On spectral properties of periodic quantum graph systems

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(Joint work with Pavel Exner)

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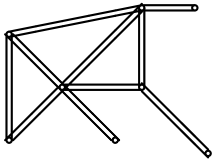
Applications of quantum graphs:

models of nanosized graph-like systems

Real system

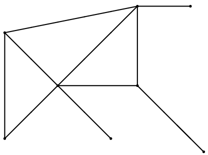


electron on an object from **thin wires**
(semiconductors etc.)

$$H = -\Delta$$

3-D

Model: quantum graph



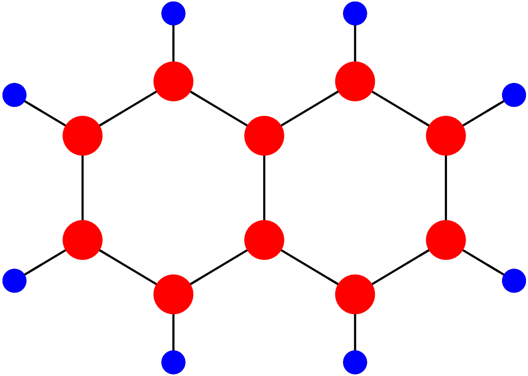
particle on a **graph**

$$H = -\frac{\mathrm{d}^2}{\mathrm{d}x^2}$$

1-D

$\Rightarrow$ *simpler analysis*

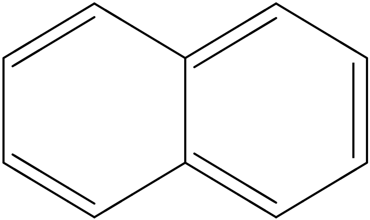
Naphtalene molecule ($C_{10}H_8$)



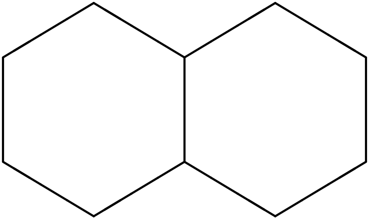
● = carbon atom ● = hydrogen atom

Calculations of spectra of molecules

Naphtalene molecule ($C_{10}H_8$) – skeletal formula



Naphtalene molecule ($C_{10}H_8$)



Ruedenberg and Scherr (1953):

This graph is a good model of the $C_{10}H_8$ molecule.
(The spectrum obtained with an error ≈10%.)

Applications of quantum graphs

- Study of nanosized objects (molecules, nanoparticles)
  - spectral properties
  - scattering properties
- Characteristics of new materials (graphene, graphene nanotubes etc.)
- Description of propagation of waves in waveguides (because quantum graphs and waveguides have similar features)

Periodic quantum graphs

Applications of periodic quantum graphs:

- models of natural crystalline materials
- study and design of new materials

Typical spectral property of periodic quantum graph systems

- the spectrum has a band-gap structure

The **arrangement of bands and gaps** in the spectrum of a periodic graph depends on

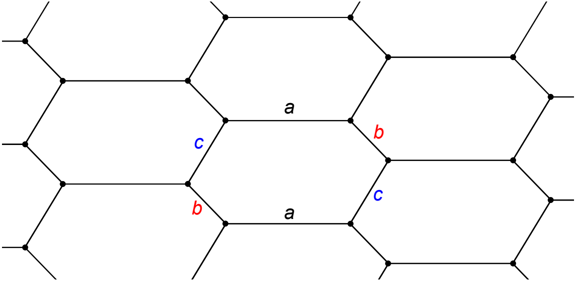
- topology of the graph
- lengths of the edges
- couplings in the vertices (i.e., point potentials in the vertices)
- potentials on the edges

Nevertheless, the relation between the these parameters and the arrangement of gaps is generally **not well understood yet**.

Example:

Spectrum of a dilated honeycomb network

Dilated honeycomb network

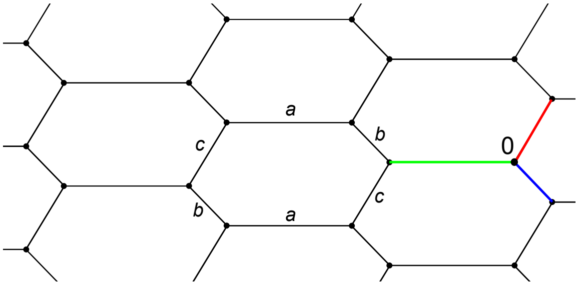


Potential on the edges: 0 (free motion)

Potential in the vertices: δ potential of strength α

(i.e., Dirac delta function multiplied by α)

Dilated honeycomb network



Potential on the edges: 0 (free motion)

Potential in the vertices: δ potential of strength α (i.e., Dirac delta function multiplied by α)

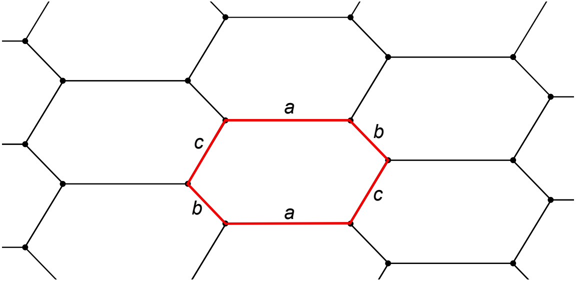
Hamiltonian: $H : \psi \mapsto -\psi''$

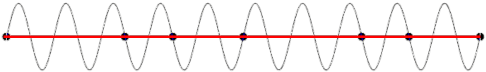
$$\psi_1(0) = \psi_2(0) = \psi_3(0) =: \psi(0)\,, \qquad \psi_1'(0)+\psi_2'(0)+\psi_3'(0) = \alpha\psi(0)$$

Discrete spectrum

Proposition

$k^2 \in \sigma_{\mathrm{p}}(H) \quad \Leftarrow \quad ka,\ kb,\ kc$ - *integer multiples of* π.



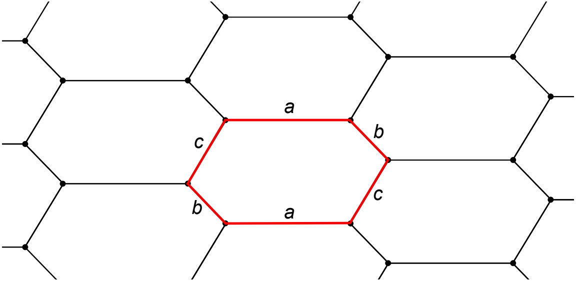


$\psi(x) = \sin(kx)$

Discrete spectrum

Theorem

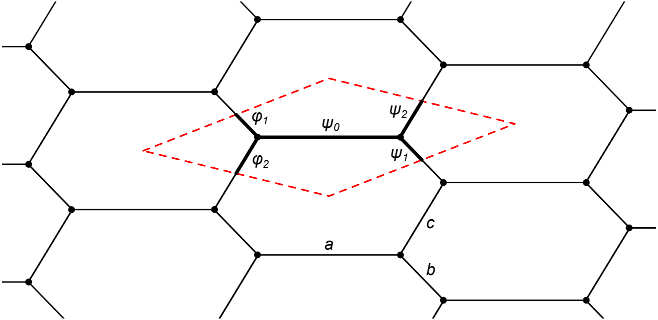
$k^2 \in \sigma_{\mathrm{p}}(H) \quad \Leftrightarrow \quad ka,\ kb,\ kc$ - *integer multiples of* π



Corollary

$\sigma_{\mathrm{p}}(H) \neq \emptyset \quad \Leftrightarrow \quad a, b, c$ *are commensurable numbers*

Elementary cell:

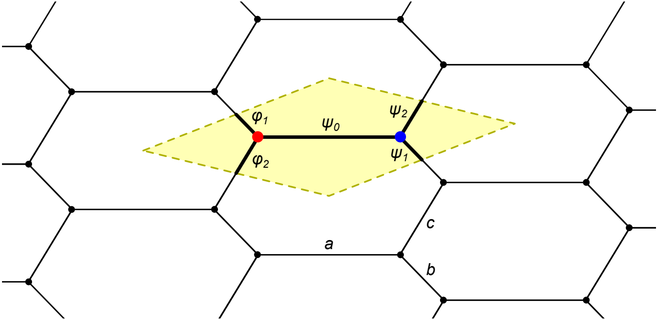


$$H : \psi \mapsto -\psi'' , \quad \text{hence} \quad k^2 \in \sigma(H) \quad \Leftrightarrow \quad -\psi'' = k^2\psi$$

$$\Rightarrow \qquad \psi_j(x) = C_j^+ \mathrm{e}^{\mathrm{i}kx} + C_j^- \mathrm{e}^{-\mathrm{i}kx} \qquad j = 0, 1, 2$$

$$\varphi_j(x) = D_j^+ \mathrm{e}^{\mathrm{i}kx} + D_j^- \mathrm{e}^{-\mathrm{i}kx} \qquad j = 1, 2$$

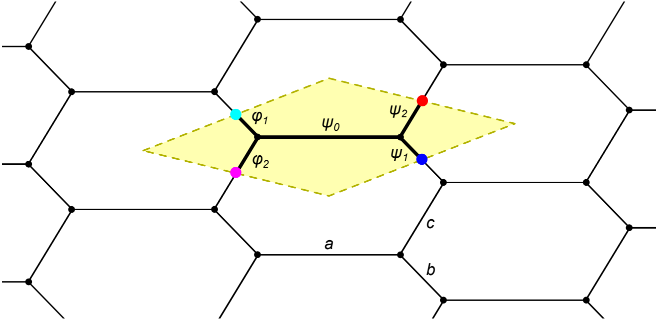
Boundary conditions in the vertices



Potential δ in the vertices:

$$\varphi_1(\color{red}{\bullet}) = \varphi_2(\color{red}{\bullet}) = \psi_0(\color{red}{\bullet})$$
$$-\varphi_1'(\color{red}{\bullet}) - \varphi_2'(\color{red}{\bullet}) + \varphi_1'(\color{red}{\bullet}) = \alpha\varphi_1(\color{red}{\bullet})$$

$$\psi_1(\color{blue}{\bullet}) = \psi_2(\color{blue}{\bullet}) = \psi_0(\color{blue}{\bullet})$$
$$\psi_1'(\color{blue}{\bullet}) + \psi_2'(\color{blue}{\bullet}) - \psi_0'(\color{blue}{\bullet}) = \alpha\psi_0(\color{blue}{\bullet})$$



Floquet–Bloch conditions

$$\psi_1(\bullet) = e^{i\theta_1}\varphi_1(\bullet) \qquad \psi_2(\bullet) = e^{i\theta_2}\varphi_2(\bullet)$$
$$\psi_1'(\bullet) = e^{i\theta_1}\varphi_1'(\bullet) \qquad \psi_2'(\bullet) = e^{i\theta_2}\varphi_2'(\bullet)$$

for certain $\theta_1, \theta_2 \in (-\pi, \pi]$.

We have: **10 unknowns** $(C_j^+, C_j^-, j = 0,1,2;\ D_j^+, D_j^-, j = 1,2)$
10 equations (b.c., F.–B. conditions)

$k^2 \in \sigma_c(H)$
$\Leftrightarrow$ there is a nontrivial solution $(C_j^\pm, D_j^\pm)$

$$\Leftrightarrow \quad \det \begin{pmatrix} 1 & 1 & -1 & -1 \\ \mathrm{e}^{\mathrm{i}(bk-\theta_1)} & \mathrm{e}^{\mathrm{i}(-bk-\theta_1)} & -\mathrm{e}^{\mathrm{i}(ck-\theta_2)} & -\mathrm{e}^{\mathrm{i}(-ck-\theta_2)} \\ m_{31} & m_{32} & \mathrm{i} & -\mathrm{i} \\ m_{41} & m_{42} & -\mathrm{i}\mathrm{e}^{\mathrm{i}(ck-\theta_2)} & \mathrm{i}\mathrm{e}^{\mathrm{i}(-ck-\theta_2)} \end{pmatrix} = 0$$

for certain $\theta_1, \theta_2 \in (-\pi, \pi]$, where

$$m_{3\ell} = \frac{\mathrm{e}^{-\mathrm{i}(-1)^\ell ak} + \mathrm{e}^{-\mathrm{i}((-1)^\ell bk+\theta_1)}}{\sin ak} - \frac{\alpha}{k}$$

$$m_{4\ell} = \frac{-\mathrm{e}^{-\mathrm{i}((-1)^\ell(ak+bk)+\theta_1)} + 1}{\sin ak} - \frac{\alpha}{k}\mathrm{e}^{-\mathrm{i}((-1)^\ell bk+\theta_1)}$$

Spectral gaps

$E = k^2$ is in a spectral gap, if it holds (1) or (2):

(1):

$$\left|\operatorname{cotg} ak + \operatorname{cotg} bk + \operatorname{cotg} ck + \frac{\alpha}{k}\right| > \frac{1}{|\sin ak|} + \frac{1}{|\sin bk|} + \frac{1}{|\sin ck|}$$

(2):

$$\left|\operatorname{cotg} ak + \operatorname{cotg} bk + \operatorname{cotg} ck + \frac{\alpha}{k}\right| <$$
$$2\max\left\{\frac{1}{|\sin ak|}, \frac{1}{|\sin bk|}, \frac{1}{|\sin ck|}\right\} - \left(\frac{1}{|\sin ak|} + \frac{1}{|\sin bk|} + \frac{1}{|\sin ck|}\right)$$

Gaps in negative spectrum

$E = -\kappa^2$ is in a spectral gap, if it holds (1) or (2):

(1):

$$\left|\coth a\kappa + \coth b\kappa + \coth c\kappa + \frac{\alpha}{\kappa}\right| > \frac{1}{\sinh a\kappa} + \frac{1}{\sinh b\kappa} + \frac{1}{\sinh c\kappa}$$

(2):

$$\left|\coth a\kappa + \coth b\kappa + \coth c\kappa + \frac{\alpha}{\kappa}\right| < \frac{2}{\sinh \ell_m\kappa} - \frac{1}{\sinh a\kappa} - \frac{1}{\sinh b\kappa} - \frac{1}{\sinh c\kappa}$$

where $\ell_m := \min\{a, b, c\}$.

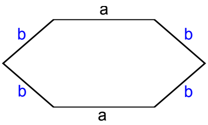
Proposition

The negative part of $\sigma(H)$ contains a gap adjacent to zero exactly in the following two cases:

- $|\alpha| > \frac{2}{a} + \frac{2}{b} + \frac{2}{c}$;
- $\frac{2}{\ell_{\min}} > \frac{1}{a} + \frac{1}{b} + \frac{1}{c} \quad \wedge \quad \frac{2}{a} + \frac{2}{b} + \frac{2}{c} - \frac{2}{\ell_{\min}} < |\alpha| < \frac{2}{\ell_{\min}}$.

Case $b = c$

Let $b = c$.



- **(1):**

$$\left|\operatorname{cotg} ak + 2\operatorname{cotg} bk + \frac{\alpha}{k}\right| > \frac{1}{|\sin ak|} + \frac{2}{|\sin bk|}$$

- **(2):**

$$\frac{1}{|\sin ak|} - \frac{2}{|\sin bk|} > \left|\operatorname{cotg} ak + 2\operatorname{cotg} bk + \frac{\alpha}{k}\right|$$

We set $\theta = \frac{a}{b}$.

“Badly approximable” and “Last admissible” irrational numbers

$\theta \in \mathbb{R} \backslash \mathbb{Q}$ is called *badly approximable* if

$$\exists\, \gamma > 0 : \qquad \left| \theta - \frac{p}{q} \right| > \frac{\gamma}{q^2} \qquad \forall\, p, q \in \mathbb{N}$$

$\theta \in \mathbb{R} \backslash \mathbb{Q}$ is called *Last admissible* if

$$\exists \text{ integer seq. } \{p_n\}_{n=1}^{\infty} \,,\, \{q_n\}_{n=1}^{\infty} : \qquad \lim_{n \to \infty} q_n^2 \left| \theta - \frac{p_n}{q_n} \right| = 0$$

Remark: badly approximable $\cup$ Last admissible $= \mathbb{R} \backslash \mathbb{Q}$

Condition (1) for $b = c$

(1): $$\left|\operatorname{cotg} ak + 2\operatorname{cotg} bk + \frac{\alpha}{k}\right| > \frac{1}{|\sin ak|} + \frac{2}{|\sin bk|}$$

Theorem

α	$\theta := \frac{a}{b}$	*number of gaps (1)*
0	*any*	0
$\neq 0$ $\neq 0$ $\lvert\alpha\rvert \geq \frac{\pi^2}{2\sqrt{5}} \min\{\frac{2}{a}, \frac{1}{b}\}$	$\in \mathbb{Q}$ *Last admissible* *badly approximable*	∞
$0 < \lvert\alpha\rvert \leq \alpha_0$	*badly approximable*	$< \infty$

Proof, case $\alpha = 0$

We aim to prove that for $\alpha = 0$, the condition

$$(1): \qquad \left|\operatorname{cotg} ak + 2\operatorname{cotg} bk + \frac{\alpha}{k}\right| > \frac{1}{|\sin ak|} + \frac{2}{|\sin bk|}$$

has no solution for $k > 0$.

$$\alpha = 0: \qquad |\operatorname{cotg} ak + 2\operatorname{cotg} bk| > \frac{1}{|\sin ak|} + \frac{2}{|\sin bk|}$$

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has no solution for $k > 0$.

$$\alpha = 0: \qquad |\operatorname{cotg} ak + 2\operatorname{cotg} bk| > \frac{1}{|\sin ak|} + \frac{2}{|\sin bk|}$$

Trivially:

$$|\operatorname{cotg} ak + 2\operatorname{cotg} bk| \leq |\operatorname{cotg} ak| + 2|\operatorname{cotg} bk| \leq \frac{1}{|\sin ak|} + \frac{2}{|\sin bk|}$$

hence $$|\operatorname{cotg} ak + 2\operatorname{cotg} bk| \not> \frac{1}{|\sin ak|} + \frac{2}{|\sin bk|}$$

$\Rightarrow$ no gaps

Proof, case $\theta \in \mathbb{Q}$

(1): $$\left|\operatorname{cotg} ak + 2\operatorname{cotg} bk + \frac{\alpha}{k}\right| > \frac{1}{|\sin ak|} + \frac{2}{|\sin bk|}$$

Proof, case $\theta \in \mathbb{Q}$

(1): $$\left|\operatorname{cotg} ak + 2\operatorname{cotg} bk + \frac{\alpha}{k}\right| > \frac{1}{|\sin ak|} + \frac{2}{|\sin bk|}$$

$\frac{a}{b} \in \mathbb{Q} \quad \Rightarrow \quad \exists L > 0,\ \exists_{\infty} m \in \mathbb{N} : aLm, bLm$ – even numbers

Let $\quad k = Lm\pi + \operatorname{sgn}(\alpha) \cdot \delta \quad$ for $\delta > 0,\ \delta \ll 1$

(1): $\left|\operatorname{cotg} ak + 2\operatorname{cotg} bk + \frac{\alpha}{k}\right| > \frac{1}{|\sin ak|} + \frac{2}{|\sin bk|}$

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$$\frac{\alpha}{k} = \operatorname{sgn}(\alpha)\cdot\frac{|\alpha|}{Lm\pi + \operatorname{sgn}(\alpha)\delta}, \quad |\sin ak| = |\sin a\delta|, \quad |\sin bk| = |\sin b\delta|$$

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$$\frac{\alpha}{k} = \operatorname{sgn}(\alpha)\cdot\frac{|\alpha|}{Lm\pi + \operatorname{sgn}(\alpha)\delta}, \quad |\sin ak| = |\sin a\delta|, \quad |\sin bk| = |\sin b\delta|$$

$$(1) \Leftrightarrow \frac{1}{|\sin a\delta|} - |\operatorname{cotg} a\delta| + 2\left(\frac{1}{|\sin b\delta|} - |\operatorname{cotg} b\delta|\right) < \frac{|\alpha|}{Lm\pi + \operatorname{sgn}(\alpha)\delta}$$

Proof, case $\theta \in \mathbb{Q}$

(1): $\left|\operatorname{cotg} ak + 2\operatorname{cotg} bk + \frac{\alpha}{k}\right| > \frac{1}{|\sin ak|} + \frac{2}{|\sin bk|}$

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$$\frac{\alpha}{k} = \operatorname{sgn}(\alpha)\cdot\frac{|\alpha|}{Lm\pi + \operatorname{sgn}(\alpha)\delta}, \quad |\sin ak| = |\sin a\delta|, \quad |\sin bk| = |\sin b\delta|$$

$$(1) \Leftrightarrow \underbrace{\frac{1}{|\sin a\delta|} - |\operatorname{cotg} a\delta|}_{\stackrel{\delta\to 0}{\longrightarrow} 0} + 2\underbrace{\left(\frac{1}{|\sin b\delta|} - |\operatorname{cotg} b\delta|\right)}_{\stackrel{\delta\to 0}{\longrightarrow} 0} < \underbrace{\frac{|\alpha|}{Lm\pi + \operatorname{sgn}(\alpha)\delta}}_{\stackrel{\delta\to 0}{\longrightarrow} \frac{|\alpha|}{Lm\pi} = const > 0}$$

Proof, case $\theta \in \mathbb{Q}$

(1): $$\left|\text{cotg}\, ak + 2\,\text{cotg}\, bk + \tfrac{\alpha}{k}\right| > \frac{1}{|\sin ak|} + \frac{2}{|\sin bk|}$$

$\frac{a}{b} \in \mathbb{Q} \quad \Rightarrow \quad \exists L > 0,\ \exists_\infty m \in \mathbb{N} : aLm, bLm$ – even numbers

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$$(1) \Leftrightarrow \underbrace{\frac{1}{|\sin a\delta|} - |\text{cotg}\, a\delta|}_{\xrightarrow{\delta\to 0} \delta \to 0} + 2\underbrace{\left(\frac{1}{|\sin b\delta|} - |\text{cotg}\, b\delta|\right)}_{\xrightarrow{\delta\to 0} 0} < \underbrace{\frac{|\alpha|}{Lm\pi + \text{sgn}(\alpha)\delta}}_{\xrightarrow{\delta\to 0} \frac{|\alpha|}{Lm\pi} = const > 0}$$

Condition (1) is satisfied for k in a neighbourhood of $m\pi$ for infinitely many m.

Proof, case θ – Last admissible

(1): $$\left|\operatorname{cotg} ak + 2\operatorname{cotg} bk + \frac{\alpha}{k}\right| > \frac{1}{|\sin ak|} + \frac{2}{|\sin bk|}$$

$\frac{a}{b}$ – L.a. $\Rightarrow$ $\exists\ \{p_n\}_{n=1}^{\infty}\ ,\ \{q_n\}_{n=1}^{\infty}$: $\lim_{n\to\infty} q_n^2 \left|\theta - \frac{p_n}{q_n}\right| = 0$

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$\{p_n\}_{n=1}^{\infty}\ ,\ \{q_n\}_{n=1}^{\infty}$ can be chosen such that $\operatorname{sgn}\left(\theta - \frac{p_n}{q_n}\right) = \operatorname{sgn}(\alpha)$

Let $\delta > 0$, $\delta \ll 1$, $k = \frac{q_n\pi}{b} + \operatorname{sgn}(\alpha)\cdot\delta$

Proof, case θ – Last admissible

(1): $$\left|\operatorname{cotg} ak + 2\operatorname{cotg} bk + \frac{\alpha}{k}\right| > \frac{1}{|\sin ak|} + \frac{2}{|\sin bk|}$$

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Let $\delta > 0$, $\delta \ll 1$, $k = \frac{q_n\pi}{b} + \operatorname{sgn}(\alpha)\cdot\delta$

$$(1) \Leftrightarrow \quad \frac{1}{\left|\sin\left(\frac{a}{b}q_n\pi + \operatorname{sgn}(\alpha)\delta a\right)\right|} - \left|\operatorname{cotg}\left(\frac{a}{b}q_n\pi + \operatorname{sgn}(\alpha)\delta a\right)\right| + 2\left(\frac{1}{|\sin b\delta|} - |\operatorname{cotg} b\delta|\right) < \frac{|\alpha|}{\frac{q_n\pi}{b} + \delta}$$

Proof, case θ – Last admissible

(1): $\left|\operatorname{cotg} ak + 2\operatorname{cotg} bk + \frac{\alpha}{k}\right| > \frac{1}{|\sin ak|} + \frac{2}{|\sin bk|}$

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$$(1) \Leftrightarrow \frac{1}{\left|\sin\left(\frac{a}{b}q_n\pi + \operatorname{sgn}(\alpha)\delta a\right)\right|} - \left|\operatorname{cotg}\left(\frac{a}{b}q_n\pi + \operatorname{sgn}(\alpha)\delta a\right)\right| + 2\left(\frac{1}{|\sin b\delta|} - |\operatorname{cotg} b\delta|\right) < \frac{|\alpha|}{\frac{q_n\pi}{b} + \delta}$$

$$\cdot q_n\,,\ \delta\to 0:\quad \underbrace{q_n\left(\frac{1}{\left|\sin\frac{a}{b}q_n\pi\right|} - \left|\operatorname{cotg}\frac{a}{b}q_n\pi\right|\right)}_{\approx q_n^2\left(\theta - \frac{p_n}{q_n}\right)\frac{\pi}{2}\xrightarrow{n\to\infty} 0} + 2q_n\cdot 0 < \underbrace{\frac{|\alpha| b}{\pi}}_{const>0}$$

(1) satisfied for k in a neighbourhood of $\frac{q_n\pi}{b}$ for all n.

Proof, case θ – badly approximable

(1): $$\left|\operatorname{cotg} ak + 2\operatorname{cotg} bk + \frac{\alpha}{k}\right| > \frac{1}{|\sin ak|} + \frac{2}{|\sin bk|}$$

(1) $\Rightarrow$ $$F(k) := \left|\operatorname{tg}\left(\left\{\frac{ak}{\pi}\right\}\frac{\pi}{2}\right)\right| + 2\left|\operatorname{tg}\left(\left\{\frac{bk}{\pi}\right\}\frac{\pi}{2}\right)\right| < \frac{|\alpha|}{k}$$

local minima of $F(k)$: $k = \frac{m\pi}{b}$, $k = \frac{m\pi}{a}$

Proof, case θ – badly approximable

(1): $\left|\operatorname{cotg} ak + 2\operatorname{cotg} bk + \frac{\alpha}{k}\right| > \frac{1}{|\sin ak|} + \frac{2}{|\sin bk|}$

(1) $\Rightarrow$ $F(k) := \left|\operatorname{tg}\left(\left\{\frac{ak}{\pi}\right\}\frac{\pi}{2}\right)\right| + 2\left|\operatorname{tg}\left(\left\{\frac{bk}{\pi}\right\}\frac{\pi}{2}\right)\right| < \frac{|\alpha|}{k}$

local minima of $F(k)$: $k = \frac{m\pi}{b}$, $k = \frac{m\pi}{a}$

$$F\left(\frac{m\pi}{b}\right) = \left|\operatorname{tg}\left(\left\{\frac{a}{b}m\right\}\frac{\pi}{2}\right)\right| > \left|\left\{\frac{a}{b}m\right\}\right|\frac{\pi}{2} = \left|\theta - \frac{\|\theta m\|}{m}\right| m\frac{\pi}{2} > \frac{\gamma}{m^2}\frac{m\pi}{2}$$

$$k \in \left[(m-\frac{1}{2})\frac{\pi}{b}, (m+\frac{1}{2})\frac{\pi}{b}\right] \wedge\ m \gg 1 \quad \Rightarrow \quad \frac{|\alpha|}{k} \approx \frac{|\alpha| b}{m\pi}$$

$$|\alpha| \leq \frac{\gamma\pi^2}{2b} \quad \Rightarrow \quad F\left(\frac{m\pi}{b}\right) \not< |\alpha|\left(\frac{m\pi}{b}\right)^{-1}$$

Also: $|\alpha| \leq \frac{\gamma\pi^2}{a} \quad \Rightarrow \quad F\left(\frac{m\pi}{a}\right) \not< |\alpha|\left(\frac{m\pi}{a}\right)^{-1}$

$0 < |\alpha| \leq \gamma\pi^2 \min\{\frac{1}{a}, \frac{1}{2b}\} \quad \Rightarrow \quad F(k) \not< \frac{|\alpha|}{k} \quad \forall k > 0 \quad \Rightarrow$ no spectral gaps

Proof, case θ – badly approximable

Theorem (Hurwitz): $\forall\theta\in\mathbb{R}\backslash\mathbb{Q}\quad\exists\ \{p_n\}_{n=1}^{\infty}\ ,\ \{q_n\}_{n=1}^{\infty}$
$p_n,q_n\in\mathbb{N}\,,\ \lim_{n\to\infty}q_n=\infty\,,\qquad\left|\theta-\frac{p_n}{q_n}\right|<\frac{1}{\sqrt{5}q_n^2}$

Proof, case θ – badly approximable

Theorem (Hurwitz): $\forall\theta \in \mathbb{R}\backslash\mathbb{Q} \quad \exists \ \{p_n\}_{n=1}^{\infty}\ ,\ \{q_n\}_{n=1}^{\infty}$

$p_n, q_n \in \mathbb{N}\,,\ \lim_{n\to\infty} q_n = \infty\,, \qquad \left|\theta - \frac{p_n}{q_n}\right| < \frac{1}{\sqrt{5}q_n^2}$

$\{p_n\}_{n=1}^{\infty}\ ,\ \{q_n\}_{n=1}^{\infty}$ can be chosen such that $\operatorname{sgn}\left(\theta - \frac{p_n}{q_n}\right) = \operatorname{sgn}(\alpha)$

Let $\delta > 0$, $\delta \ll 1$, $\qquad k = \frac{q_n\pi}{b} + \operatorname{sgn}(\alpha)\cdot\delta$

Proof, case θ – badly approximable

Theorem (Hurwitz): $\forall \theta \in \mathbb{R} \backslash \mathbb{Q} \quad \exists \ \{p_n\}_{n=1}^{\infty} \ , \ \{q_n\}_{n=1}^{\infty}$

$p_n, q_n \in \mathbb{N}\,, \ \lim_{n\to\infty} q_n = \infty\,, \qquad \left|\theta - \frac{p_n}{q_n}\right| < \frac{1}{\sqrt{5}q_n^2}$

$\{p_n\}_{n=1}^{\infty} \ , \ \{q_n\}_{n=1}^{\infty}$ can be chosen such that $\operatorname{sgn}\left(\theta - \frac{p_n}{q_n}\right) = \operatorname{sgn}(\alpha)$

Let $\delta > 0$, $\delta \ll 1$, $\quad k = \frac{q_n \pi}{b} + \operatorname{sgn}(\alpha)\cdot\delta$

$$(1) \Leftrightarrow \quad \frac{1}{\left|\sin\left(\frac{a}{b}q_n\pi + \operatorname{sgn}(\alpha)\delta a\right)\right|} - \left|\operatorname{cotg}\left(\frac{a}{b}q_n\pi + \operatorname{sgn}(\alpha)\delta a\right)\right| + 2\left(\frac{1}{|\sin b\delta|} - |\operatorname{cotg} b\delta|\right) < \frac{|\alpha|}{\frac{q_n\pi}{b} + \delta}$$

Theorem (Hurwitz): $\forall\theta\in\mathbb{R}\backslash\mathbb{Q}\quad\exists\ \{p_n\}_{n=1}^{\infty}\ ,\ \{q_n\}_{n=1}^{\infty}$

$p_n,q_n\in\mathbb{N}\,,\ \lim_{n\to\infty}q_n=\infty\,,\qquad\left|\theta-\frac{p_n}{q_n}\right|<\frac{1}{\sqrt{5}q_n^2}$

$\{p_n\}_{n=1}^{\infty}\ ,\ \{q_n\}_{n=1}^{\infty}$ can be chosen such that $\operatorname{sgn}\left(\theta-\frac{p_n}{q_n}\right)=\operatorname{sgn}(\alpha)$

Let $\delta>0$, $\delta\ll 1$, $\quad k=\frac{q_n\pi}{b}+\operatorname{sgn}(\alpha)\cdot\delta$

$$(1)\Leftrightarrow\quad\frac{1}{\left|\sin\left(\frac{a}{b}q_n\pi+\operatorname{sgn}(\alpha)\delta a\right)\right|}-\left|\operatorname{cotg}\left(\frac{a}{b}q_n\pi+\operatorname{sgn}(\alpha)\delta a\right)\right|+2\left(\frac{1}{|\sin b\delta|}-|\operatorname{cotg} b\delta|\right)<\frac{|\alpha|}{\frac{q_n\pi}{b}+\delta}$$

$$\cdot q_n;\ \delta\to 0:\quad\underbrace{q_n\left(\frac{1}{\left|\sin\frac{a}{b}q_n\pi\right|}-\left|\operatorname{cotg}\frac{a}{b}q_n\pi\right|\right)}_{\approx q_n^2\left(\theta-\frac{p_n}{q_n}\right)\frac{\pi}{2}<\frac{1}{\sqrt{5}}\cdot\frac{\pi}{2}}+2q_n\cdot 0<\frac{|\alpha|b}{\pi}$$

$|\alpha|>\frac{\pi^2}{2\sqrt{5}b}\quad\Rightarrow\quad\forall n$, (1) satisfied in a neighbourhood of $\frac{q_n\pi}{b}$

$|\alpha|>\frac{\pi^2}{4\sqrt{5}a}\quad\Rightarrow\quad\forall n$, (1) satisfied in a neighbourhood of $\frac{q_n\pi}{a}$

Condition (2) for $b = c$

(2): $$\frac{1}{|\sin ak|} - \frac{2}{|\sin bk|} > \left|\operatorname{cotg} ak + 2\operatorname{cotg} bk + \frac{\alpha}{k}\right|$$

Theorem

α	$\theta := \frac{a}{b}$	*number of gaps (2)*
0	*any*	0
$\neq 0$	$\in \mathbb{Q}$	$< \infty$
$\neq 0$ $\|\alpha\| \geq \frac{4\pi}{\sqrt{5}a}$	*Last admissible* *badly approximable*	∞
$0 < \|\alpha\| \leq \alpha_0$	*badly approximable*	$< \infty$

Summary for $b = c$

Number of gaps in $\sigma(H)$:

$\lvert\alpha\rvert$	$\theta := \frac{a}{b}$	number of gaps (1)	number of gaps (2)	**number of gaps (total)**
0	any	0	0	0
$\neq 0$	$\in \mathbb{Q}$	∞	$< \infty$	
$\neq 0$	Last admissible	∞	∞	∞
large	badly approximable	∞	∞	
small	badly approximable	$< \infty$	$< \infty$	$< \infty$

Summary

1. Quantum graphs are used as models of graph-like nanostructures (including new materials).

2. Periodic quantum graphs have band-gap spectra.

3. The number, size and positions of gaps depend on
   - topology of the graph
   - lengths of edges
   - couplings in vertices
   - potentials on edges

4. Each of this four properties may have a substantial effect on the structure of gaps in the spectrum.

5. The relation between the graph parameters and the structure of gaps is not well understood yet, and is subject to further examination.

Thank you for your attention!