The momentum band density of periodic graphs

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Joint work with Gregory Berkolaiko

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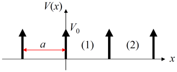
Periodic potentials

Waves\electrons in a periodic medium

E.g., Kronnig-Penny model $\left(-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V_0 \sum_{n=-\infty}^{\infty} \delta\left(x - na\right)\right)\psi = k^2\psi$



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

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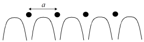

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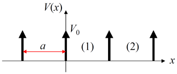

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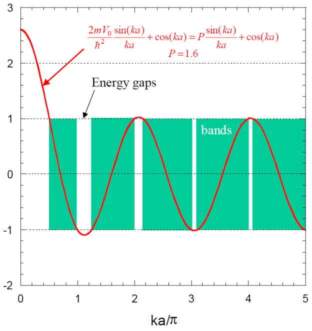

momentum band density

p_σ :=probability that a random (uniformly chosen) momentum belongs to the spectrum.

Example (Kronig-Penny model)

$$\left.\begin{array}{c} \text{Band width} \underset{k\to\infty}{\longrightarrow} \text{constant} \\ \text{Gap width} \underset{k\to\infty}{\longrightarrow} 0 \end{array}\right\} \Rightarrow p_\sigma = 1$$

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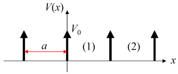

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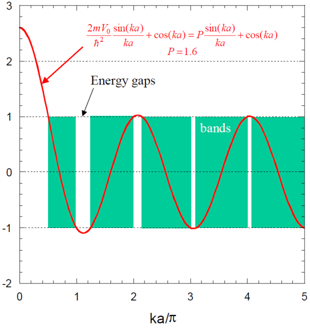

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- Gap creation mechanisms
- Bethe-Sommerfeld conjecture -
  occurence of a finite number of gaps

Periodic graphs

Consider $-\frac{\mathrm{d}^2}{\mathrm{d}x^2}\psi = k^2\psi$ on a $\mathbb{Z}^d$-periodic graph,

with Neumann vertex conditions: ψ is continuous at v ***and*** $\sum \psi'|_v = 0$.

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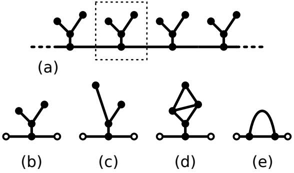
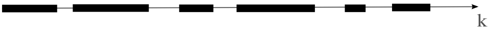


How does p_σ depend on the decoration?



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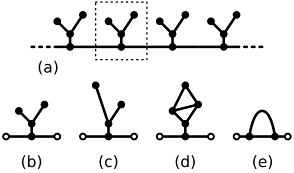
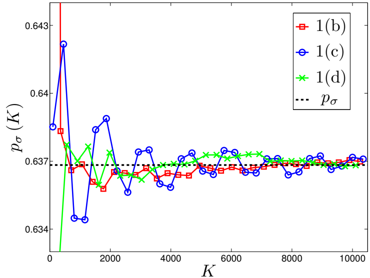


How does p_σ depend on the decoration?

Denote $p_\sigma(K) := \frac{|\sigma \cap [0,K]|}{K}$, the band density in $[0, K]$

so that $p_\sigma := \lim_{K\to\infty} p_\sigma(K)$



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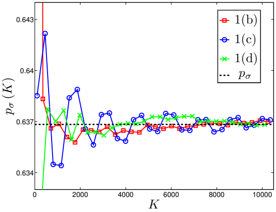

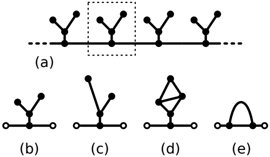

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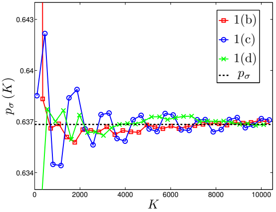
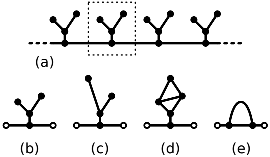




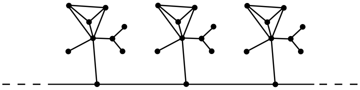
Theorem (RB, Berkolaiko)

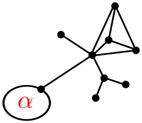
Consider a d-dimensional periodic graph. Then

1. *The limit $p_\sigma := \lim_{K\to\infty} p_\sigma(K)$ exists.*
2. *If there exists at least one gap, then $p_\sigma < 1$.*
   If there exists at least one non-flat band, then $p_\sigma > 0$.
3. *If the edge lengths are incommensurate,*
   then p_σ does not depend on their specific values.
4. *p_σ is independent on some details of the decoration's topology.*

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:

$$\left(-i\frac{\mathrm{d}}{\mathrm{d}x}+A(x)\right)^2\psi=k^2\psi\ ,$$

with magnetic flux $\alpha=\oint_{\text{cycle}}A\left(x\right)\mathrm{dx}$.

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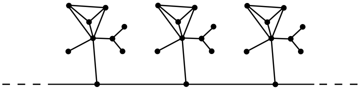

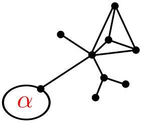

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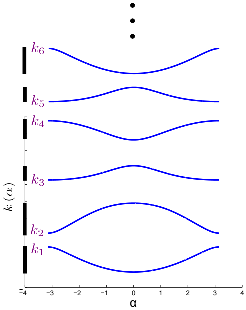
The n^{th} band is $B_n:=\left[\min_\alpha k_n\left(\alpha\right),\max_\alpha k_n\left(\alpha\right)\right]$

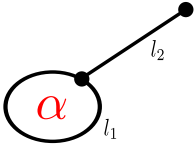
$$p_\sigma\left(K\right):=\frac{\left|\left(\cup_n B_n\right)\cap[0,K]\right|}{\left|[0,K]\right|}$$

$$p_\sigma:=\lim_{K\to\infty}p_\sigma\left(K\right)$$



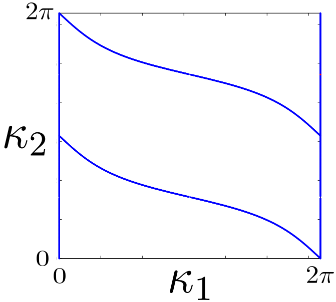
A glance at the proof

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



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

Zero magnetic flux
$\{F\left(\kappa_1, \kappa_2; 0\right) = 0\}$



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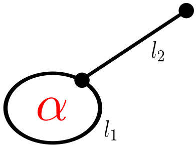

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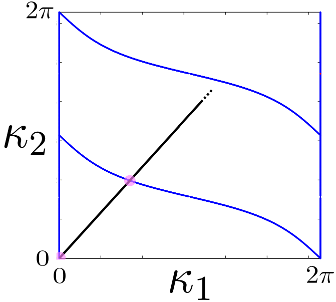

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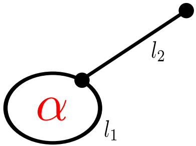

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Torus idea from Barra, Gaspard ('00)

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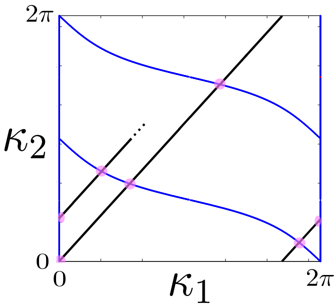

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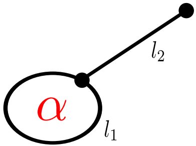

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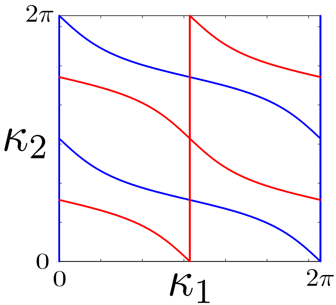

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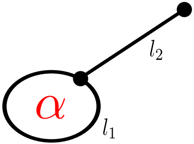

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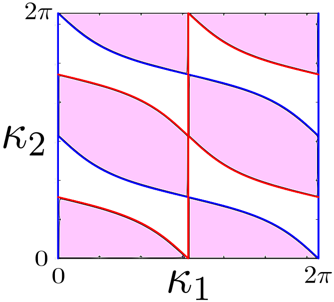

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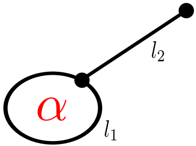

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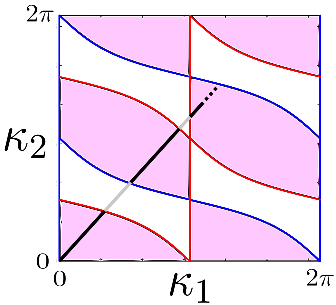

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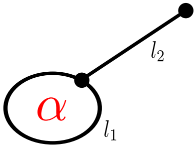

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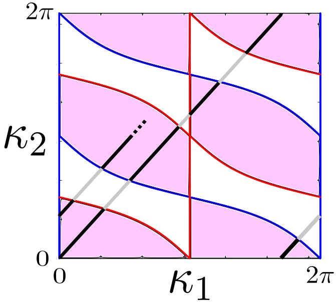

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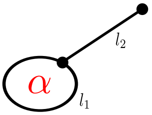

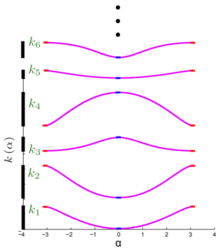

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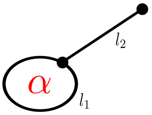

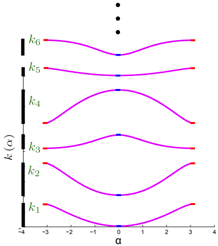

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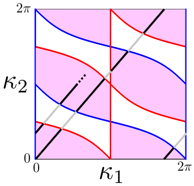

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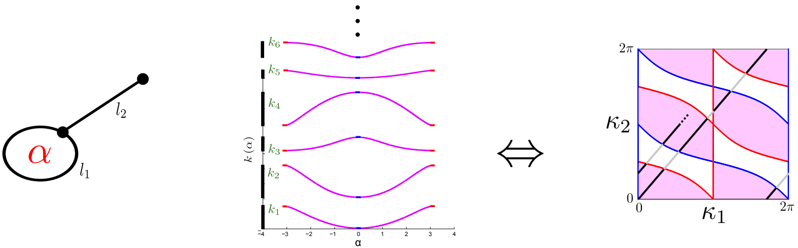

Due to ergodic motion, p_σ equals the ratio of shaded area within the torus.

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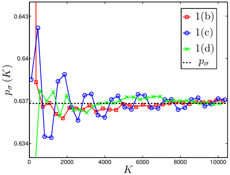
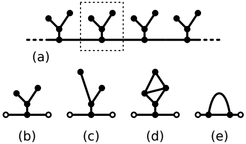
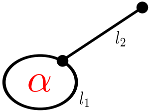
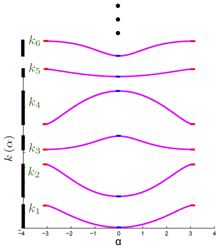


$$p_\sigma = \frac{2}{\pi^2}\int_0^{\pi} \arctan\left(2\cot\left(\theta/2\right)\right)d\theta$$
$$\approx 0.637$$

for all decorations (b)-(d)







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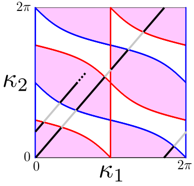

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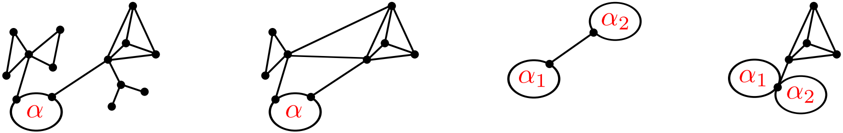
Further directions

- How does p_σ depend on the topology of the decoration and the periodicity?



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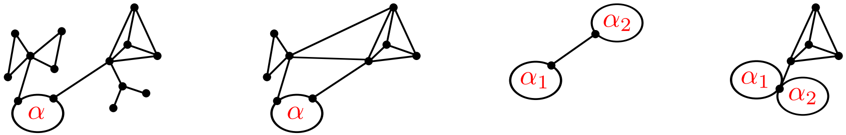
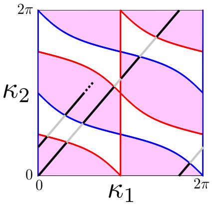


- Bounds on possible sizes of bands and gaps



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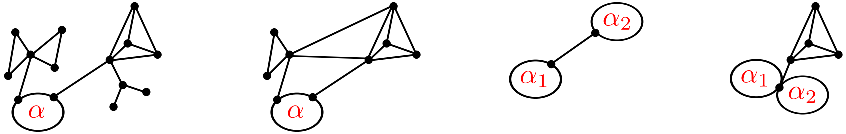
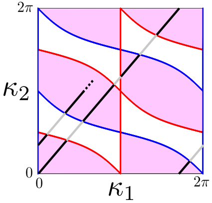


- Bounds on possible sizes of bands and gaps
- Understanding better the gap openning mechanism



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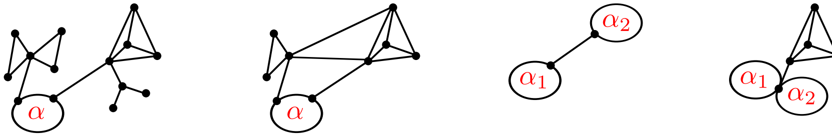

- Bounds on possible sizes of bands and gaps
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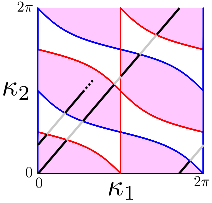

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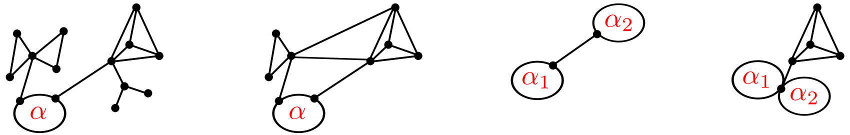

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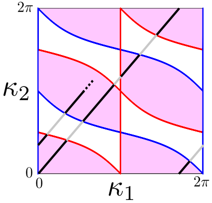

- Nodal count of the eigenfunctions on the edges of the Brillouin zone

The momentum band density of periodic graphs

Ram Band

University of Bristol

Joint work with Gregory Berkolaiko

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