The momentum band density of periodic graphs

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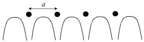
University of Bristol

Joint work with Gregory Berkolaiko

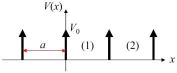
6th Workshop on Quantum Chaos and Localisation Phenomena, Warsaw, May 2013

Periodic potentials

Electrons in a periodic structure



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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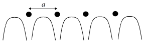

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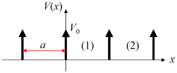

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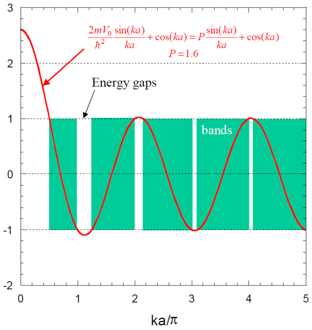

- Band width $\underset{k\to\infty}{\longrightarrow}$ constant
- Gap width $\underset{k\to\infty}{\longrightarrow}$ 0

$\Rightarrow$ Average band density $= 1$

figures taken from http://nanohub.org/

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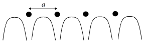

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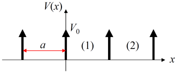

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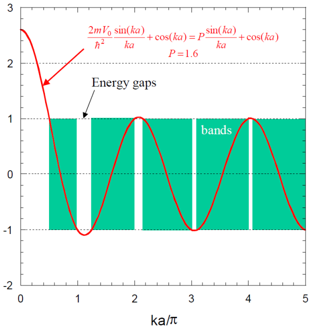

- Band width $\underset{k\to\infty}{\longrightarrow}$ constant
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$\Rightarrow$ Average band density $= 1$

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

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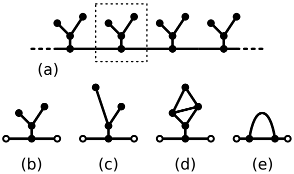
Periodic graphs

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

$p_\sigma :=$ the band density, i.e., the probability that a randomly chosen momentum belongs to the spectrum σ.

How does p_σ depends on the decoration graph?



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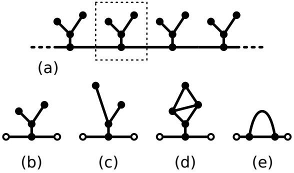

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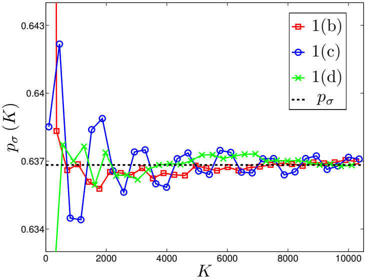
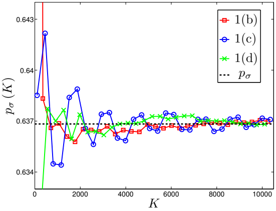
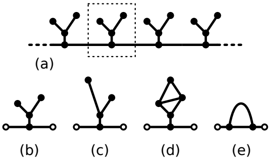


Denote by $p_\sigma(K)$ the band density in $[0, K]$

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

Periodic graphs





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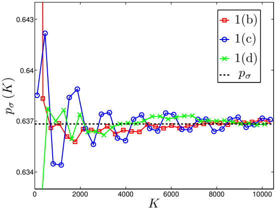
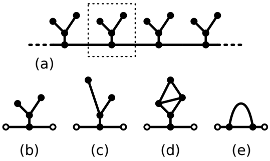




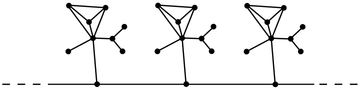
Theorem (RB, Berkolaiko)

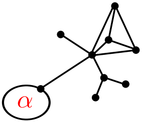
1. *The limit* $p_\sigma := \lim_{K\to\infty} p_\sigma(K)$ *exists.*
2. *If there exists at least one gap, then* $p_\sigma < 1$.
   If there exists at least one non-flat band, then $p_\sigma > 0$.
3. *If the edge lengths are incommensurate,*
   then p_σ *does not depend on their specific values.*
4.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

Remark - the theorem is also valid for more than $1d$ periodicity.

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)





Fact (An equivalent problem)

a compact graph with a magnetic flux:

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

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

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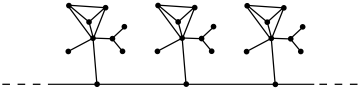

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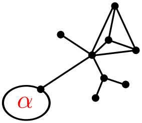
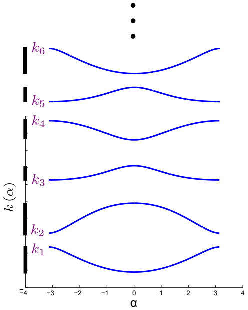
The n^{th} *band is* $B_n:=\left[\min_\alpha k_n\left(\alpha\right),\max_\alpha k_n\left(\alpha\right)\right]$

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

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





A glance at the proof

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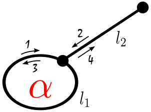

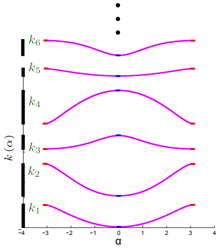

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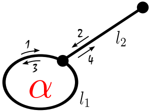

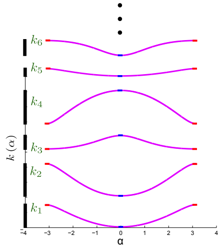

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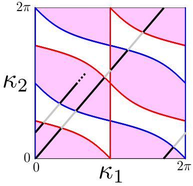

Torus idea from Barra, Gaspard ('00)

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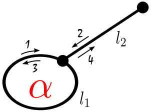

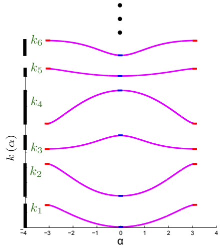

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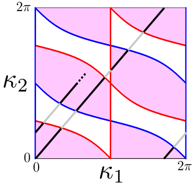

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Due to ergodic motion, p_σ equals the shaded area on the torus.

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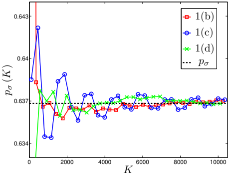
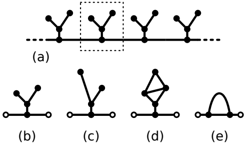
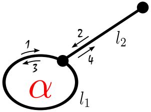


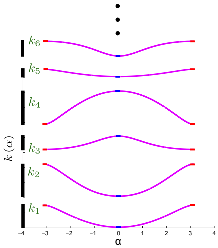
$$p_\sigma = \frac{2}{\pi^2}\int_0^\pi \arctan\left(2\cot\left({}^{\theta}/_{2}\right)\right)d\theta$$

$$\approx 0.637$$

for all decorations (b)-(d)







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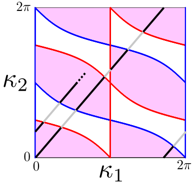

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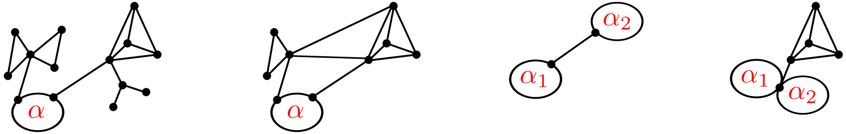
Further directions

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



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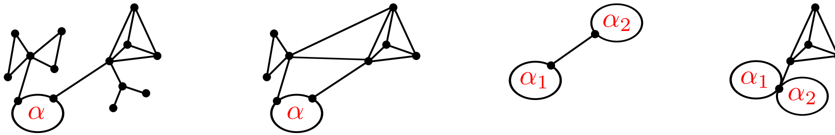
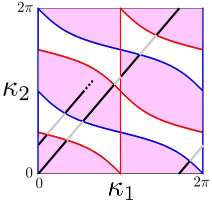


- Bounds on possible sizes of bands and gaps



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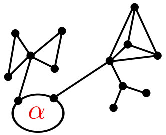

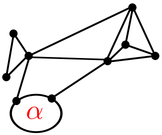

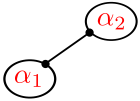

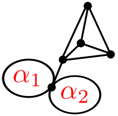

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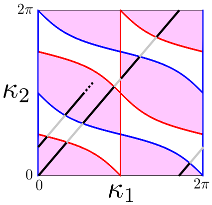
- Understanding better the gap openning mechanism



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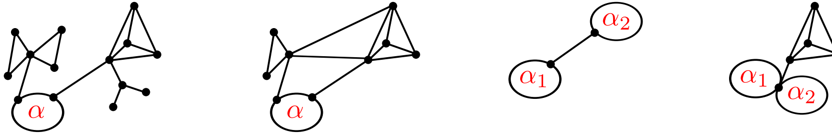

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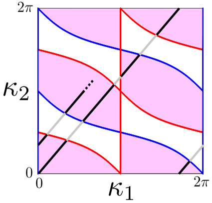

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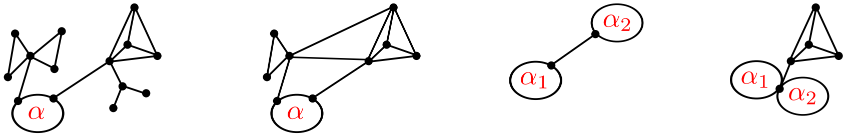

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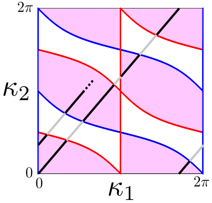

- Nodal count of the eigenfunctions on the edges of the Brillouin zone