Atypical spectral and dynamical properties of non-locally finite crystals (and hopefully a second part)

based on joint work with O. Post, M. Sabri, and M. Täufer (and P. Bifulco and C. Rose)

Joachim Kerner

Walkshop in Mathematical Physics at the Constructor University Bremen

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Part I: Atypical spectral and dynamical properties of non-locally finite crystals

J. Kerner, O. Post, M. Sabri, M. Täufer, *The curious spectra and dynamics of non-locally finite crystals*, arXiv:2411.14965 (2024), to appear in Communications in Mathematical Physics

Basic setup

- We study discrete Schrödinger operators $\mathcal{H}_\Gamma = \mathcal{A}_\Gamma + Q$ on infinite periodic graphs with finite fundamental cells
- We go beyond the (typical) locally-finite setting and allow a vertex to be connected to *infinitely* many other vertices in the graph; we assume the associated edge weights to be summable
- The **main message** of the first part: such periodic graphs (or crystals) exhibit various atypical phenomena that are absent in the locally-finite setting and that are interesting from a theoretical as well as experimental point of view

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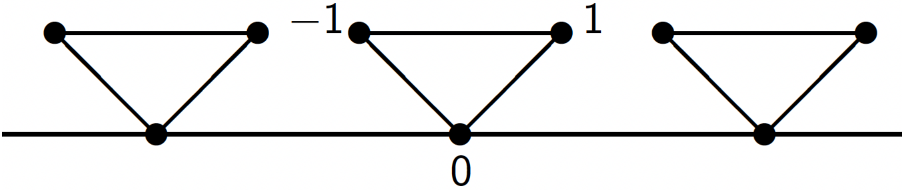
What is typical in the loc.-fin. setting?



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- The Floquet eigenvalues $E_j(\theta)$, $\theta \in \mathbb{T}^d$, are analytic almost everywhere
- An energy band cannot be partly flat; to each (entirely) flat band there corresponds an eigenvector with *compact* support
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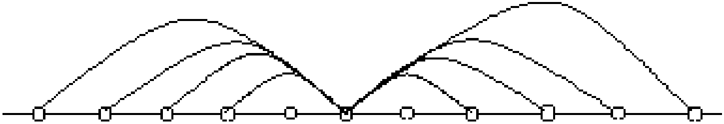
An example graph

- As an example, we consider such a graph



What are some new features?

- Non-locally finite graphs can exhibit *partly* flat bands and eigenfunctions need not be compactly supported anymore
- Already graphs with a single vertex in the fundamental cell may exhibit a (partly) flat band
- There exists a non-locally finite graph that exhibits purely singular continuous spectrum
- Regarding transport: there exist graphs with purely absolutely continuous spectrum that exhibit ballistic transport but *no* dispersion (this solves a question raised in the community)
- There exist non-locally finite graphs with super-ballistic motion

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The framework

- We assume

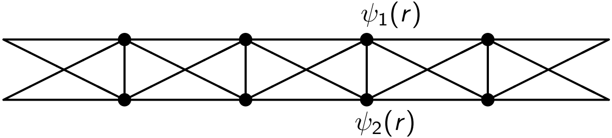
$$\Gamma = V_f + \mathbb{Z}^d_{\mathfrak{a}}$$

with $|V_f| = \nu < \infty$; let $I_{ij} = \{k \in \mathbb{Z}^d : v_j + k_{\mathfrak{a}} \sim v_i\}$

- Hilbert space is $\ell^2(\Gamma) \equiv \ell^2(\mathbb{Z}^d)^\nu$
- Let $Q = (Q_1, \ldots, Q_\nu) \in \mathbb{R}^\nu$ be the potential and introduce the Schrödinger operator

$$(\mathcal{H}_\Gamma \psi)_i(r) = \sum_{j=1}^{\nu} \sum_{k \in I_{ij}} w_{ij}(k)\psi_j(r+k) + Q_i\psi_i(r)$$

for $i = 1, \ldots, \nu$, $r \in \mathbb{Z}^d$



We assume

(1) $w_{ij}(k) > 0$ for all $i, j \in \{1, \ldots, \nu\}$ and $k \in I_{ij}$,

(2) $0 \notin I_{ii} \quad \forall\, i \in \{1, \ldots, \nu\}$,

(3) $w_{ji}(-k) = w_{ij}(k)$ for all $i, j \in \{1, \ldots, \nu\}$ and $k \in I_{ij}$,

(4) $\sum_{k \in I_{ij}} w_{ij}(k) < \infty$ for all $i, j \in \{1, \ldots, \nu\}$.

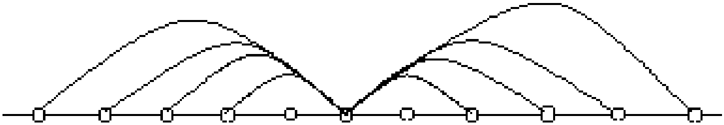
Special case: $\nu = 1$. Then

$$(\mathcal{H}_\Gamma \psi)(r) = \sum_{k \in \mathbb{Z}^d} w(k)\psi(r + k) + Q\psi(r)$$

with $w(k) \geq 0$, $w(-k) = w(k)$, $\sum w(k) < \infty$.

An example graph

- As an example, we consider a graph Γ with $\nu = 1$ and $d = 1$



- The most important (and expected) ingredient here is the unitary Floquet transform $U : \ell^2(\mathbb{Z}^d)^\nu \to L^2(\mathbb{T}^d)^\nu$ defined via,

$$(U\psi)_j(\theta) = \sum_{k\in\mathbb{Z}^d} \mathrm{e}^{2\pi i\theta\cdot k}\psi_j(k) \ , \quad j \in \{1, \dots, \nu\} \ .$$

- Then $\mathcal{H}_\Gamma$ is unitarily equivalent to $\mathcal{M}_H$, a multiplication operator on $L^2(\mathbb{T}^d)^\nu$ acting as the matrix function

$$H(\theta) = (h_{ij}(\theta))_{i,j=1}^{\nu} \ .$$

- One has

$$h_{ij}(\theta) = \begin{cases} \sum_{k\in I_{ij}} w_{ij}(k)\mathrm{e}^{2\pi i\theta\cdot k} \ , & i \neq j \ , \\ \sum_{k\in I_{ii}} w_{ii}(k)\mathrm{e}^{2\pi i\theta\cdot k} + Q_i \ , & i = j \ . \end{cases}$$

- This implies

$$\sigma(\mathcal{H}_\Gamma) = \bigcup_{j=1}^{\nu} \sigma_j \ ,$$

where $\sigma_j = \mathrm{ran}\ E_j(\cdot)$; $E_j(\theta)$ are the real eigenvalues of $H(\theta)$.

Theorem (Singular continuous spectrum)

Consider the $\mathbb{Z}$-periodic graph Γ with $\nu = 1$ and weights

$$w(k) = \begin{cases} \frac{1}{4k\sqrt{\log_2(2k)}} & \text{if } k = 2^{n-1} \text{ for some } n \geq 1, \\ 0 & \text{otherwise,} \end{cases}$$

for $k \geq 0$ and $w(-k) := w(k)$. Furthermore, let $Q = 0$. Then $\mathcal{H}_\Gamma$ has purely singular continuous spectrum.

Ballistic transport and dispersion

- Assume that $\psi \neq 0$ is some initial state (typically, with compact support). In order to prove ballistic transport one aims to show that

$$\lim_{t \to \infty} \frac{\|x \mathrm{e}^{-it\mathcal{H}_\Gamma} \psi\|^2}{t^2} > 0 \ ,$$

where x is some suitable "position operator". In a regime of *localization*, the limit would be zero.

- Dispersion: In order to prove dispersion for some inital state $\psi \neq 0$ one would like to establish estimates of the form

$$\|\mathrm{e}^{-it\mathcal{H}_\Gamma} \psi\|_\infty \leq ct^{-\alpha} \cdot \|\psi\|_1 \ ,$$

with $\alpha, c > 0$. Intuitively, dispersion means that the state flattens out as time increases.

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Some results: II-IV

3.1. **One-dimensional examples with one-element fundamental cell.** Let us consider the following simple examples which already induce crystals with remarkable properties, as we will see later in the article. We define

$$a(\theta) = \left(\theta - \frac{1}{2}\right)^2 \tag{3.1a}$$

$$b(\theta) = \begin{cases} \frac{1}{2} - \theta\,, & \theta \in [0, \frac{1}{2}], \\ \theta - \frac{1}{2}\,, & \theta \in [\frac{1}{2}, 1], \end{cases} \tag{3.1b}$$

$$c(\theta) = \begin{cases} \frac{1}{4} - \theta\,, & \theta \in [0, \frac{1}{4}], \\ 0\,, & \theta \in [\frac{1}{4}, \frac{3}{4}]\,, \\ \theta - \frac{3}{4}\,, & \theta \in [\frac{3}{4}, 1]. \end{cases} \tag{3.1c}$$

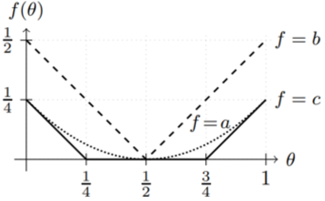

FIGURE 5. The functions a (dotted), b (dashed) and c (continuous line).

Some results II

Theorem (Ballistic but absence of dispersion – $b(\theta)$)

Consider the $\mathbb{Z}$-periodic graph Γ with $\nu = 1$, $Q = \frac{1}{4}$ and weights

$$w(k) = \begin{cases} \frac{1}{\pi^2 k^2} & \text{if } k \text{ odd}, \\ 0 & \text{if } k \text{ even.} \end{cases}$$

Then $\mathcal{H}_\Gamma$ has purely absolutely continuous spectrum. Any initial state $\psi \neq 0$ (with finite first momentum) spreads out at ballistic speed. However, Γ violates dispersion. More explicitly, one has

$$\|e^{-it\mathcal{H}_\Gamma}\delta_n\|_\infty > \frac{1}{\pi}$$

for all $t > 0$.

This theorem provides a negative answer to a question raised by Damanik et al. in [2].

Some results III

Theorem (Faster dispersion than $\mathbb{Z} - a(\theta)$)

Consider the $\mathbb{Z}$-periodic graph Γ with $\nu = 1$, $Q = \frac{1}{12}$ and weights

$$w(k) = \frac{1}{2\pi^2 k^2} \ .$$

Then $\mathcal{H}_\Gamma$ has purely absolutely continuous spectrum. Furthermore, any initial state $\psi \neq 0$ (with finite first momentum) spreads out at ballistic speed. Moreover, $\mathcal{H}_\Gamma$ disperses faster than $\mathcal{H}_\mathbb{Z} = \mathcal{A}_\mathbb{Z}$: one has

$$\|e^{-it\mathcal{H}_\Gamma}\psi\|_\infty \leq 8t^{-1/2}\|\psi\|_1 \ .$$

Note here that for $\mathcal{A}_\mathbb{Z}$ on has $\sim t^{-1/3}$ instead (Stefanov, Kevrekidis (2004)). So, in our setting one is somehow closer to the continuum.

Some results IV

Theorem (Another graph with no dispersion and a partly flat band – $c(\theta)$)

Consider the $\mathbb{Z}$-periodic graph Γ with $\nu = 1$, $Q = \frac{1}{16}$ and weights

$$w(k) = \begin{cases} \frac{1}{2\pi^2 k^2} & \text{if } k \text{ odd }, \\ \frac{1-(-1)^{k/2}}{2\pi^2 k^2} & \text{if } k \text{ even.} \end{cases}$$

Then $\mathcal{H}_\Gamma$ has a partly flat band (infinitely degenerate eigenvalue), it violates dispersion, and in fact, a sizable mass of the initial state δ_0 stays at the origin at all times (but in this state one has ballistic transport).

Open questions

- What is the “generic spectral type” of crystals?
- ...

Part II: Spectral comparison results

P. Bifulco, J. Kerner, C. Rose, *Spectral comparison results for Laplacians on discrete graphs*, arXiv:2412.15937 (2024)

- **Basic idea**: Compare the eigenvalues of two operators with each other, one being the perturbation of the other and both defined on the same structure
- We will be looking at the eigenvalue *differences*
- Such results have been studied recently on domains (Rudnick et al.), on finite quantum graphs (Band et al., Bifulco/K) and infinite quantum graphs (Bifulco/K)
- Question: What about similar results on discrete graphs?
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- Let X be a non-empty set, $b : X \times X \to [0, \infty)$ symmetric with $b(x, x) = 0$ and $\sum_{y \in X} b(x, y) < \infty$ for all $y \in X$
- Introduce the maps $c : X \to [0, \infty)$ (external potential) and $m : X \to (0, \infty)$ (vertex measure)
- We consider discrete graphs (b, c) over the discrete measure space (X, m). The underlying Hilbert space is

$$\ell^2(X, m)$$

- We consider certain self-adjoint realizations of the discrete Laplacian acting via

$$(\mathcal{L}_{b,c}f)(x) = \frac{1}{m(x)} \sum_{y \in X} b(x,y)(f(x) - f(y)) + \frac{c(x)}{m(x)} f(x) \ , \quad x \in X \ .$$

- The associated quadratic form is given by

$$\mathcal{Q}_{b,c}(f,g) = \frac{1}{2} \sum_{x,y \in X} b(x,y)(f(x) - f(y))(g(x) - g(y)) + \sum_{x \in X} c(x)(fg)(x),$$

on a suitable form domain $D(Q) \subset \ell^2(X,m)$.

- We require that the corresponding form domain $D(Q)$ is such that $D(Q^{(D)}) \subset D(Q) \subset D(Q^{(N)})$
- $D(Q^{(D)})$ is the closure of the compactly supported funtions with respect to the form norm and $D(Q^{(N)})$ is the maximal domain
- We also require that the form domain of $\mathcal{L}_{b,c=0}$ is compactly embedded in $\ell^2(X, m)$. This implies that the spectra of $\mathcal{L}_{b,c}$ as well as $\mathcal{L}_{b,c=0}$ are purely discrete

Theorem (Spectral comparison result)

Assume that $\mathcal{L}_{b,c=0}$ has purely discrete spectrum and let an external potential $c : X \to [0,\infty)$ be given. Then

$$\sum_{n=1}^{\dim \ell^2(X,m)} (\lambda_n(c) - \lambda_n(0)) = \sum_{x \in X} \frac{c(x)}{m(x)}$$

Theorem (Local Weyl law)

Assume that $\mathcal{L}_{b,c=0}$ has purely discrete spectrum and let an external potential $c : X \to [0, \infty)$ be given. Let $f_n^c \in \ell^2(X, m)$ denote the normalized orthogonal eigenfunctions of $\mathcal{L}_{b,c}$. Then

$$\sum_{n=1}^{\dim \ell^2(X,m)} |f_n^c(x)|^2 = \frac{1}{m(x)} , \quad x \in X .$$

- Let $X = \mathbb{N}$ with $m(n) := n^{-4}$ be given. We consider the path graph over (X, m) defined via $b(n+1, n) = b(n, n+1) = n^2$ and $b(n, m) = 0$ whenever $|n - m| > 1$. Moreover, we suppose that $c(n) = 0$ for all $n \in \mathbb{N}$. Then, one has that $D(Q^{(N)})$ is compactly embedded in $\ell^2(X, m)$ and hence any self-adjoint realization has purely discrete spectrum.

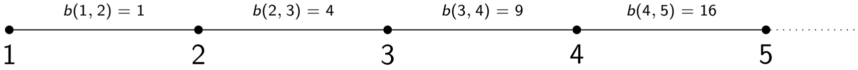

Figure: The infinite path graph b over $(\mathbb{N}, m)$.

- For $c(n) = n^{-6}$ the eigenvalues differences sum up to $\frac{\pi^2}{6}$.

Thank you for your attention!