Spectral properties of half-periodic systems

David Gontier

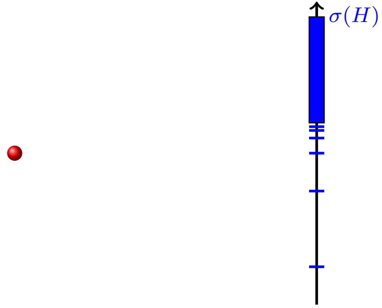
CEREMADE, Université Paris-Dauphine & DMA, École Normale Supérieure de Paris

Joint work with Hanne Van Den Bosch and Camilo Gómez Araya

June 5, 2024

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

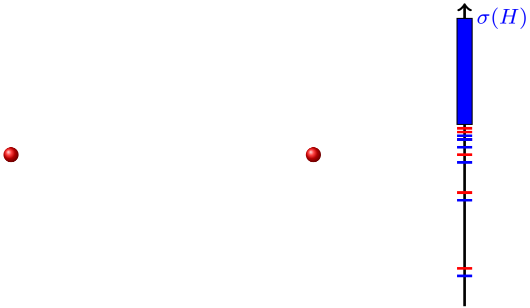
$$H = -\Delta + V(\mathbf{x}), \quad \text{e.g.} \quad V(\mathbf{x}) = \frac{-Z}{|\mathbf{x}|}.$$



- Discrete spectrum (= eigenvalues). The energy levels are *quantized*.
- The N fermions occupies the N first eigenvectors/orbitals (associated to the N lowest eigenvalues).

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

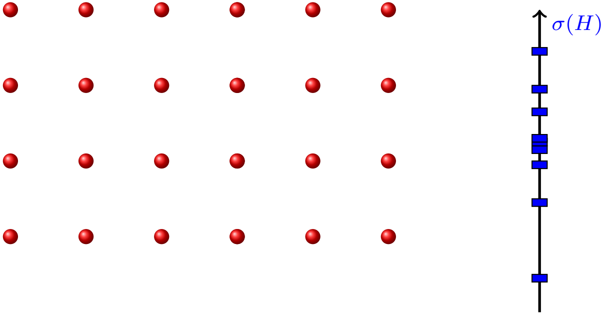
$$H = -\Delta + V\left(\mathbf{x} - \frac{R}{2}\right) + V\left(\mathbf{x} + \frac{R}{2}\right).$$



- 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!
One band = one electron per unit cell.

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

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

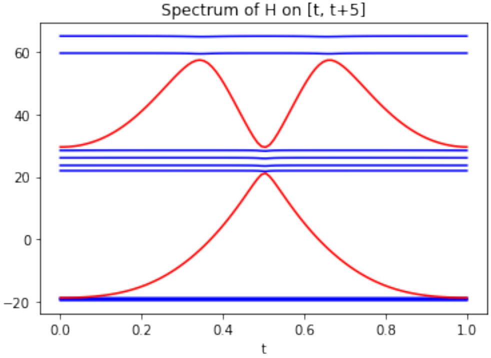
The potential V is 1-periodic. We expect a band-gap structure for the spectrum.
We study H in a box $[t, t+L]$ with Dirichlet boundary conditions, and with finite difference.

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.



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.

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 (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.
These eigenvalues are simple, and their associated eigenvectors are exponentially localised (= edge modes).

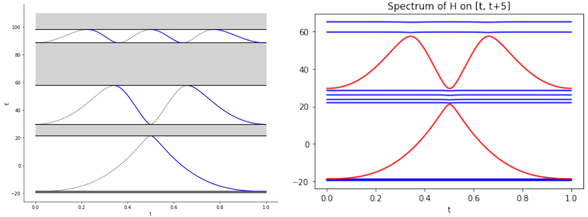


Figure: (Left) Spectrum of $H^\sharp(t)$ for $t \in [0, 1]$. (Right) Spectrum of the operator on $[t, t + L]$.

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

Idea of the proof

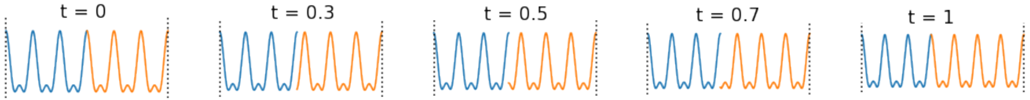
Step 1. Prove the result for *dislocations* (following *Hempel and Kohlmann*).
Introduce the dislocated operator

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

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

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

with periodic boundary conditions.



Remarks

- The branches of eigenvalues of $t \mapsto H_{L,t}^{\mathrm{disloc}}$ 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.

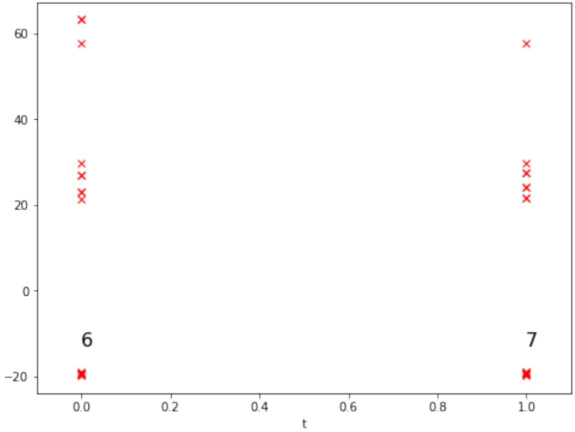


Figure: Spectrum of $H_{L,t}^{\text{disloc}}$ for $L = 6$ at $t = 0$ (6 cells) and $t = 1$ (7 cells).

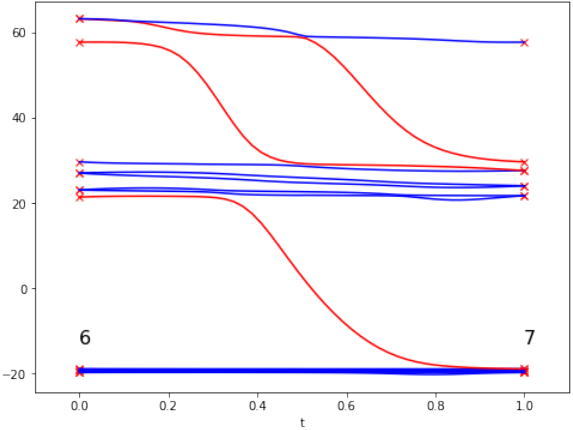


Figure: Spectrum of $H_{L,t}^{\text{disloc}}$ for all $t \in [0, 1]$.

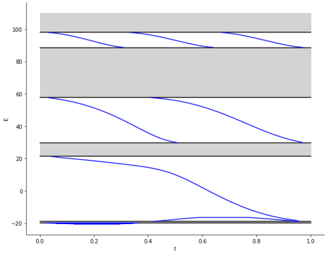
The presence and the number of the red lines are independent of $L \in \mathbb{N}$.
They survive in the limit $L \to \infty$.

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

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

Consider the cut Hamiltonian

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

and with Dirichlet boundary conditions at $x=0$ (only the domain differs).

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

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

So

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

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

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

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 $\mathrm{Sf}\left(H_t^{\text{junct}}, E\right) = \mathcal{N}_R(E)$.

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 $\mathrm{Sf}\left(H_t^{\text{junct}}, E\right) = \mathcal{N}_R(E)$.

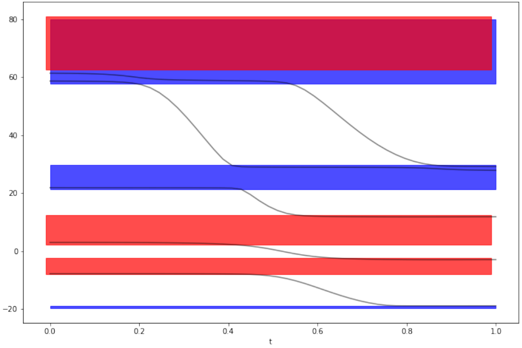


Figure: Spectrum of H_t^{junc} as a function of t.

A «fun» analogy

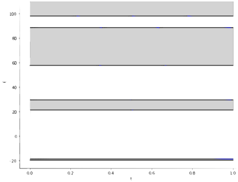
The *«Grand Hilbert Hotel»*
An infinite number of floors, and an infinite number of rooms per floor.

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

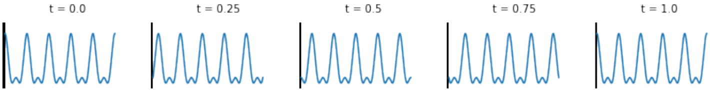
... Floor 3.

... Floor 2.

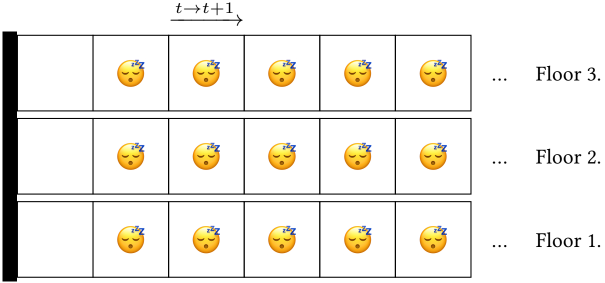
... Floor 1.

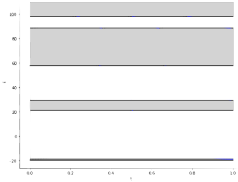


As t moves from 0 to 1...

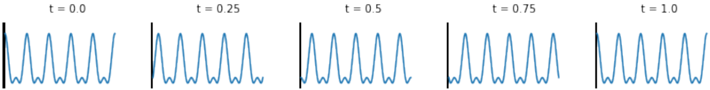


... a new room is created on each floor!

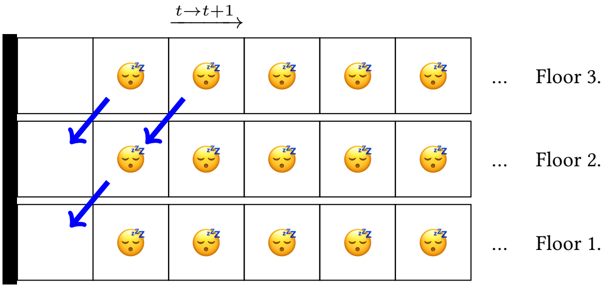


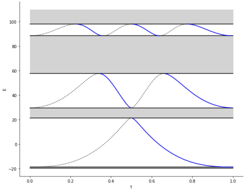


As t moves from 0 to 1...



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

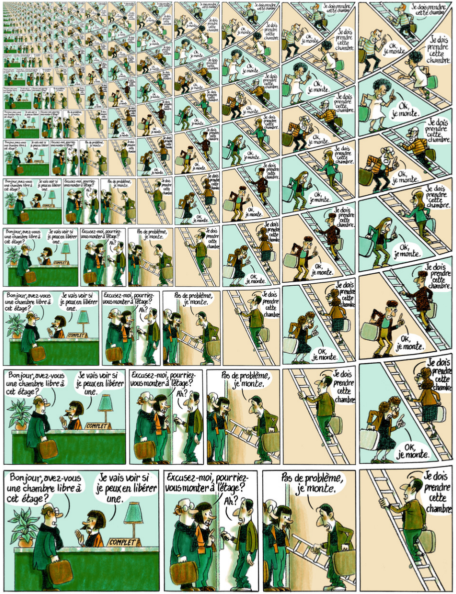




In order to fill the new rooms,

- 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.

If we reverse the motion, (we delete rooms, or new guests arrive), then people climb up instead.

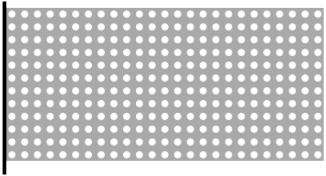


The Grand Hilbert Hotel, by Étienne Lécroart.

The two-dimensional case.

Let V be a $\mathbb{Z}^2$-periodic potential. We study the edge operator

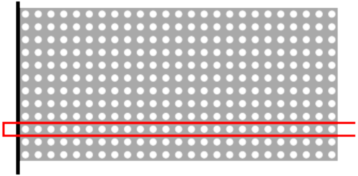
$$H^\sharp(t) = -\Delta + V(x-t, y), \quad \text{on} \quad L^2(\mathbb{R}_+ \times \mathbb{R}), \quad \text{with Dirichlet boundary conditions.}$$



The two-dimensional case.

Let V be a $\mathbb{Z}^2$-periodic potential. We study the edge operator

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



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

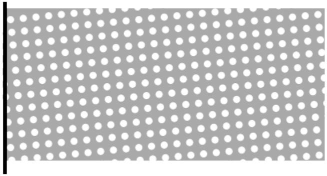
$$H_k^\sharp(t) = -\partial_{xx}^2 + (-\mathrm{i}\partial_y + k)^2 + V(x-t, y), \quad \text{on the **tube**} \quad L^2(\mathbb{R}_+ \times [0,1]).$$

- 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 $\Longrightarrow$ 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.

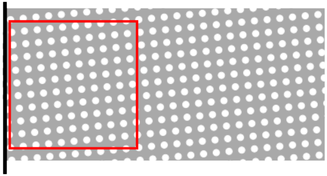
The two-dimensional twisted case.

We rotate V by θ.



The two-dimensional twisted case.

We rotate V by θ.



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»

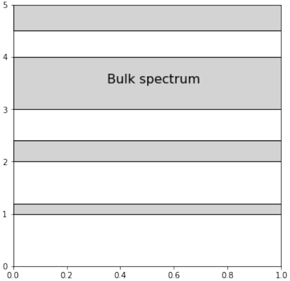
In-commensurate case ($\tan\theta \notin \mathbb{Q}$, corresponds to $L \to \infty$)

Theorem (DG 2021)

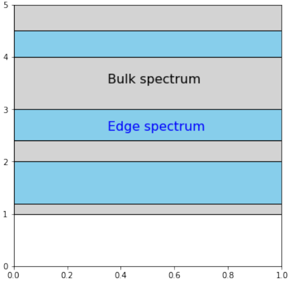
If $\tan\theta \notin \mathbb{Q}$, *the spectrum of* $H_\theta^\sharp$ *is of the form* $[\Sigma, \infty)$.

Remarks:

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



(a) Uncut two-dimensional material



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

Open question

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

In the Tight–Binding Approximation (TBA)

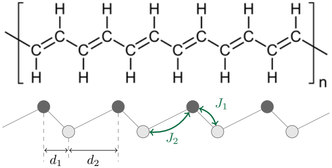
joint work with Hanne Van Den Bosch & Camilo Gómez Araya

In the (one dimensional) TBA, bulk operators are of the form

$$(H\psi)_n = a_* \psi_{n-1} + b\psi_n + a\psi_n \qquad = (h * \psi) \quad \text{(=convolution)}.$$

$$H = \left(\begin{array}{ccc|ccc} \ddots & \ddots & & & & \\ \ddots & b & a & & & \\ & a^* & b & a & & \\ \hline & & a^* & \color{red}{b} & \color{red}{a} & \\ & & & \color{red}{a^*} & \color{red}{b} & \color{red}{\ddots} \\ & & & & \color{red}{\ddots} & \color{red}{\ddots} \end{array}\right).$$

Motivation (Example): Su–Schrieffer-Heeger (SSH) chain (polyacetylene)



$$H = \begin{pmatrix} \ddots & \ddots & & & & \\ \ddots & 0 & J_1 & & & \\ & J_1^* & 0 & J_2 & & \\ & & J_2^* & 0 & J_1 & \\ & & & J_1^* & 0 & \ddots \\ & & & & \ddots & \ddots \end{pmatrix}, \quad a = \begin{pmatrix} 0 & 0 \\ J_2 & 0 \end{pmatrix}, \quad b = \begin{pmatrix} 0 & J_1 \\ J_1 & 0 \end{pmatrix}.$$

Lemma (Exercice)

If $|J_1| < |J_2|$, then 0 is an eigenvalue of multiplicity 1 of the cut operator $H^\sharp$.
If $|J_2| < |J_1|$, then 0 is not an eigenvalue of $H^\sharp$.

In the first case, the corresponding eigenvector (= edge state) is **topologically stable** $\equiv$ *Majorana fermions*?

Question: Can we prove spectral flows for TBA models?

Problem

There is no *cut parameter*... The naïve one will give a discontinuous family of operators.

$\Longrightarrow$ **no Spectral Flows**.

Idea: use a *Soft wall* instead of a *hard truncation*

Soft wall ? $w(x)$ a ν-Lipschitz function with $w(-\infty) = +\infty$ and $w(+\infty) = 0$.

Wall operator $(W_t \psi)_n = W(n-t)\psi_n$ (multiplication operator).

Cut operator

$$\boxed{H_t^\sharp \psi = W_t \psi + h * \psi} \qquad \text{(multiplication + convolution).}$$

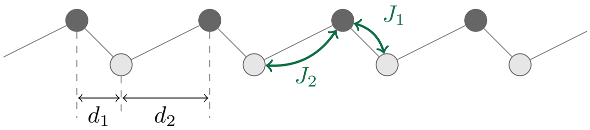
Remarks

- In the TBA setting, the bulk operator is bounded perturbation of the (unbounded) wall operator.
- When $t \mapsto t+1$, the wall is moving to the right. We expect branches of eigenvalues going **upwards**.

Lemma (DG, Gómez Araya, Van Den Bosch, 20??)

We have $\mathrm{Sf}(H_t^\sharp, E) = -\mathcal{N}(E)$.
In addition, for all $t_0 \in \mathbb{R}$ *the operator* $H^\sharp(t_0)$ *has at least* $\mathcal{N}(E)$ *eigenvalues in each interval of the form* $(\lambda, \lambda + \nu]$ *in this gap.*

Numerical simulations for the SSH chain



We took $d_1 = 1/4$, $d_2 = 3/4$, $J_1 = 3/2$ and $J_2 = 1/2$, and the soft wall $w(x) := \begin{cases} 0 & \text{for} \quad x \geq 0 \\ \nu|x| & \text{for} \quad x \leq 0 \end{cases}$,

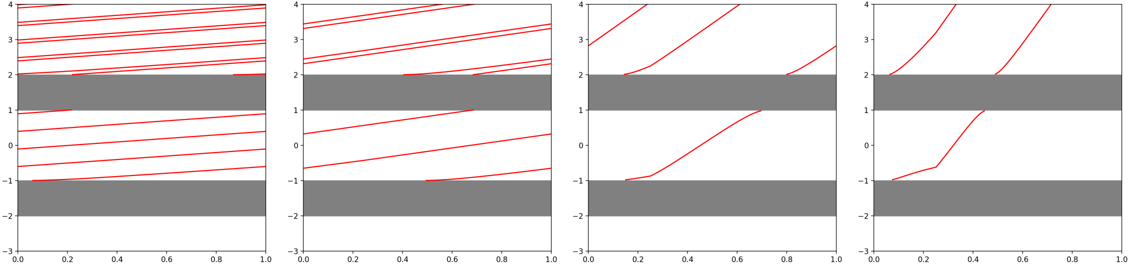


Figure: From left to right, $\nu = 0.5$, $\nu = 1$, $\nu = 5$ and $\nu = 10$.

There is no fundamental difference between the $|J_1| > |J_2|$ and $|J_2| < |J_1|$ cases!
In this soft–wall setting, it is unclear whether the edge modes are topologically protected.

Numerical simulations for graphene (2d)

The *hard–truncation* theory

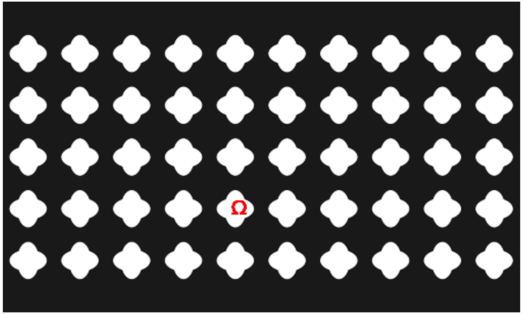
The spectrum of $H^\sharp(k_2)$ (Bloch in the direction orthogonal to the wall) depends on the orientation of the cut:

- For the *zigzag* cut, there is a flat band appearing between the two *Dirac cones*;
- For the *armchair* cut, there is no extra edge modes;
- For another (commensurate orientation), a flat band appears (expect in few rare cases).

Appendix

A degenerate case

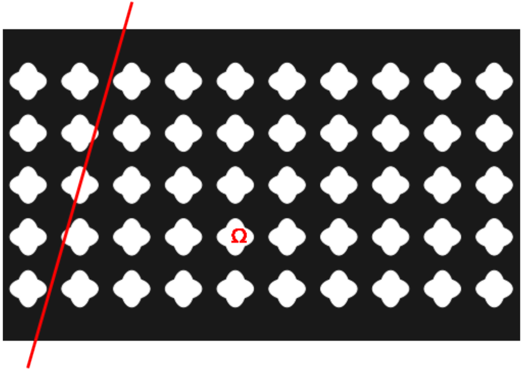
Consider $\Omega \subset \mathbb{R}^2$ a nice bounded set, and repeat it on a $\mathbb{Z}^2$ grid.
Consider $H = -\Delta$ on $L^2(\mathbb{R}^2)$, with Dirichlet boundary conditions «everywhere».



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

A degenerate case

Consider $\Omega \subset \mathbb{R}^2$ a nice bounded set, 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.
In the cut situation:

- If $\tan\theta \in \mathbb{Q}$, a finite number of new motifs appear, each one appears infinitely many times
  $\Longrightarrow$ 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: The cut Landau operator

Consider the **Landau** Hamiltonian (it describes a 2d electron gas in a constant magnetic field B.)

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

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 Fourier momentum k_y plays the role of the shift.

Lemma

If $B \neq 0$, the bulk Hamiltonian has discrete spectrum. $\sigma(H_B) = |B|(2\mathbb{N}_0 + 1)$. (Landau operator).
The edge Hamiltonian $H_{B,t}^\sharp$ has flows of eigenvalues, going downwards.
In particular $\sigma(H_B^\sharp) = [|B|, \infty)$.