The momentum band density of periodic graphs

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Joint work with Gregory Berkolaiko

Spectral Theory of Laplace and Schrödinger Operators, Banff, Aug 2013
Periodic potentials

Waves\ electrons in a periodic medium

E.g., Kronig-Penny model

\[
\left(-\frac{d^2}{dx^2} + V_0 \sum_{n=-\infty}^{\infty} \delta(x - na) \right) \psi = k^2 \psi
\]

gives rise to band structure (measured in terms of \(k\)).
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momentum band density

\( p_{\sigma} := \text{probability that a random (uniformly chosen) momentum belongs to the spectrum.} \)

Example (Kronig-Penny model)

Band width \( \rightarrow \) constant \( k \rightarrow \infty \)

Gap width \( \rightarrow \) 0 \( k \rightarrow \infty \)

\( \Rightarrow p_{\sigma} = 1 \)
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**momentum band density**

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**Example (Kronig-Penny model)**

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\text{Band width} & \rightarrow \text{constant} \\
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\end{align*}
\]

\(\Rightarrow p_\sigma = 1\)

- Gap creation mechanisms
- Bethe-Sommerfeld conjecture - occurrence of a finite number of gaps
Consider \(-\frac{d^2}{dx^2} \psi = k^2 \psi\) on a \(\mathbb{Z}^d\)-periodic graph,
with Neumann vertex conditions: \(\psi\) is continuous at \(v\) \text{ and } \sum \psi' |_v = 0.

\(p_\sigma\) := probability that a random (uniformly chosen) momentum, \(k\), belongs to the spectrum, \(\sigma\).

How does \(p_\sigma\) depend on the decoration?
Periodic graphs

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\(p_\sigma :=\) probability that a random (uniformly chosen) momentum, \(k\), belongs to the spectrum, \(\sigma\).

How does \(p_\sigma\) depend on the decoration?

Denote \(p_\sigma(K) := \frac{|\sigma \cap [0,K]|}{K}\), the band density in \([0,K]\) so that \(p_\sigma := \lim_{K \to \infty} p_\sigma(K)\).
Theorem (RB, Berkolaiko)

Consider a $d$-dimensional periodic graph. Then

1. The limit $p_\sigma: = \lim_{K \to \infty} p_\sigma(K)$ exists.

2. If there exists at least one gap, then $p_\sigma < 1$.

3. If there exists at least one non-flat band, then $p_\sigma > 0$.

4. If the edge lengths are incommensurate, then $p_\sigma$ does not depend on their specific values.

5. $p_\sigma$ is independent on some details of the decoration's topology.
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Periodic is Magnetic

The band structure of graphs - previous results:

*metric* - Avron, Exner, Last ('94); Kuchment ('04);
  Brüning, Geyler, Pankrashkin ('07)
*discrete* - Schenker, Aizenman ('00)

An equivalent problem is

a compact graph with a magnetic flux:

\[
\left( -i \frac{d}{dx} + A(x) \right)^2 \psi = k^2 \psi ,
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with magnetic flux \( \alpha = \int_{\text{cycle}} A(x) \, dx \).
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The \( n^{\text{th}} \) band is \( B_n := [\min_\alpha k_n(\alpha), \max_\alpha k_n(\alpha)] \)

\[
p_\sigma(K) := \frac{|(\bigcup_n B_n) \cap [0,K]|}{|0,K|}
\]

\[
p_\sigma := \lim_{K \to \infty} p_\sigma(K)
\]
A glance at the proof

For a graph with \( E \) edges, the eigenvalues are \( \{k^2; F(kl_1, \ldots, kl_E; \vec{\alpha}) = 0\} \), where \( F \) is \( 2\pi \)-periodic in its first \( E \) variables.

\[ \Rightarrow \text{Eigenvalues described by a flow on a torus, } \mathbb{T} = [0, 2\pi)^E: \]
\[ k \text{ is “time” and } (\kappa_1, \ldots \kappa_E) = (kl_1, \ldots kl_E) \]

Zero magnetic flux
\( \{F(\kappa_1, \kappa_2; 0) = 0\} \)
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For a graph with $E$ edges, the eigenvalues are \( \{k^2; F(kl_1, \ldots, kl_E; \vec{\alpha}) = 0\} \), where $F$ is $2\pi$-periodic in its first $E$ variables.

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Torus idea from Barra, Gaspard ('00)

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\[ p_\sigma = \frac{2}{\pi^2} \int_0^\pi \arctan \left( 2 \cot \left( \frac{\theta}{2} \right) \right) d\theta \]

\[ \approx 0.637 \]

for all decorations (b)-(d)

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Further directions

- How does $p_\sigma$ depend on the topology of the decoration and the periodicity?
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- Bounds on possible sizes of bands and gaps

- Understanding better the gap opening mechanism
- Adding potentials and non-trivial vertex conditions
- Nodal count of the eigenfunctions on the edges of the Brillouin zone
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