Habilitation à diriger la recherche : Periodic and half-periodic fermionic systems

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Fermions (= electrons in this talk)

Pauli principle: *«two identical fermions cannot be in the same quantum state».*

A system of N (uncorrelated) fermions is described by N-**orthonormal** functions (the *orbitals*)... or by the orthogonal projector on these N functions.

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In this habilitation, we are interested in systems with infinitely many fermions \equiv orthogonal projectors of infinite rank.

Outline of the manuscript:

• Low energy spectrum of periodic systems

(with É. Cancès, H. Cornean, V. Ehrlacher, A. Levitt, D. Lombardi, D. Monaco, S. Perrin-Roussel, S. Siraj-Dine). Wannier functions, homotopy of projectors, Brillouin zone integration, ...

Semi-periodic systems

Bulk-edge correspondence, edge modes, spectral flows, ...

• The Hartree-Fock gas (and Peierls model)

(with M. Lewin, Ch. Hainzl, A. Kouandé. É. Séré). Spin symmetry breaking, spatial symmetry breaking, SSH model for polyacetylene, ...

• Lieb-Thirring (and related) inequalities

(with R.L. Frank, M. Lewin, F.Q. Nazar). Lieb-Thirring inequalities, fermionic non-linear Schrödinger, ...

Semi-periodic systems

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

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



• The N fermions occupies the N first eigenvectors/orbitals (associated to the N lowest eigenvalues).

 $\sigma(H)$

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



- 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)



- 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 »;
- $\bullet\,$ 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).

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Motivation: Spectral pollution

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

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

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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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 $H^2(\mathbb{R}^+) \cap H^1_0(\mathbb{R}^+)$). Since V is 1-periodic, the map $t \mapsto H^{\sharp}_t$ 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].

R. Hempel and M. Kohlmann, J. Math. Anal. Appl., 381(1):166-178, 2011.

D. Gontier, J. Math. Phys. 61, 2020.

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E. Korotyaev, Commun. Math. Phys., 213(2):471-489, 2000.

Idea of the proof

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

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

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

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

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 $H_{L,t}^{\text{disloc}}$ 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 $t\mapsto H_t^{\rm disloc}.$

The Spectral flow

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

Sf (A_t, E) := number of eigenvalues going **downwards** in the essential gap where E lies.



The previous result can be formulated as:

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

Facts :

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

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

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

$$Sf(f(A_t), f(E)) = Sf(A_t, E)$$

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

Recall that the dislocated operator is

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

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 (only the domain differs).

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

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

So

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

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

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

The case of junctions

Take two 1-periodic potentials

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

Consider the junction Hamiltonian

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

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

The case of junctions

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



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

A typical spectrum contains:

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

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.



As $t \bmod 0$ to 1...

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



As $t \bmod 0$ 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.

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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 $\mathbb{Z}^2\text{-periodic potential. We study the edge operator$

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

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The two-dimensional twisted case.

We rotate V by θ .



The two-dimensional twisted case.

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

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 $t \mapsto H^{\sharp}_{\theta}(t)$ is now 1/L-periodic (up to some x_2 shifts)
- So the map $t \mapsto \sigma(H^{\sharp}_{\theta}(t))$ 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_{θ}^{\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.



Open question

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

D. Gontier, Comptes Rendus Mathématique, 359(8), 949-958 (2021).

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The Grand Hilbert Hotel, by Étienne Lécroart.

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Crystallization in Lieb-Thirring inequalities

Joint work with Rupert L. FRANK, Mathieu LEWIN and Faizan Q. NAZAR.

Keller problem (1961). Among all potentials V with $\int_{\mathbb{R}^d} V^p$ fixed, which one minimizes $\lambda_1(-\Delta - V)$?

- Existence of an optimal potential in all dimensions (explicit in dimension d = 1).
- Links with Gagliardo-Niremberg inequality, non-linear Schrödinger equation, ...

Theorem (Keller/Gagliardo-Niremberg inequality)

For all $\gamma > \max(0, 1 - \frac{d}{2})$, there is an optimal (smallest) constant $L_{\gamma,d}^{(1)}$ so that, for all $V \in L^{\gamma + \frac{d}{2}}(\mathbb{R}^d, \mathbb{R}^+)$,

 $|\lambda_1(-\Delta-V)|^{\gamma} \le L_{\gamma,d}^{(1)} \int_{\mathbb{R}^d} V^{\gamma+\frac{d}{2}}.$ (Keller inequality).

J.B. Keller, J. Mathematical Phys. 2 (1961), 262–266. E.H. Lieb, W.E. Thirring, Phys. Rev. Lett. 35 (1975), 687–689. E.H. Lieb, W.E. Thirring, Studies in Math. Phys. (1976), 269–303. Keller problem (1961). Among all potentials V with $\int_{\mathbb{R}^d} V^p$ fixed, which one minimizes $\lambda_1(-\Delta - V)$?

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This inequality was then extended by Lieb and Thirring to the (infinite) sum of eigenvalues:

Theorem (Lieb-Thirring inequality, '75-76)

For all $\gamma > \max(0, 1 - \frac{d}{2})$, there is an optimal (smallest) constant $L_{\gamma,d}$ so that, for all $V \in L^{\gamma + \frac{d}{2}}(\mathbb{R}^d, \mathbb{R}^+)$,

$$\sum_{n=1}^{\infty} |\lambda_n(-\Delta-V)|^{\gamma} \le L_{\gamma,d} \int_{\mathbb{R}^d} V^{\gamma+\frac{d}{2}}.$$
 (Lieb-Thirring inequality).

"Open question": is there an optimal potential V for Lieb–Thirring?

J.B. Keller, J. Mathematical Phys. 2 (1961), 262-266.

E.H. Lieb, W.E. Thirring, Phys. Rev. Lett. 35 (1975), 687-689.

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Finite rank Lieb-Thirring.

For all $\gamma > \max(0, 1 - \frac{d}{2})$, there is an optimal (smallest) constant $L_{\gamma,d}^{(N)}$ so that $\sum_{n=1}^{N} |\lambda_n(-\Delta - V)|^{\gamma} \le L_{\gamma,d}^{(N)} \int_{\mathbb{R}^d} V^{\gamma + \frac{d}{2}}.$

Basic fact: The sequence $N \mapsto L_{\gamma,d}^{(N)}$ is increasing, and $L_{\gamma,d} = \lim \uparrow L_{\gamma,d}^{(N)}$.

Theorem (R.L. Frank, DG, M. Lewin (2024?))

For all $\gamma > \max(0, 1 - \frac{d}{2})$, and all integer N > 0, there is an optimal potential $V_N \in L^{\gamma + \frac{d}{2}}(\mathbb{R}^d, \mathbb{R}^+)$. In addition, if $\gamma > \max(0, 2 - \frac{d}{2})$, then $L_{\gamma,d}^{(2N)} > L_{\gamma,d}^{(N)}$. In particular, if $\gamma > \max(0, 2 - \frac{d}{2})$, then $L_{\gamma,d} > L_{\gamma,d}^{(N)}$ for all N.

If the problem defining $L_{\gamma,d}$ has an optimal potential V_* (?), then this one must generate an infinite number of eigenvalues.

R.L. Frank, D. Gontier, M. Lewin, accepted in American Journal of Mathematics.

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Proof of the second part: Consider the test function

$$V_R(x) := \left[V_N^q \left(x - \frac{R}{2} \right) + V_N^q \left(x + \frac{R}{2} \right) \right]^{\frac{1}{q}}, \quad q := \gamma + \frac{d}{2} - 1 \ge 0,$$

and compute the contribution of the *tunnelling* effect. If q > 1, we find $L_{\kappa,d}^{(2N)} > L_{\kappa,d}^{(N)}$.

R.L. Frank, D. Gontier, M. Lewin, accepted in American Journal of Mathematics.

Similar phenomenon for the fermionic non-linear Schrödinger inequality



D. Gontier, M. Lewin, F.Q. Nazar. ARMA 240(3), 1203-1254 (2021).

Similar phenomenon for the fermionic non-linear Schrödinger inequality



Figure: Optimal density for $J_{p,d}^{\text{NLS}}$ in the case d = 2, p = 1.5 and for N from 1 to 7.

D. Gontier, M. Lewin, F.Q. Nazar. ARMA 240(3), 1203-1254 (2021).

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\Rightarrow There is a **crystallization phenomenon**! **Conjecture:** If $\gamma > \max\{0, 2 - \frac{d}{2}\}$, The sequence $(V_N)_N$ "converges" to a periodic potential.

D. Gontier, M. Lewin, F.Q. Nazar. ARMA 240(3), 1203-1254 (2021).

Periodic Lieb-Thirring inequality

Lemma (R.L. Frank, DG, M. Lewin (2021))

Let
$$\gamma > \max\{0, 1 - \frac{d}{2}\}$$
. Then, for all periodic $V \in L^{\gamma + \frac{d}{2}}_{\text{loc}}(\mathbb{R}^d, \mathbb{R}^+)$, we have
$$\underline{\operatorname{Tr}}\left((-\Delta - V)^{\gamma}_{-}\right) \leq L_{\gamma, d} \oint V^{\gamma + \frac{d}{2}}.$$

with the same best Lieb–Thirring constant $L_{\gamma,d}$.

Remark. Taking the test function V = cst shows that

$$L_{\gamma,d} \ge L_{\gamma,d}^{\rm sc} := \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} (|\mathbf{k}|^2 - 1)^{\gamma} d\mathbf{k}. \qquad (\textit{semi-classical constant})$$

Lieb-Thirring "conjecture": $L_{\gamma,d} \stackrel{?}{=} \max\{L_{\gamma,d}^{(1)}, L_{\gamma,d}^{sc}\}.$

The optimal scenario is either the one-bound state, or the semi-classical one = fluid phase.

R.L. Frank, D. Gontier, M. Lewin. Partial Differential Equations, Spectral Theory, and Mathematical Physics. The Ari Laptev Anniversary Volume, volume 18. EMS Publishing House (2021).

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The optimal scenario is either the one-bound state, or the semi-classical one = fluid phase.

Facts.

• In all dimensions d, there is $1 \le \gamma_{
m sc}(d) \le \frac{3}{2}$ so that

$$\begin{cases} \text{if } \gamma < \gamma_{\text{sc}}(d), \qquad L_{\gamma,d} > L_{\gamma,d}^{\text{sc}} \\ \text{if } \gamma \geq \gamma_{\text{sc}}(d), \qquad L_{\gamma,d} = L_{\gamma,d}^{\text{sc}}. \end{cases}$$

• In dimension d = 2, we have $\gamma_{sc}(2) \ge 1.165378$.

In dimension d = 2, for $\gamma \in (1, \gamma_{sc}(2))$, we expect crystallization.

R.L. Frank, D. Gontier, M. Lewin. Partial Differential Equations, Spectral Theory, and Mathematical Physics. The Ari Laptev Anniversary Volume, volume 18. EMS Publishing House (2021).





Figure: Numerical computation of the optimal periodic potential in dimension d = 2, for $\gamma = 1.165400$.

The integrable case $\gamma = 3/2$ in dimension d = 1.

In the original article by Lieb-Thirring 1976, they proved

$$L_{3/2,1} = L_{3/2,1}^{(1)} = L_{3/2,1}^{(N)} = L_{3/2,1}^{\rm sc} = \frac{3}{16}.$$

The optimal potentials for $L_{\gamma,d}^{(N)}$ is the set of *N*-solitons (links with the Korteweg-de-Vries equation)

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Theorem (R.L. Frank, DG, M. Lewin (2021))

For all 0 < k < 1, the potential $V_k(x) := 1 + k^2 - 2k^2 \operatorname{sn}(x|k)^2$ with minimal period 2K(k), is an optimizer for the periodic problem at $\gamma = 3/2$ and d = 1. Here, $\operatorname{sn}(\cdot|k)$ is the Jacobi elliptic function, and $K(\cdot)$ is the complete elliptic integral of the first kind. In addition,

$$\lim_{k \to 0} V_k(x) = 1 \text{ (semi-classical)} \quad and \quad \lim_{k \to 1} V_k(x) = \frac{2}{\cosh^2(x)} \text{ (1-soliton)}.$$

This potential is sometime called the periodic Lamé potential, or the cnoidal wave.



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Known facts about Lieb-Thirring

- $\gamma \mapsto L_{\gamma,d}/L_{\gamma,d}^{sc}$ is decreasing (Aizenmann-Lieb, 1978), and ≥ 1 . There is a unique point $\gamma_{c}(d) > 0$ so that $L_{\gamma,d} = L_{\gamma,d}^{sc}$ iff $\gamma \geq \gamma_{c}(d)$.
- $\gamma = 3/2$ in dimension d = 1. $L_{\gamma,d} = L_{\gamma,d}^{(N)} = L_{\gamma,d}^{\text{sc}} = \frac{3}{16}$. (Lieb-Thirring 1976).
- $\gamma \geq 3/2$ is semi-classical: $L_{\gamma,d} = L_{\gamma,d}^{\mathrm{sc}}$ for all $\gamma \geq \frac{3}{2}$. (Laptev-Weidl 2000) .
- $\gamma = 1/2$ in dimension d = 1. $L_{\frac{1}{2},1} = L_{\frac{1}{2},1}^{(1)}$. (Hundertmark-Lieb-Thomas, 1998).
- $\gamma < 1$ is not semi-classical. $L_{\gamma,d} > L_{\gamma,d}^{\mathrm{sc}}$ for all $\gamma < 1$. (Hellfer-Robert, 2010).



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 $\sigma(-\Delta|_{\Omega})$, 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 $\sigma(-\Delta|_{\Omega})$, 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 \implies 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
 - \implies pure-point spectrum everywhere.