Periodic quantum graphs and the Bethe–Sommerfeld conjecture

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(Joint work with Pavel Exner)

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Introduction

Quantum graphs

Quantum graph:

$$(\Gamma, H),$$

where

- Γ – a metric graph;
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Applications:

Models of thin wires, networks and waveguides.

Examples

- A line of length L with Hamiltonian

$$H\psi(x) = -\frac{\hbar^2}{2m}\psi''(x)$$

with boundary conditions

$$\psi'(0) = \psi'(L) = 0.$$

Convention: $\hbar = 2m = 1$, $H\psi(x) = -\psi''(x)$

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- An infinite line with Hamiltonian

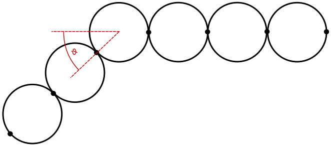
$$H\psi(x) = -\psi''(x)$$

and Dirac δ potential of strength α in each point $x = n \in \mathbb{N}$:

$$\psi(n_-) = \psi(n_+)$$
$$\psi'(n_+) - \psi'(n_-) = \alpha \cdot \psi(n_+)$$

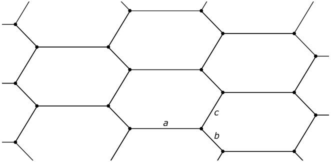
Other examples

- Bent chain



Hamiltonian: $H\psi(x) = -\psi''(x)$ on every line,
boundary conditions (representing "potentials") in the vertices.

- Hexagonal lattice



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Bethe–Sommerfeld conjecture

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A quantum system periodic in more than one direction has a finite number of gaps in the spectrum.

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Remarks:

- The property was taken for granted,
- but mathematically it is a hard problem;
- it took decades before it was proved for most “ordinary” cases.

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Observation (1980s):

The B-S conjecture is **false for quantum graphs**.

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The B-S conjecture is **false for quantum graphs**.

For every quantum graph studied in the literature for 30 years, the number of gaps always turned out to be either infinite or zero.

Results

Question:

Does there exist a graph having a finite nonzero number of gaps in its spectrum?

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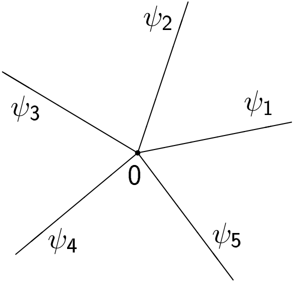
We will present 2 results:

1. We find (sufficient) conditions for a graph to violate the Bethe–Sommerfeld conjecture (to have either infinitely many spectral gaps).

2. We prove that a quantum graph with a finite nonzero number of gaps exists.

Graphs violating the Bethe–Sommerfeld conjecture

Boundary conditions



$$\Psi := \begin{pmatrix} \psi_1(0_+) \\ \vdots \\ \psi_n(0_+) \end{pmatrix}$$

$$\Psi' := \begin{pmatrix} \psi_1'(0_+) \\ \vdots \\ \psi_n'(0_+) \end{pmatrix}$$

ST-form of boundary conditions:

$$\begin{pmatrix} I^{(r)} & T \\ 0 & 0 \end{pmatrix} \Psi' = \begin{pmatrix} S & 0 \\ -T^* & I^{(n-r)} \end{pmatrix} \Psi$$

for certain r, S, and T, where $I^{(r)}$ is the identity matrix of order r.

Scale-invariang couplings

$$\text{B.c.:} \qquad \begin{pmatrix} I^{(r)} & T \\ 0 & 0 \end{pmatrix} \Psi' = \begin{pmatrix} S & 0 \\ -T^* & I^{(n-r)} \end{pmatrix} \Psi,$$

Scattering matrix $\mathcal{S}(k)$ in a vertex of degree n:

$|[\mathcal{S}(k)]_{j\ell}|^2$ =probability, that a particle of energy k^2 coming from the ℓ-th edge is scattered to the j-th edge.

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$$\mathcal{S}(k) = -I^{(n)} + 2 \begin{pmatrix} I^{(r)} \\ T^* \end{pmatrix} \left(I^{(r)} + TT^* - \frac{1}{\mathrm{i}k} S \right)^{-1} \begin{pmatrix} I^{(r)} & T \end{pmatrix}$$

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Observation.

$\mathcal{S}(k)$ is k-independent iff $S = 0$.

Graphs with scale-invariant couplings

Proposition.

Let all the vertex couplings in an infinite periodic quantum graph be scale-invariant. Then the implication holds:

(i) If $\sigma(H_0)$ contains a gap, then $\sigma(H_0)$ contains infinitely many gaps.

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(ii) If $\sigma(H_0)$ has a gap of size s, then for every $\epsilon > 0$ there is an infinite sequence of gaps of sizes at least $s - \epsilon$ (in terms of momentum).

(iii) If all the graph edge lengths are rationally dependent, then the momentum spectrum is periodic.

Associated scale-invariant vertex coupling

Definition

Let a vertex coupling be given by

$$\begin{pmatrix} I^{(r)} & T \\ 0 & 0 \end{pmatrix} \Psi' = \begin{pmatrix} S & 0 \\ -T^* & I^{(n-r)} \end{pmatrix} \Psi \,.$$

The **associated scale-invariant vertex coupling** is given by

$$\begin{pmatrix} I^{(r)} & T \\ 0 & 0 \end{pmatrix} \Psi' = \begin{pmatrix} 0 & 0 \\ -T^* & I^{(n-r)} \end{pmatrix} \Psi \,.$$

Graphs with general vertex couplings

Proposition.

Let

- $\sigma(H)$ be the spectrum of a periodic graph with general couplings at the vertices;
- $\sigma(H_0)$ be the spectrum of the same graph, in which all vertex couplings are replaced by the *associated scale-invariant couplings*.

Then

(i) If $\sigma(H_0)$ has a gap, then $\sigma(H)$ has infinitely many gaps.

(ii) If $\sigma(H_0)$ has a gap of size s, then there are infinitely many gaps in $\sigma(H)$ of sizes at least $s - \epsilon$ (in terms of momentum).

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Then

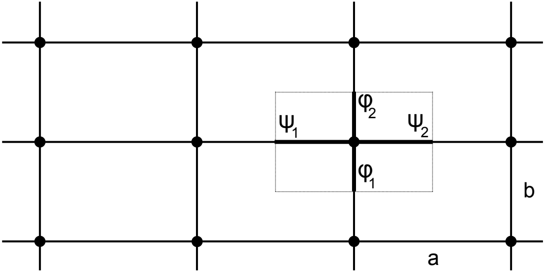
(i) If $\sigma(H_0)$ has a gap, then $\sigma(H)$ has infinitely many gaps.

(ii) If $\sigma(H_0)$ has a gap of size s, then there are infinitely many gaps in $\sigma(H)$ of sizes at least $s - \epsilon$ (in terms of momentum).

Any quantum graph with scale-invariant couplings that has spectral gaps allows to construct a large family of counterexamples to the Bethe–Sommerfeld conjecture.

A quantum graph with a finite nonzero number of spectral gaps

Rectangular lattice



Proposition. $k^2 > 0$ belongs to a gap iff

$$\tan\left(\frac{ka}{2} - \frac{\pi}{2}\left\lfloor\frac{ka}{\pi}\right\rfloor\right) + \tan\left(\frac{kb}{2} - \frac{\pi}{2}\left\lfloor\frac{kb}{\pi}\right\rfloor\right) < \frac{\alpha}{2k} \qquad (\text{case } \alpha > 0)$$

$$\cot\left(\frac{ka}{2} - \frac{\pi}{2}\left\lfloor\frac{ka}{\pi}\right\rfloor\right) + \cot\left(\frac{kb}{2} - \frac{\pi}{2}\left\lfloor\frac{kb}{\pi}\right\rfloor\right) < \frac{|\alpha|}{2k} \qquad (\text{case } \alpha < 0)$$

Number-theoretic preliminaries

A number $\theta \in \mathbb{R}$ is called *badly approximable* if there exists a $c > 0$ such that

$$\left|\theta - \frac{p}{q}\right| > \frac{c}{q^2}$$

for all $p, q \in \mathbb{Z}$ with $q \neq 0$.

Theorem (Exner'96)

The positive spectrum of a rectangular lattice may have a finite number of gaps only if $\frac{a}{b}$ is a badly approximable number.

Definition

For $\theta \in \mathbb{R}$ we define

$$\upsilon(\theta) = \inf\left\{c > 0 \;\middle|\; (\exists_\infty (p,q) \in \mathbb{N}^2)\left(0 < \theta - \frac{p}{q} < \frac{c}{q^2}\right)\right\}.$$

Best Diophantine approximations

A $\frac{p}{q} \in \mathbb{Q}$ with $p, q \in \mathbb{Z}$ is a **best Diophantine approximation of the first kind** to a given $\theta \in \mathbb{R}$ if

$$\left|\theta - \frac{p}{q}\right| < \left|\theta - \frac{p'}{q'}\right|$$

for all $\frac{p'}{q'} \neq \frac{p}{q}$ such that $p', q' \in \mathbb{Z}$ and $0 < q' \leq q$.

A $\frac{p}{q} \in \mathbb{Q}$ with $p, q \in \mathbb{Z}$ is a **best Diophantine approximation of the second kind** to a given $\theta \in \mathbb{R}$ if

$$|q\theta - p| < |q'\theta - p'|$$

for all $\frac{p'}{q'} \neq \frac{p}{q}$ such that $p', q' \in \mathbb{Z}$ and $0 < q' \leq q$.

Theorem: Every best approximation of the second kind is a convergent $\frac{p_n}{q_n}$ of the continued fraction corresponding to θ.

Best Diophantine approximations from below/above

Definition

Let $\theta \in \mathbb{R}$ and $p, q \in \mathbb{Z}$.

- A $\frac{p}{q}$ is a **best approximation from below of the third kind** to θ if

$$0 < q(q\theta - p) < q'(q'\theta - p')$$

for all $\frac{p'}{q'} \geq \theta$ such that $\frac{p'}{q'} \neq \frac{p}{q}$, $p', q' \in \mathbb{Z}$ and $0 < q' \leq q$.

- A $\frac{p}{q}$ is a **best approximation from above of the third kind** to θ if

$$0 < q(p - q\theta) < q'(p' - q'\theta)$$

for all $\frac{p'}{q'} \leq \theta$ such that $\frac{p'}{q'} \neq \frac{p}{q}$, $p', q' \in \mathbb{Z}$ and $0 < q' \leq q$.

Best Diophantine approximations from below/above

Proposition

Every best approximation from below of the third kind to a $\theta \in \mathbb{R}$ is a convergent of θ.

Proposition

Every best approximation from above of the third kind to a $\theta \in \mathbb{R}$ is either $\lceil \theta \rceil$, or a convergent of θ.

Number of spectral gaps

Case $\alpha > 0$ (repulsive Dirac δ potential)

Proposition

Let $\theta = \frac{a}{b}$.

- *Every gap in the positive spectrum is adjacent to one of the points* $k^2 = \left(\frac{m\pi}{a}\right)^2$ *and* $k^2 = \left(\frac{m\pi}{b}\right)^2$ *for* $m \in \mathbb{N}_0$.
- *A gap adjacent to* $k^2 = \left(\frac{m\pi}{a}\right)^2$ *is present iff*

$$\frac{2m\pi}{a} \tan\left(\frac{\pi}{2}(m\theta^{-1} - \lfloor m\theta^{-1} \rfloor)\right) < \alpha.$$

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Case $\alpha > 0$ (repulsive Dirac δ potential)

Corollary

Let $\theta = \frac{a}{b}$. *If the following two conditions are satisfied for all* $m \in \mathbb{N}$,

$$\frac{2m\pi}{a} \tan\left(\frac{\pi}{2}(m\theta^{-1} - \lfloor m\theta^{-1} \rfloor)\right) \geq \alpha$$
$$\frac{2m\pi}{b} \tan\left(\frac{\pi}{2}(m\theta - \lfloor m\theta \rfloor)\right) \geq \alpha,$$

then there are no gaps in the positive spectrum.

Proposition

Let $\theta = \frac{a}{b}$. *If*

$$\alpha < \pi^2 \cdot \min\left\{\frac{\upsilon(\theta)}{b}, \frac{\upsilon(\theta^{-1})}{a}\right\},$$

then the number of gaps in the positive spectrum is at most finite.

Case $\alpha > 0$ (repulsive Dirac δ potential)

Partial summary.

Rectangular lattice with edge lengths a, b, (repulsive) Dirac δ potential of strength $\alpha > 0$.

- Gaps are present iff

$$\frac{2m\pi}{a} \tan\left(\frac{\pi}{2}(m\theta^{-1} - \lfloor m\theta^{-1} \rfloor)\right) < \alpha.$$

  or

$$\frac{2m\pi}{b} \tan\left(\frac{\pi}{2}(m\theta - \lfloor m\theta \rfloor)\right) < \alpha.$$

  for some $m \in \mathbb{N}$.

- If

$$\alpha < \pi^2 \cdot \min\left\{\frac{\upsilon(\theta)}{b}, \frac{\upsilon(\theta^{-1})}{a}\right\},$$

  the number of gaps is at most finite.

Case $\alpha > 0$ (repulsive Dirac δ potential)

Theorem

Let $\theta = \frac{a}{b}$ and

$$\gamma_+ := \min\left\{ \inf_{m\in\mathbb{N}} \left\{ \frac{2m\pi}{a} \tan\left(\frac{\pi}{2}(m\theta^{-1} - \lfloor m\theta^{-1} \rfloor)\right) \right\}, \inf_{m\in\mathbb{N}} \left\{ \frac{2m\pi}{b} \tan\left(\frac{\pi}{2}(m\theta - \lfloor m\theta \rfloor)\right) \right\} \right\}.$$

If the strength α of the Dirac δ potential satifies

$$\gamma_+ < \alpha < \pi^2 \cdot \min\left\{ \frac{\upsilon(\theta)}{b}, \frac{\upsilon(\theta^{-1})}{a} \right\},$$

then there is a <u>nonzero and finite</u> number of gaps in the positive spectrum.

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Let $\theta = \frac{a}{b}$ *and*

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If the strength α *of the Dirac* δ *potential satifies*

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Question: Are there a, b such that $\gamma_+ < \pi^2 \cdot \min\left\{ \frac{\upsilon(\theta)}{b}, \frac{\upsilon(\theta^{-1})}{a} \right\}$?

Case $\alpha < 0$ (attractive Dirac δ potential)

Proposition

Let $\alpha < 0$ *and* $\theta = \frac{a}{b}$.

- *Every gap in the positive spectrum is adjacent to one of the points* $k^2 = \left(\frac{m\pi}{a}\right)^2$ *and* $k^2 = \left(\frac{m\pi}{b}\right)^2$ *for* $m \in \mathbb{N}_0$.
- *A gap adjacent to* $k^2 = \left(\frac{m\pi}{a}\right)^2$ *is present if and only if*

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- If

$$|\alpha| < \pi^2 \cdot \min\left\{\frac{\upsilon(\theta^{-1})}{b}, \frac{\upsilon(\theta)}{a}\right\},$$

  the number of gaps is at most finite.

Case $\alpha < 0$ (attractive Dirac δ potential)

Corollary

If the following two conditions are satisfied for all $m \in \mathbb{N}$,

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Theorem

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If

$$\gamma_- < |\alpha| < \pi^2 \cdot \min\left\{ \frac{\upsilon(\theta^{-1})}{b}, \frac{\upsilon(\theta)}{a} \right\},$$

there is a nonzero and finite number of gaps in the positive spectrum.

Case $\alpha < 0$ (attractive Dirac δ potential)

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Question: Are there a, b such that $\gamma_- < \pi^2 \cdot \min\left\{\frac{\upsilon(\theta^{-1})}{b}, \frac{\upsilon(\theta)}{a}\right\}$?

Example: golden–mean lattice

Golden–mean lattice

Proposition. For $\frac{a}{b} = \phi = \frac{\sqrt{5}+1}{2}$, we have

$$\upsilon(\phi) = \upsilon(\phi^{-1}) = \frac{1}{\sqrt{5}}$$

hence

$$\pi^2 \cdot \min\left\{\frac{\upsilon(\theta)}{b}, \frac{\upsilon(\theta^{-1})}{a}\right\} = \frac{\pi^2}{\sqrt{5}a} \approx \frac{4.414}{a}$$
$$\pi^2 \cdot \min\left\{\frac{\upsilon(\theta^{-1})}{b}, \frac{\upsilon(\theta)}{a}\right\} = \frac{\pi^2}{\sqrt{5}a} \approx \frac{4.414}{a}$$

At the same time, we have

$$\gamma_+ \geq \frac{\pi^2}{\sqrt{5}a} \approx \frac{4.414}{a}$$
$$\gamma_- \leq \frac{2\pi}{a} \tan\left(\frac{3-\sqrt{5}}{4}\pi\right) \approx \frac{4.298}{a}$$

Golden–mean lattice

Theorem

Let $\frac{a}{b} = \phi = \frac{\sqrt{5}+1}{2}$. *Then:*

(i) *If* $\alpha > \frac{\pi^2}{\sqrt{5}a}$ *or* $\alpha \le -\frac{\pi^2}{\sqrt{5}a}$, *there are infinitely many spectral gaps.*

(ii) *If*

$$-\frac{2\pi}{a}\tan\left(\frac{3-\sqrt{5}}{4}\pi\right) \le \alpha \le \frac{\pi^2}{\sqrt{5}a},$$

there are no gaps in the positive spectrum.

(iii) *If*

$$-\frac{\pi^2}{\sqrt{5}a} < \alpha < -\frac{2\pi}{a}\tan\left(\frac{3-\sqrt{5}}{4}\pi\right),$$

there is a nonzero and finite number of gaps in the positive spectrum.

Golden–mean lattice

Corollary

Quantum graphs with a finite nonzero number of gaps exist.

Remark

- A finite nonzero number of gaps in the positive spectrum of the golden mean lattice can occur only for $\alpha < 0$.
- If $\alpha > 0$, there are either no gaps in the spectrum or infinitely many of them in accordance with a numerical observation made in [Exner and Gawlista 1996].
- The window in which the golden-mean lattice has the Bethe–Sommerfeld property is narrow, roughly can be characterized as $4.298 \lesssim -\alpha a \lesssim 4.414$.

Golden–mean lattice

We are able to control the number of gaps in the Bethe–Sommerfeld regime:

Theorem

For a given $N \in \mathbb{N}$, there are exactly N gaps in the positive spectrum if and only if α is chosen within the bounds

$$-\frac{2\pi\left(\phi^{2(N+1)}-\phi^{-2(N+1)}\right)}{\sqrt{5}a}\tan\left(\frac{\pi}{2}\phi^{-2(N+1)}\right) \le \alpha < -\frac{2\pi\left(\phi^{2N}-\phi^{-2N}\right)}{\sqrt{5}a}\tan\left(\frac{\pi}{2}\phi^{-2N}\right).$$

Constructing graphs with the Bethe–Sommerfeld property

Bethe–Sommerfeld property for both repulsive and attractive potentials

Theorem

Let the edge ratio be

$$\theta = \frac{2t^3 - 2t^2 - 1 + \sqrt{5}}{2(t^4 - t^3 + t^2 - t + 1)} \quad \text{for} \;\; t \in \mathbb{N},\; t \geq 3\,;$$

then there is a nonzero and finite number of gaps in the positive spectrum for a certain $\alpha > 0$ and for a certain $\alpha < 0$ as well.

Remark

- $\theta = \frac{t\phi+1}{(t^2+1)\phi+t}$ for $\phi = \frac{1+\sqrt{5}}{2}$ being the golden mean;
- the continued-fraction representation of θ is $[0; t, t, 1, 1, 1, 1, \ldots]$.

Explicit construction of Bethe–Sommerfeld regime

1. Take a β with an infinite continued-fraction representation
$$\beta = [0; c_1, c_2, c_3, \ldots]$$
such that the terms $c_1, c_2, c_3, \ldots$ are bounded.
2. Define ρ, ς and τ with continued-fraction representations
$$\begin{aligned} \rho &= [0; t, c_1, c_2, c_3, \ldots] \\ \varsigma &= [0; 1, t, c_1, c_2, c_3, \ldots] \\ \tau &= [0; t, t, c_1, c_2, c_3, \ldots] \end{aligned}$$
3. If t is chosen such that
$$\frac{2}{\pi} \tan\left(\frac{\pi}{2t}\right) < \min\{\upsilon(\beta), \upsilon(\beta^{-1})\}$$
the number of gaps is guaranteed to be finite nonzero
   - for $a/b = \rho$ and certain repulsive potentials ($\alpha > 0$);
   - for $a/b = \varsigma$ and certain attractive potentials ($\alpha < 0$);
   - for $a/b = \tau$ and certain potentials of both repulsive ($\alpha > 0$) and attractive ($\alpha < 0$) type.

Thank you for your attention!