# Spectral properties of materials cut in half 

David Gontier<br>CEREMADE, Université Paris-Dauphine \& DMA, École Normale Supérieure de Paris

May 202022
Séminaire du groupe analyse du LMR, Reims

## Dauphine $\mid$ PSL* CEREMADE

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 $\Rightarrow$ 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!
Rigorous proof using 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

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

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.


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

$$
H_{t}^{\sharp}=-\partial_{x x}^{2}+V(x-t) \quad \text { on } \quad L^{2}\left(\mathbb{R}^{+}\right)
$$

with Dirichlet boundary conditions, that is with domain $H^{2}\left(\mathbb{R}^{+}\right) \cap H_{0}^{1}\left(\mathbb{R}^{+}\right)$.
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 $[t, t+L]$.
We provide here two proofs, applications, and extensions of this theorem.
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.

## First proof: «compute» everything

## Preliminaries.

Potential: Let $V \in C^{1}(\mathbb{R}, \mathbb{R})$ be any potential (not necessarily 1-periodic).
Hamiltonian: $\quad H:=-\partial_{x x}^{2}+V$ as an operator on $L^{2}(\mathbb{R})$.
Associated ODE: $\quad-u^{\prime \prime}+V(x) u=E u$, on $\mathbb{R}$.
Vector space of solutions: Let $\mathcal{L}_{V}(E)$ denote the vectorial space of solutions of the ODE.
Since it is a second order ODE, $\operatorname{dim} \mathcal{L}_{V}(E)=2$, and

$$
\mathcal{L}_{V}(E)=\operatorname{Ran}\left\{c_{E}, s_{E}\right\}, \quad\left\{\begin{array}{l}
-c_{E}^{\prime \prime}+V c_{E}=E c_{E} \\
c_{E}(0)=1, c_{E}^{\prime}(0)=0
\end{array}, \quad\left\{\begin{array}{l}
-s_{E}^{\prime \prime}+V s_{E}=E s_{E} \\
s_{E}(0)=0, s_{E}^{\prime}(0)=1
\end{array} .\right.\right.
$$

## Lemma (definition?)

$E \in \mathbb{R}$ is an eigenvalue of $H$ iff $\mathcal{L}_{V}(E) \cap L^{2}(\mathbb{R}) \neq \emptyset$.
Transfer matrix

$$
T_{E}(x):=\left(\begin{array}{ll}
c_{E}(x) & c_{E}^{\prime}(x) \\
s_{E}(x) & s_{E}^{\prime}(x)
\end{array}\right) .
$$

## Lemma

For all $x \in \mathbb{R}$, we have $\operatorname{det} T_{E}(x)=1$
Indeed, $\operatorname{det} T_{E}$ is the Wronskian of the ODE. At $x=0$, we have $T_{E}(0)=\mathbb{I}_{2}$, and

$$
\left(\operatorname{det} T_{E}\right)^{\prime}=\left(c_{E} s_{E}^{\prime}-s_{E} c_{E}^{\prime}\right)^{\prime}=c_{E} s_{E}^{\prime \prime}-s_{E} c_{E}^{\prime \prime}=c_{E}(V-E) s_{E}-s_{E}(V-E) c_{E}=0
$$

## Case of periodic potentials.

We now assume that $V$ is 1-periodic.
If $u(x)$ is solution to the ODE, then so is $u(\cdot+1)$. In particular there are constants $\alpha, \beta, \gamma, \delta$ such that

$$
\left\{\begin{array}{l}
c_{E}(x+1)=\alpha c_{E}(x)+\beta s_{E}(x) \\
s_{E}(x+1)=\gamma c_{E}(x)+\delta s_{E}(x) .
\end{array} \quad \text { or equivalently } \quad T_{E}(x+1)=\left(\begin{array}{cc}
\alpha & \gamma \\
\beta & \delta
\end{array}\right) T_{E}(x) .\right.
$$

At $x=0$, we recognise $T_{E}(x=1)$, so $T_{E}(x+1)=T_{E}(1) T_{E}(x)$.
So for any solution $u \in \mathcal{L}_{E}$, we have

$$
\binom{u(x+n)}{u^{\prime}(x+n)}=\left[T_{E}(1)\right]^{n}\binom{u(x)}{u^{\prime}(x)} .
$$

$\Longrightarrow$ The behaviour of solutions at infinity is given by the singular values of $T_{E}(1)$.
If $\lambda_{1}$ and $\lambda_{2}$ are the singular values of $T_{E}(1)$, then

- $\lambda_{1} \lambda_{2}=\operatorname{det} T_{E}(1)=1$.
- $\lambda_{1}+\lambda_{2}=\operatorname{Tr}\left(T_{E}\right) \in \mathbb{R}$.


## Two cases.

- if $\left|\lambda_{1}\right|>1$, then $\left|\lambda_{2}\right|<1$. This implies $\lambda_{1}, \lambda_{2} \in \mathbb{R}$ and $\left|\operatorname{Tr}\left(T_{E}\right)\right|>2$.

There is one mode exponentially increasing at $+\infty$ and exponentially decreasing at $-\infty$.
There is one mode exponentially increasing at $-\infty$ and exponentially decreasing at $+\infty$. The elements of $\mathcal{L}_{E}$ cannot be approximated in $L^{2}$, which implies $E \notin \sigma(H)$.

- if $\left|\lambda_{1}\right|=1$, then $\left|\lambda_{2}\right|=1$. This implies $\left|\lambda_{1}\right|=1, \lambda_{2}=\overline{\lambda_{1}}$ and $\left|\operatorname{Tr}\left(T_{E}\right)\right| \leq 2$.

All solutions in $\mathcal{L}_{E}$ are bounded (quasi-periodic).
All solutions in $\mathcal{L}_{E}$ can be approximated in $L^{2}$, which implies $E \in \sigma_{\text {ess }}(H)$.

The spectrum of $H$ can be read from the (continuous) map $E \mapsto \operatorname{Tr}\left(T_{E}\right)$.

Example: for $V(x):=50 \cdot \cos (2 \pi x)+10 \cdot \cos (4 \pi x)$,


## Theorem (Spectrum of 1-dimensional periodic operators)

If $V$ is 1-periodic, the spectrum $H:=-\partial_{x x}^{2}+V(x)$ is purely essential (no eigenvalues). It is composed of bands:

$$
\sigma(H)=\sigma_{\mathrm{ess}}(H)=\bigcup_{n \geq 1}\left[E_{n}^{-}, E_{n}^{+}\right]
$$

Essential gap: The interval $g_{n}:=\left(E_{n}^{+}, E_{n+1}^{-}\right)$is called the n-th essential gap of the operator $H$. Physical interpretation:

- If $E \in \sigma(H)$, electrons with energy $E$ can travel through the medium (quasi-periodic solutions);
- If $E \notin \sigma(H)$, electrons cannot propagate: they are exponentially attenuated in the medium.

Example: If $V=0$, then $H=-\partial_{x x}^{2}$. We have $-u^{\prime \prime}=E u$ if $u=\alpha \mathrm{e}^{\mathrm{i} \sqrt{E}}+\beta \mathrm{e}^{-\mathrm{i} \sqrt{E}}$.

- If $E \geq 0, \sqrt{E} \in \mathbb{R}$, and we have travelling waves;
- If $E<0, \sqrt{E} \in \mathrm{i} \mathbb{R}$, and we have exponential waves.
- The spectrum of $-\partial_{x x}^{2}$ is $[0, \infty)$.


## How about the half system?

Let $E \notin \sigma(H)$. The set of solutions can be split as

$$
\mathcal{L}_{V}(E)=\mathcal{L}_{V}^{+}(E) \oplus \mathcal{L}_{V}^{-}(E), \quad \mathcal{L}_{V}^{ \pm}(E):=\left\{u \in \mathcal{L}_{V}(E), \quad u \in L^{2}\left(\mathbb{R}^{ \pm}\right)\right\}
$$

They are both of dimension 1 .
We define the discrete set $\mathcal{Z}_{V}^{+}[u]:=u^{-1}(\{0\})$ for $u \in \mathcal{L}_{V}^{+}(E)$.

- The set $\mathcal{Z}_{V}^{+} \subset \mathbb{R}$ depends only on $\mathcal{L}_{V}^{+}($not on $u)$.
- The set $\mathcal{Z}_{V}^{+}$is 1-periodic (because if $u \in \mathcal{L}_{V}^{+}(E)$, then $u(\cdot-1) \in \mathcal{L}_{V}^{+}(E)$, hence $u(\cdot-1)=\alpha u$ ).

Key remark: If $0 \in \mathcal{Z}^{+}$, then $E$ is an eigenvalue of $H^{\sharp}$ (with corresponding eigenspace $\mathcal{L}_{V}^{+}$).

## How about the half system?

Let $E \notin \sigma(H)$. The set of solutions can be split as

$$
\mathcal{L}_{V}(E)=\mathcal{L}_{V}^{+}(E) \oplus \mathcal{L}_{V}^{-}(E), \quad \mathcal{L}_{V}^{ \pm}(E):=\left\{u \in \mathcal{L}_{V}(E), \quad u \in L^{2}\left(\mathbb{R}^{ \pm}\right)\right\}
$$

They are both of dimension 1 .
We define the discrete set $\mathcal{Z}_{V}^{+}[u]:=u^{-1}(\{0\})$ for $u \in \mathcal{L}_{V}^{+}(E)$.

- The set $\mathcal{Z}_{V}^{+} \subset \mathbb{R}$ depends only on $\mathcal{L}_{V}^{+}($not on $u)$.
- The set $\mathcal{Z}_{V}^{+}$is 1-periodic (because if $u \in \mathcal{L}_{V}^{+}(E)$, then $u(\cdot-1) \in \mathcal{L}_{V}^{+}(E)$, hence $u(\cdot-1)=\alpha u$ ).

Key remark: If $0 \in \mathcal{Z}^{+}$, then $E$ is an eigenvalue of $H^{\sharp}$ (with corresponding eigenspace $\mathcal{L}_{V}^{+}$).
Consider now $V_{t}(x)=V(x-t), H_{t}=-\partial_{x^{x}}^{2}+V_{t}, \mathcal{L}_{t}^{ \pm}(E)=\mathcal{L}_{V_{t}}^{ \pm}(E), \mathcal{Z}_{t}^{+}:=\mathcal{Z}_{V_{t}}^{+}, \ldots$

- We have $\mathcal{Z}_{t}^{+}=\mathcal{Z}_{0}^{+}+t$ (the set of roots is shifted);
- If $0 \in \mathcal{Z}_{t}^{+}$, then $E \in \sigma\left(H_{t}^{\sharp}\right)$.

So, the number of $t \in[0,1)$ so that $E \in \sigma\left(H_{t}^{\sharp}\right)$ equals the number of points of $\mathcal{Z}_{V}^{+}$in $(-1,0]$.

## Lemma

If $E$ is in the $n$-th gap, and if $u \in \mathcal{L}_{V}(E)$ is any non null solution, then $u$ has $n$ zeros in $(-1,0]$.

## Proof.

Step 1. If $x_{0} \in \mathcal{Z}_{0}$, then $x_{0}+1 \in \mathcal{Z}_{0}$.
In particular, $\left(E,\left.u_{t=0}\right|_{\left[x_{0}, x_{0}+1\right]}\right)$ is an eigenpair of the Dirichlet problem

$$
\left\{\begin{array}{l}
\left(-\partial_{x x}^{2}+V(x)\right) u=E u, \quad \text { on } \quad\left(x_{0}, x_{0}+1\right) \\
u\left(x_{0}\right)=u\left(x_{0}+1\right)=0 .
\end{array}\right.
$$

We want to evaluate $\mathcal{M}$, the number of roots of $u$ in $\left[x_{0}, x_{0}+1\right)$
Step 2 (deformation). For $0 \leq s \leq 1$, we introduce $\left(E(s), \widetilde{u_{s}}\right)$ the Dirichlet eigenpair of

$$
\left\{\begin{array}{l}
\left(-\partial_{x x}^{2}+s V(x)\right) \widetilde{u_{s}}=E_{s} \widetilde{u_{s}}, \quad \text { on } \quad\left(x_{0}, x_{0}+1\right) \\
\widetilde{u_{s}}\left(x_{0}\right)=\widetilde{u_{s}}\left(x_{0}+1\right)=0
\end{array}\right.
$$

which is a continuation of $(E, u)$ at $s=1$, and by $\mathcal{M}_{s}$ the number of zeros of $\widetilde{u_{s}}$ in the interval $\left[x_{0}, x_{0}+1\right)$.

By continuity, $E(s)$ cannot cross the essential spectrum, so $E(s)$ is always in the $n$-th gap. By Cauchy-Lipschitz, two zeros cannot merge, so $\mathcal{M}_{s}$ is independent of $s$, and $\mathcal{M}=\mathcal{M}_{s=1}$. At $s=0$, we recover the usual Laplacian (hence $u_{s=0}(x) \approx \sin (\pi(n+1) x)$ )

We deduce that $E(s)$ is the branch of $n$-th eigenvalues, and that $\mathcal{M}=n$.

## Lemma

If $\widetilde{E}(t)$ is a branch of eigenvalues of $H_{t}^{\sharp}$ in the gap, then $E^{\prime}(t)<0$ (all branches go downwards).
If $(\widetilde{E}(t), \widetilde{u}(t))$ is a branch of eigenpair for $H_{t}^{\sharp}$ with $\left\|\widetilde{u}_{t}\right\|^{2}=1$. We have $H(t) \widetilde{u}(t)=\widetilde{E}(t)$, and $\widetilde{E}(t)=\langle\widetilde{u}(t), H(t) \widetilde{u}(t)\rangle$. Differentiating in $t$ gives (Hellmann-Feynman argument)

$$
\begin{aligned}
\widetilde{E}^{\prime}(t) & =\left\langle\widetilde{u_{t}}, \partial_{t} H_{t} \widetilde{u_{t}}\right\rangle+\left\langle\partial_{t} \widetilde{u_{t}}, H_{t} \widetilde{u_{t}}\right\rangle+\left\langle\widetilde{u_{t}}, H_{t} \partial_{t} \widetilde{u_{t}}\right\rangle \\
& =\left\langle\widetilde{u_{t}},\left(\partial_{t} V_{t}\right) \widetilde{u_{t}}\right\rangle+\widetilde{E}(t) \underbrace{\left(\left\langle\partial_{t} \widetilde{u_{t}}, \widetilde{u_{t}}\right\rangle+\left\langle\widetilde{u_{t}}, \partial_{t} \widetilde{u_{t}}\right\rangle\right)}_{=\partial_{t}\left\|\widetilde{u_{t}}\right\|^{2}=0}=\int_{0}^{\infty}\left(\partial_{t} V_{t}\right)\left|\widetilde{u_{t}}\right|^{2} \mathrm{~d} x .
\end{aligned}
$$

On the other hand, if $u(t)=u(x-t)$ is a branch of functions in $\mathcal{L}_{t}^{+}(E)$ ( E is fixed now), then

$$
\left(-\partial_{x x}^{2}+V_{t}-E\right) u_{t}=0
$$

These functions do not satisfy Dirichlet in general! Differentiating in $t$ gives

$$
\left(-\partial_{x x}^{2}+V_{t}-E\right) \partial_{t} u_{t}+\left(\partial_{t} V_{t}\right) u_{t}=0 .
$$

We multiply by $u_{t}$ and integrate on $\mathbb{R}^{+}$. We integrate by part and obtain (now we have boundary terms)

$$
\int_{0}^{\infty}\left(\partial_{t} V_{t}\right)\left|u_{t}\right|^{2}=\partial_{x} u_{t}(0) \partial_{t} u_{t}(0)
$$

Of course, at the point $t$, we have $u_{t}=\widetilde{u_{t}}$. Since $u_{t}(x)=u(x-t)$, we obtain

$$
\widetilde{E}^{\prime}(t)=-\left|\partial_{t} u_{t}\right|^{2}(0)<0
$$

## An application: junctions and dislocations

## The Spectral flow

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

Sf $\left(A_{t}, E\right):=$ number of eigenvalues going downwards in the essential gap where $E$ lies.


The previous result can be formulated as:

$$
\mathrm{Sf}\left(H_{t}^{\sharp}, E\right)=\mathcal{N}(E), \quad \mathcal{N}(E):=\text { number of bands below } E .
$$

Facts :

- If $t \mapsto K_{t}$ is a 1-periodic continuous family of compact operators, then

$$
\operatorname{Sf}\left(A_{t}, E\right)=\operatorname{Sf}\left(A_{t}+K_{t}, E\right)
$$

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

$$
\operatorname{Sf}\left(f\left(A_{t}\right), f(E)\right)=\operatorname{Sf}\left(A_{t}, E\right)
$$

## Application: Junctions between two materials

Let $V_{L}$ and $V_{R}$ be two 1-periodic potentials. We consider the junction operator

$$
H_{t}^{\text {junction }}:=-\partial_{x x}^{2}+\left[V_{L}(x) \mathbb{1}(x<0)+V_{R}(x-t) \mathbb{1}(x>0)\right] \quad \text { on } \quad L^{2}(\mathbb{R})
$$

## Theorem

If $E \in \mathbb{R}$ is in the resolvent set of all left and right bulk operators, then

$$
\operatorname{Sf}\left(H_{t}^{\text {junction }}, E\right)=\mathcal{N}^{+}(E)
$$

## Application: Junctions between two materials

Let $V_{L}$ and $V_{R}$ be two 1-periodic potentials. We consider the junction operator

$$
H_{t}^{\text {junction }}:=-\partial_{x x}^{2}+\left[V_{L}(x) \mathbb{1}(x<0)+V_{R}(x-t) \mathbb{1}(x>0)\right] \quad \text { on } \quad L^{2}(\mathbb{R})
$$

## Theorem

If $E \in \mathbb{R}$ is in the resolvent set of all left and right bulk operators, then

$$
\operatorname{Sf}\left(H_{t}^{\text {junction }}, E\right)=\mathcal{N}^{+}(E) .
$$

## Idea of the proof

Consider the cut Hamiltonian

$$
H_{t}^{\text {cut }}:=-\partial_{x x}^{2}+\left[V_{L}(x) \mathbb{1}(x<0)+V_{R}(x-t) \mathbb{1}(x>0)\right] \quad \text { on } \quad L^{2}(\mathbb{R})=L^{2}\left(\mathbb{R}^{-}\right) \cup L^{2}\left(\mathbb{R}^{+}\right)
$$

and with Dirichlet boundary conditions at $x=0$.
For any $\Sigma$ negative enough (below the essential spectra of all operators), we have

$$
K_{t}:=\left(\Sigma-H_{t}^{\text {cut }}\right)^{-1}-\left(\Sigma-H_{t}^{\text {junction }}\right)^{-1} \quad \text { is compact (here, it is finite rank). }
$$

So

$$
\operatorname{Sf}\left(\left(\Sigma-H_{t}^{\text {junction }}\right)^{-1},(\Sigma-E)^{-1}\right)=\operatorname{Sf}\left(\left(\Sigma-H_{t}^{\text {cut }}\right)^{-1},(\Sigma-E)^{-1}\right)
$$

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

$$
\operatorname{Sf}\left(H_{t}^{\text {junction }}, E\right)=\operatorname{Sf}\left(H_{t}^{\text {cut }}, E\right)=\operatorname{Sf}\left(H_{t}^{\sharp,+}, E\right)=\mathcal{N}^{+}(E) .
$$

## Remarks on this first proof

## Good points

Can be generalized in different settings.
Instead of a flow of roots (the set $\mathcal{Z}_{V}^{+}$), we use the notion of Maslov index = crossings of Lagrangian planes (tools of symplectic geometry).

- Vector valued operators

$$
H_{t}:=-\Delta+\mathbb{V}_{t}(x), \quad \text { on } \quad L^{2}\left(\mathbb{R}, \mathbb{C}^{N}\right)
$$

We prove that if $E \notin \sigma(H)$, then $\operatorname{dim}\left(\mathcal{L}_{V}^{ \pm}\right)$are both of dimension $N$.

- We can change the boundary conditions (and have a $t$-dependent boundary conditions). For instance, we prove that for the family of operators

$$
H_{t}^{\sharp}:=-\Delta+V(x), \quad \text { with Robin domain } \quad \sin (\pi t) u(0)=\cos (\pi t) u^{\prime}(0)
$$

we have $\operatorname{Sf}\left(H_{t}^{\sharp}, E\right)=-1$ in all gaps (including the 0-th one!)
Bad point
Not really adapted to the two-dimensional setting...

## Second proof(by Hempel and Kohlmann)

## Idea of the proof

Idea: Prove the result in the dislocated case.
Let $L \in \mathbb{N}$ be a (large) integer. Consider the family of operators

$$
\mathcal{H}_{L, t}^{\text {junction }}:=-\partial_{x x}^{2}+[V(x) \mathbb{1}(x<0)+V(x-t) \mathbb{1}(x>0)], \quad \text { on } \quad L^{2}\left(\left[-\frac{1}{2} L, \frac{1}{2} L+t\right]\right)
$$

with periodic boundary conditions.

- The branches of eigenvalues of $t \mapsto \mathcal{H}_{L, t}^{\text {junction }}$ 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.
$\Rightarrow$ The extra eigenvalue must come from an upper band...
$\Rightarrow$ There is a «spectral flow» of 1 between the second band and the first one There is a «spectral flow» of 2 between the third band and the second one, ...

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.

$\qquad$

As $t$ moves from 0 to $1 \ldots$

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


As $t$ moves from 0 to $1 \ldots$

$$
t=0.0
$$

$t=0.25$
$t=0.5$
$t=0.75$
$t=1.0$



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



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.

Remark: the proof can be generalized to higher dimensions!

## The two-dimensional case

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

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

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

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



- For $L \in \mathbb{N}$, consider the model in the tube $\mathbb{R}_{+} \times[0, L]$ with periodic boundary conditions in $x_{2}$.
- Consider the «Two-dimensional Grand Hilbert Hotel».
- As $t$ moves from 0 to $1, L$ new rooms are created on each floor.
- Let $L \rightarrow \infty$...

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 $\theta$.

The two-dimensional twisted case.
We rotate $V$ by $\theta$.


Commensurate case $\left(\tan \theta=\frac{p}{q}\right.$ )
Considering a Supercell of size $L=\sqrt{p^{2}+q^{2}}$, we recover a $L \mathbb{Z}^{2}$-periodic potential. «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 $t \mapsto \sigma\left(H_{\theta}^{\sharp}(t)\right)$ is $1 / L$ periodic.
«Ast moves from 0 to $\frac{1}{L}, 1$ new room is created»

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

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


## Theorem (DG, Comples Rendus. Mathématique, Tome 359 (ev21) )

If $\tan \theta \notin \mathbb{Q}$, the spectrum of $H_{\theta}^{\sharp}$ 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... so the convergence of the spectrum is not guaranteed, and we need to prove it by hand.

Limiting procedure
Consider a sequence $\theta_{n} \rightarrow \theta$, with $\tan \left(\theta_{n}\right)=\frac{p_{n}}{q_{n}} \in \mathbb{Q}$, and set $L_{n}:=\sqrt{p_{n}^{2}+q_{n}^{2}}$.
By the commensurate case result, there is $t_{n} \in\left[0, \frac{1}{L_{n}}\right]$ and $\phi_{n} \in L_{\text {per }}^{2}\left(\mathbb{R}^{+} \times\left[0, L_{n}\right]\right)$ so that

$$
\left(-\Delta+V_{\theta_{n}}\left(t-t_{n}\right)-E\right) \phi_{n}=0, \quad \int_{\mathbb{R}^{+} \times\left[0, L_{n}\right]}\left|\phi_{n}\right|^{2}=1 .
$$

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

## Idea of the proof

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

Limiting procedure
Consider a sequence $\theta_{n} \rightarrow \theta$, with $\tan \left(\theta_{n}\right)=\frac{p_{n}}{q_{n}} \in \mathbb{Q}$, and set $L_{n}:=\sqrt{p_{n}^{2}+q_{n}^{2}}$.
By the commensurate case result, there is $t_{n} \in\left[0, \frac{1}{L_{n}}\right]$ and $\phi_{n} \in L_{\mathrm{per}}^{2}\left(\mathbb{R}^{+} \times\left[0, L_{n}\right]\right)$ so that

$$
\left(-\Delta+V_{\theta_{n}}\left(t-t_{n}\right)-E\right) \phi_{n}=0, \quad \int_{\mathbb{R}^{+} \times\left[0, L_{n}\right]}\left|\phi_{n}\right|^{2}=1 .
$$

It is tempting to extract a weak-limit of $\phi_{n}$, but this will fail (we would get $\phi_{*}=0$ at the end)...
Idea: Normalize the functions in $L^{\infty}$
Consider the functions

$$
\Psi_{n}:=\frac{\phi_{n}}{\left\|\phi_{n}\right\|_{L^{\infty}}}, \quad \text { so that } \quad\left(-\Delta+V_{\theta_{n}}\left(t-t_{n}\right)-E\right) \Psi_{n}=0, \quad\left\|\Psi_{n}\right\|_{L^{\infty}}=1
$$

(the parameter $L_{n}$ is no longer here).

$$
\left(-\Delta+V_{\theta_{n}}\left(t-t_{n}\right)-E\right) \Psi_{n}=0, \quad\left\|\Psi_{n}\right\|_{L^{\infty}}=1
$$

## Step 1: Control the mass

Consider $x_{n} \in \mathbb{R}^{2}$ so that $\Psi_{n}\left(x_{n}\right)>\frac{1}{2}$.

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

$$
\left(-\Delta+V_{\theta}\left(x-t^{*}\right)-E\right) \Psi_{*}=0
$$

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

$$
\left(-\Delta+V_{\theta_{n}}\left(t-t_{n}\right)-E\right) \Psi_{n}=0, \quad\left\|\Psi_{n}\right\|_{L^{\infty}}=1
$$

## Step 1: Control the mass

Consider $x_{n} \in \mathbb{R}^{2}$ so that $\Psi_{n}\left(x_{n}\right)>\frac{1}{2}$.

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

$$
\left(-\Delta+V_{\theta}\left(x-t^{*}\right)-E\right) \Psi_{*}=0
$$

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


## Open question

Is $E$ an eigenvalue of $H_{\theta}$ ( $\sim$ Anderson localization), or in the essential spectrum (travelling waves).

## Another application: the definition of the kilo

May 20, 2019: New definition of the kg by the Bureau International des Poids et Mesures (BIPM) ${ }^{1}$ :
"Le kilogramme, symbole kg, est l'unité de masse du SI. Il est défini en prenant la valeur numérique fixée de la constante de Planck, h, égale à 6, $62607015 \times 10^{-34}$ f.s."

Question: How do you measure $h$ ? How do you measure $h$ with $10^{-9}$ accuracy?
Comments by von Klitzing ${ }^{2}$ : "The discovery of the QHE led to a new type of electrical resistor [...]. This resistor is universal for all 2D electron systems in strong magnetic fields with an uncertainty of less than one part in $10^{10}$."

QHE = Quantum Hall Effect ${ }^{3}$ (von Klitzing got Nobel prize in 1985 for discovery of Quantum Hall Effect).


[^0]In this setting, the magnetic field $A$ plays the role of the pump.

$$
H_{B}=-\partial_{x x}^{2}+\left(-\mathrm{i} \partial_{y}+B x\right)^{2}
$$

After a Fourier transform in $y$, we get

$$
H_{B, k_{y}}=-\partial_{x x}^{2}+\left(k_{y}+B x\right)^{2}=-\partial_{x x}^{2}+B^{2}(x-t)^{2}, \quad \text { with } \quad t=\frac{-k_{y}}{B}
$$

## Lemma

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

The plateaus observed by von Klitzing correspond to these spectral flows.

In this setting, the magnetic field $A$ plays the role of the pump.

$$
H_{B}=-\partial_{x x}^{2}+\left(-\mathrm{i} \partial_{y}+B x\right)^{2}
$$

After a Fourier transform in $y$, we get

$$
H_{B, k_{y}}=-\partial_{x x}^{2}+\left(k_{y}+B x\right)^{2}=-\partial_{x x}^{2}+B^{2}(x-t)^{2}, \quad \text { with } \quad t=\frac{-k_{y}}{B}
$$

## Lemma

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

The plateaus observed by von Klitzing correspond to these spectral flows.

## Thank you for your attention!


[^0]:    ${ }^{1}$ https://www.bipm.org/fr/measurement-units/
    ${ }^{2}$ von Klitzing, Nature Physics 13, 2017
    ${ }^{3}$ K. von Klitzing; G. Dorda; M. Pepper, Phys. Rev. Lett. 45 (6): 494-497, 1980.

