B = -\partial_{xx}^2 + (-\mathrm{i}\partial_y + Bx)^2.$$

After a Fourier transform in y, we get

$$H_{B,k_y} = -\partial_{xx}^2 + (k_y + Bx)^2 = -\partial_{xx}^2 + B^2(x-t)^2, \quad \text{with} \quad t = \frac{-k_y}{B}.$$

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Thank you for your attention!