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Periodické kvantové grafy a Betheho–Sommerfeldova hypotéza

Periodic quantum graphs
and the Bethe–Sommerfeld conjecture

Summary

Quantum mechanics on graphs studies the behaviour of particles whose motion is restricted to a system of edges connected in vertices. A typical problem to solve concerns the energy spectrum, that is, the set of energies that are allowed for a particle confined to a graph of given topological and metric properties.

Spectra of periodic quantum systems, including quantum graphs, are known to have a band structure: intervals of allowed energies are interlaced with gaps corresponding to forbidden energies. In 1933, Bethe and Sommerfeld conjectured that the number of spectral gaps for a system periodic in more than one direction is finite. Over time the validity of the conjecture was established for numerous systems; however, it also turned out that quantum graphs do not comply with this law as their spectra have typically infinitely many gaps, or no gaps at all. These findings led to a question, which then remained open for two decades, about the existence of periodic quantum graphs with the "Bethe–Sommerfeld property", that is, featuring a nonzero finite number of gaps in the spectrum.

In the lecture, we at first find certain conditions under which a graph does not have the Bethe–Sommerfeld property. Then we present a solution to the aforementioned open problem – we demonstrate that periodic quantum graphs with a finite nonzero number of spectral gaps do indeed exist. Our proof is constructive and yields yet another result: for any chosen natural number there is a periodic quantum graph with that number of gaps in its spectrum.

Souhrn

Kvantová mechanika na grafech studuje chování částic, jejichž pohyb je omezen na soustavu hran propojených ve vrcholech. Typickou úlohou k řešení bývá nalezení energetického spektra, tedy množiny energií, které jsou přípustné pro částici vázanou na graf o daných topologických a metrických parametrech.

O spektrech periodických kvantových systémů, včetně kvantových grafů, je známo, že mají pásovou strukturu: intervaly přípustných energií se střídají s mezerami odpovídajícími zakázaným energiím. V roce 1933 vyslovili Bethe a Sommerfeld domněnku, že je-li systém periodický ve více než jednom směru, počet spektrálních mezer je konečný. Postupem času byla platnost této hypotézy potvrzena pro řadu systémů; zároveň se však ukázalo, že neplatí pro kvantové grafy – v jejich spektrech typicky nacházíme buď nekonečný počet mezer, anebo žádné mezery. Tato zjištění vedla k otázce, která poté zůstala dvě desetiletí nezodpovězená, zda vůbec existují periodické kvantové grafy s „Betheho–Sommerfeldovou vlastností“, tedy takové, v jejichž spektru je konečný nenulový počet mezer.

V přednášce nalezneme nejprve určité podmínky, za nichž graf Betheho–Sommerfeldovu vlastnost nemá. Následně představíme řešení výše zmíněné úlohy – ukážeme, že periodické kvantové grafy s konečným nenulovým počtem spektrálních mezer skutečně existují. Předložíme konstruktivní důkaz, z nějž navíc vyplyne další výsledek: pro jakékoli zvolené přirozené číslo existuje periodický kvantový graf s tímto zvoleným počtem mezer ve spektru.

Klíčová slova

kvantový graf
spektrum operátoru
periodický systém
Betheho–Sommerfeldova hypotéza
vrcholová vazba
řetězový zlomek

Keywords

quantum graph
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vertex coupling
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Contents

1 Introduction **6**
- 1.1 Quantum mechanics on graphs . . . 6
- 1.2 Bethe–Sommerfeld conjecture . . . 6

2 Basic notions **7**
- 2.1 Quantum graph . . . 7
- 2.2 Boundary conditions in quantum graph vertices . . . 8
- 2.3 Scattering matrix . . . 9
- 2.4 Special types of vertex couplings . . . 10

3 Spectra of periodic graphs: preliminary considerations **10**
- 3.1 Graphs with scale-invariant couplings . . . 11
- 3.2 Graphs with general vertex couplings . . . 11

4 Bethe–Sommerfeld quantum graphs **12**
- 4.1 Continued fractions . . . 13
- 4.2 The existence of a Bethe–Sommerfeld quantum graph . . . 14
- 4.3 Periodic graphs with a given number of spectral gaps . . . 15

5 A control of the arrangement of gaps **15**

Conclusions **16**

References **17**

Curriculum Vitae (Ing. Ondřej Turek, Ph.D.) **19**

1 Introduction

1.1 Quantum mechanics on graphs

Quantum mechanics was established in the first half of the 20th century as a response to experimental discoveries of several phenomena on atomic scale that could not be explained by classical physics. *Quantum mechanics on graphs* is its relatively new branch; it studies the behaviour of particles propagating along graph edges connected in vertices. Graphs serve as efficient models of various nanosize graph-like systems, such as electrons confined to microscopic networks or moving along bonds in large molecules.

The use of graphs as models of realistic objects is based on a simple idea: If a particle is confined to a network built of thin wires or channels, its transversal motion in the cross section of the wire is negligible with respect to its longitudal motion along the wire. Representing the wires or channels by one-dimensional lines, and the whole network-shaped object by a metric graph, substantially simplifies the mathematical description, as it practically allows to use ordinary differential equations instead of partial differential equations.

The very first application of this approach dates back probably to 1950s, when a graph was used as a model of bonds in the naphthalene molecule [RS53]. Then the concept was abandoned and nearly forgotten until its rediscovery at the end of the eighties [GP88, EŠ89] in relation to the technological progress that demanded efficient theoretical methods for examining properties of nanostructures. Since that time quantum graphs have been studied intensively. Nowadays there is an extensive literature on the subject, see e.g. proceedings [EKST08] and monograph [BK13] referring to hundreds of research works.

In addition to its applicability to practically motivated problems, quantum mechanics of graphs serves as a plentiful source of interesting solvable models illustrating quantum effects. Notorious examples in quantum mechanics textbooks, such as the particle on a line with the delta potential, the particle in a box etc., are de facto special cases of quantum graphs. Quantum mechanics on graphs offers a variety of other solvable systems, even with complicated topologies. One can utilize them for analyzing, understanding and explaining nontrivial phenomena in quantum mechanics.

In this lecture we will focus on periodic graphs. Periodic quantum systems, including quantum graphs, generally deserve attention as they naturally appear as models of crystalline structures. Periodic quantum graphs became popular especially in connection with the discovery of graphene and related material objects such as carbon nanotubes [KP07], but they are also interesting mathematically, because they may exhibit properties different from standard periodic Schrödinger operators. One of those properties is related to the famous Bethe–Sommerfeld conjecture.

1.2 Bethe–Sommerfeld conjecture

One of the most important characteristics of any quantum system is the set of its possible energies. Let us emphasize that unlike classical mechanics, where the set of allowed energies of a system is always an interval taking the form $[E_{\min}, \infty)$, the set of allowed energies of a quantum system has often a complicated structure; it may contain gaps and isolated points. By the postulates of quantum mechanics, the set of allowed energies is equal to the spectrum of the *Hamiltonian* (the operator corresponding to the total energy of the system), and usually referred to as the *spectrum* of the system.

Spectra of periodic quantum systems are generally known to have a band structure: intervals of allowed energies are interlaced with open gaps corresponding to forbidden energies. In 1933, already in the early days of the quantum theory, Bethe and Sommerfeld conjectured that if a system is periodic in more than one dimension, the number of gaps is finite [SB33]. Confirming the validity of the conjecture turned out to be a difficult mathematical problem; it took decades until an affirmative answer was obtained for most cases of the "ordinary" Schrödinger operators [Sk79, Sk85, DT82, HM98, Pa08].

At the end of the 20th century, when the Bethe–Sommerfeld conjecture was discussed in the context of quantum graphs, it was observed that periodic graphs can have an infinite number of spectral gaps [SA00, Ex96a]. In other words, the claim represented by the Bethe–Sommerfeld conjecture is false for quantum graphs. More interestingly, all cases studied in the literature in subsequent years fell into one of those two situations: no gaps, or infinitely many gaps. For two decades, there was not a single confirmed case of a periodic quantum graph whose number of spectral gaps is nonzero finite. These facts naturally gave rise to the question about the very existence of periodic quantum graphs with the "Bethe–Sommerfeld property", that is, featuring a nonzero finite number of gaps in the spectrum. This is the topic we are going to discuss in the lecture; for the brevity of expression we will speak of those graphs as of *Bethe–Sommerfeld graphs*. As the main result, we will show that Bethe–Sommerfeld graphs exist.

2 Basic notions

2.1 Quantum graph

A *metric graph* Γ is an ordered pair $\Gamma = (\mathcal{V}, \mathcal{E})$, where $\mathcal{V}$ is a set of *vertices* and $\mathcal{E}$ is a set of *edges* such that:

- The edges are undirected.
- Every edge $e \in \mathcal{E}$ has its *length* $\ell(e) \in (0, +\infty]$.
- Each edge $e \in \mathcal{E}$ having a finite length $\ell(e) < \infty$ connects two vertices, which are called *endpoints*. If the two endpoints coincide, the edge is called *loop*.
- Each edge having infinite length $\ell(e) = +\infty$ is connected to only one vertex, which is its sole endpoint.
- Multiple edges connecting two vertices are permitted.

By a *degree* of a vertex $v \in \mathcal{V}$ in the graph Γ we mean the number of occurrences of v as an endpoint among all the edges in $\mathcal{E}$.

When the motion of a quantum particle is restricted to a metric graph Γ with edges $\mathcal{E} = \{e_1, e_2, e_3, \ldots\}$, the state of this quantum system is represented by the *wave function* $\Psi = (\psi_1, \psi_2, \psi_3, \ldots)^T$, where ψ_j (the j-th component of Ψ) is a complex function with domain $(0, \ell(e_j))$ that corresponds to the j-th edge of the graph. In each of the vertices, the functions ψ_j are required to satisfy *boundary conditions* that mathematically express the physical properties of the vertex. Their formulations and important examples will be discussed in sections 2.2 – 2.4.

The term *quantum graph* stands for a metric graph Γ equipped with the differential operator corresponding to the total energy (*Hamiltonian*) H_Γ. In the simplest setting when there are no additional potentials on the graph edges, and so the particle moves freely along each edge, the Hamiltonian acts on the components of the wave function Ψ as

$$\psi_j \mapsto -\frac{\hbar^2}{2m}\psi_j'' \,, \tag{1}$$

where m is the mass of the particle and $\hbar \approx 1.054\,572 \cdot 10^{-34}$ J·s is the reduced Planck constant.

In mathematical approach to quantum graphs, it is common to set the factor $\hbar^2/(2m)$ equal to 1, which corresponds to choosing physical constants such that $\hbar = 2m = 1$. This allows to express the particle energy E and its momentum $p = \sqrt{2mE}$ in terms of the wavenumber $k = \sqrt{2mE}/\hbar$ simply as

$$E = k^2 \,, \qquad p = k \,.$$

In other words, the square root of E (frequently appearing in calculations) and the momentum can be both identified with the wavenumber k. We will follow this convention.

2.2 Boundary conditions in quantum graph vertices

Consider a quantum graph vertex of degree n and denote the wave function components on the incident edges by $\psi_1, \dots, \psi_n$ (Figure 1).

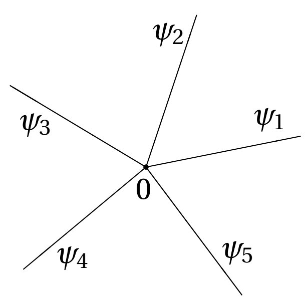

Figure 1: A quantum graph vertex (of degree 5)

Let us set

$$\Psi(0) = \begin{pmatrix} \psi_1(0_+) \\ \vdots \\ \psi_n(0_+) \end{pmatrix} \qquad \text{and} \qquad \Psi'(0) = \begin{pmatrix} \psi_1'(0_+) \\ \vdots \\ \psi_n'(0_+) \end{pmatrix},$$

where $\psi_j(0_+)$ denotes the limit of ψ_j at the vertex, and $\psi_j'(0_+)$ is the derivative of ψ_j at the vertex (the derivative in conventionally taken in the outgoing sense). The *boundary conditions* in the vertex connect the values $\psi_j(0_+)$ and $\psi_j'(0_+)$ in the form of n linear relations, commonly written in the compact way

$$A\Psi(0) + B\Psi'(0) = 0, \tag{2}$$

where A and B are complex $n \times n$ matrices such that

$$\begin{array}{ll} \bullet & \mathrm{rank}(A|B) = n, \\ \bullet & \text{the matrix } AB^* \text{ is Hermitian;} \end{array} \tag{3}$$

the symbol $(A|B)$ denotes the $n \times 2n$ matrix with A, B forming the first and the second n columns, respectively [KS99]. Properties (3) ensure the self-adjointness of the Hamiltonian, which is required by the postulates of quantum mechanics.

There exist alternative formulations of the conditions (2)&(3), in which the requirements (3) are incorporated into (2) by means of a special canonical form of the matrices A, B. One of them, proposed in [Ha00] and [KS00], expresses matrices A and B unambiguously via a unitary $n \times n$ matrix U:

$$(U - I)\Psi(0) + \mathrm{i}(U + I)\Psi'(0) = 0. \tag{4}$$

In this lecture we will take advantage of another canonical form of boundary conditions, which was derived in [CET10a] and is based on transforming A, B into block matrices as follows,

$$\begin{pmatrix} I^{(r)} & T \\ 0 & 0 \end{pmatrix} \Psi'(0) = \begin{pmatrix} S & 0 \\ -T^* & I^{(n-r)} \end{pmatrix} \Psi(0)\,, \tag{5}$$

where $r \in \{0, 1, \ldots, n\}$, the symbol $I^{(r)}$ stands for the identity matrix of order r, T is a general complex $r \times (n - r)$ matrix and S is a Hermitian matrix of order r. We call (5) *ST-form* of boundary conditions.

2.3 Scattering matrix

When a quantum particle with momentum k reaches a vertex of degree n, it is partly transmitted to the other edges and partly reflected. The scattering characteristics of the vertex are described by the *scattering matrix*

$$\mathcal{S}(k) = \begin{pmatrix} \mathcal{S}_{11}(k) & \mathcal{S}_{12}(k) & \cdots & \mathcal{S}_{1n}(k) \\ \mathcal{S}_{21}(k) & \mathcal{S}_{22}(k) & \cdots & \mathcal{S}_{2n}(k) \\ \vdots & \vdots & & \vdots \\ \mathcal{S}_{n1}(k) & \mathcal{S}_{n2}(k) & \cdots & \mathcal{S}_{nn}(k) \end{pmatrix},$$

which has the following properties:

- The elements of $\mathcal{S}(k)$ depend on the momentum k.
- The value $|\mathcal{S}_{jj}(k)|^2$ is equal to the probability of reflection on the j-th line, the value $|\mathcal{S}_{lj}(k)|^2$ for $l \neq j$ equals the probability of transmission from the j-th to the l-th line.
- Matrix $\mathcal{S}(k)$ is unitary for every k. This property may be viewed as the quantum version of Kirchhoff's law, see [KS99, KS00].

2.4 Special types of vertex couplings

Vertex couplings at a vertex of degree n form a large family, with interesting physical interpretations [CS98, CET10a, EP09] and a rich variety of scattering characteristics. Below we list three important types (or classes) that will be used in forthcoming presentation.

Free coupling

The *free coupling* is the most common type of vertex couplings. A vertex with the free coupling is characterized, in physical terms, by a free motion of particles through the vertex. It is mathematically expressed by so-called Kirchhoff boundary conditions

$$\psi_1(0) = \psi_2(0) = \cdots = \psi_n(0) =: \psi(0)\,, \qquad \sum_{j=1}^{n} \psi_j'(0) = 0\,. \tag{6}$$

δ coupling

The δ *coupling* corresponds to a repulsive or attractive potential in the vertex [Ex96b]. It is mathematically described by boundary conditions

$$\psi_j(0) = \psi_l(0) =: \psi(0)\,, \quad j, l = 1\ldots, n\,, \qquad \sum_{j=1}^{n} \psi_j'(0) = \alpha\psi(0)\,, \tag{7}$$

where $\alpha \in \mathbb{R}$ is a parameter of the coupling representing the strength and character of the potential (repulsive for $\alpha > 0$, attractive for $\alpha < 0$). The special choice $\alpha = 0$ gives the free coupling discussed above.

Scale-invariant couplings

A vertex coupling is called *scale-invariant* if the scattering matrix $\mathcal{S}(k)$ (and thus the scattering behaviour) is independent of the particle momentum k. This property is mathematically manifested in canonical forms (4) and (5) of boundary conditions in the following manner [BK13, CET10b]:

- The matrix U in boundary conditions (4) is Hermitian.
- The block S in the ST-form of boundary conditions (5) vanishes.

Scale-invariant couplings have been studied since roughly 2000 [FT00, NS00, CT10].

Example 2.1. The free coupling is scale-invariant. The δ coupling with parameter $\alpha \neq 0$ is not scale-invariant.

3 Spectra of periodic graphs: preliminary considerations

We are going to present three main results regarding the existence of Bethe–Sommerfeld quantum graphs, that is, periodic quantum graphs having a nonzero finite number of gaps in the spectrum. The first result gives a necessary condition: at least some of the vertex couplings in such a graph must lie outside the scale-invariant class.

Result 3.1. *If all the couplings at the vertices of an infinite periodic quantum graph are scale-invariant, then the graph does not have the Bethe–Sommerfeld property.*

As our second main result – the most important one – we will demonstrate that periodic quantum graphs with a nonzero finite number of spectral gaps do exist.

Result 3.2. *Bethe–Sommerfeld graphs exist.*

The third main result says that any number of spectral gaps can be attained.

Result 3.3. *For every prescribed number $N \in \mathbb{N}$, there is a periodic quantum graph having exactly N gaps in its spectrum.*

Below we prove Result 3.1 and discuss its generalization. Results 3.2 and 3.3 will be established in Section 4.

3.1 Graphs with scale-invariant couplings

The following theorem constitutes the announced Result 3.1.

Theorem 3.4 ([ET17])**.** *Let H_0 be a Hamiltonian of a periodic quantum graph with scale-invariant couplings at all the vertices. If $\sigma(H_0)$ contains a gap, then it contains infinitely many gaps.*

Sketch of the proof. If all the vertex couplings are scale-invariant, their scattering characteristics are independent of the momentum k. Using an approach developed in [BG00] and [BB13], one can show that the momentum k enters the spectral condition only via the vector

$$\vec{\phi}(k) = (\{k\ell_0\}_{(2\pi)}, \{k\ell_1\}_{(2\pi)}, \ldots, \{k\ell_d\}_{(2\pi)}),$$

where $\ell_0, \ell_1, \ldots, \ell_d$ are all the edge lengths of the graph and the symbol $\{x\}_{(2\pi)}$ stands for the difference between x and the nearest integer multiple of 2π.

Assume that a value $E = k^2$ belongs to a gap, i.e., k violates the spectral condition. For every $C > 0$ one can find a $k' > C$ such that $\vec{\phi}(k')$ becomes arbitrarily close to $\vec{\phi}(k)$, and so k' violates the spectral condition, too.

Therefore, if some $E = k^2$ belongs to a gap, then for any $C > 0$ there is an $E' = (k')^2 > C^2$ belonging to a gap. Consequently, the number of gaps is infinite.

□

3.2 Graphs with general vertex couplings

Theorem 3.4 inspires a question whether (and how) the statement can be extended to quantum graphs with vertex couplings that are not scale-invariant. Assume that the coupling in every vertex of the graph is described by boundary conditions in the ST-form, i.e.,

$$\begin{pmatrix} I^{(r)} & T \\ 0 & 0 \end{pmatrix} \Psi'(0) = \begin{pmatrix} S & 0 \\ -T^* & I^{(n-r)} \end{pmatrix} \Psi(0) \tag{8}$$

for some $n \geq r \geq 0$, some matrix $T \in \mathbb{C}^{r,n-r}$ and some Hermitian matrix S of order r. Let us emphasize that the values n and r, as well as the matrices T and S, can be different in different vertices.

In view of the fact that the scale-invariance of the coupling is broken by the presence of a nonzero matrix S in (8), we introduce the following notion:

Definition 3.5. Let a vertex coupling be given by boundary conditions (8). The *associated scale-invariant vertex coupling* is given by boundary conditions

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

That is, the coupling associated to (8) is obtained by replacing the square matrix S with the zero matrix. With this notion in hand we are ready to formulate a stronger version of Theorem 3.4.

Theorem 3.6 ([ET17])**.** *Consider a periodic graph with general couplings at the vertices and denote its spectrum as $\sigma(H)$. Let further $\sigma(H_0)$ be the spectrum of the same graph, in which all vertex couplings are replaced by the associated scale-invariant couplings. If $\sigma(H_0)$ has at least one gap, then $\sigma(H)$ has infinitely many gaps.*

Theorem 3.6 is a powerful criterion for showing that a given periodic graph with general vertex couplings cannot be of the Bethe–Sommerfeld type. The theorem allows to rule out at once the whole class of graphs sharing the same associated scale-invariant vertex couplings.

4 Bethe–Sommerfeld quantum graphs

Let us proceed to proving the existence of a periodic quantum graph with a nonzero finite number of gaps in its spectrum (Bethe–Sommerfeld graph). We will present a constructive proof that will allow us to put forward a stronger claim: there is a periodic quantum graph having any specified number of gaps in its spectrum.

To this aim we consider a rectangular lattice graph with edges of lengths a and b, see Figure 2. Since we know from the results of Section 3 that the Bethe–Sommerfeld property requires non-scale-invariant vertex couplings, let us assume that there are the δ couplings with parameter $\alpha \neq 0$ in the vertices (cf. Example 2.1). This particular model was originally

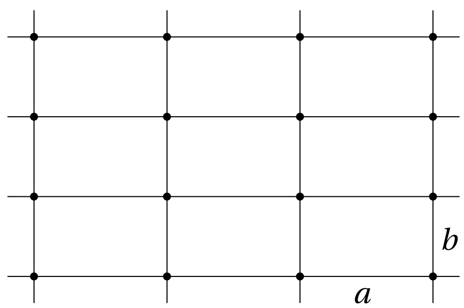

Figure 2: A rectangular lattice graph

introduced in [Ex95a] and was further discussed in [Ex96a, EG96], where the gap condition was derived. The condition depends on the sign of α (repulsive vs. attractive δ couplings).

- If $\alpha > 0$ (repulsive δ coupling), a number $k^2 > 0$ belongs to a gap if and only if the value $k > 0$ satisfies the condition

$$\tan\left(\frac{ka}{2} - \frac{\pi}{2}\left\lfloor\frac{ka}{\pi}\right\rfloor\right) + \tan\left(\frac{kb}{2} - \frac{\pi}{2}\left\lfloor\frac{kb}{\pi}\right\rfloor\right) < \frac{\alpha}{2k}\,, \tag{9}$$

where $\lfloor\cdot\rfloor$ is the floor function.

- If $\alpha < 0$ (attractive δ coupling), $k^2 > 0$ belongs to a gap if and only if $k > 0$ satisfies

$$\cot\left(\frac{ka}{2} - \frac{\pi}{2}\left\lfloor\frac{ka}{\pi}\right\rfloor\right) + \cot\left(\frac{kb}{2} - \frac{\pi}{2}\left\lfloor\frac{kb}{\pi}\right\rfloor\right) < \frac{|\alpha|}{2k}\,. \tag{10}$$

The solution of conditions (9) and (10) turns out to depend deeply on the type of irrationality of a/b. To describe the situation, we will need the apparatus of continued fractions.

4.1 Continued fractions

A *continued fraction* associated to a $\theta \in \mathbb{R}$ is a representation of θ in the form

$$\theta = a_0 + \cfrac{1}{a_1 + \cfrac{1}{a_2 + \cfrac{1}{a_3 + \cfrac{1}{\cdots}}}}\,, \tag{11}$$

where $a_0 \in \mathbb{Z}$ and $a_1, a_2, a_3, \ldots \in \mathbb{N}$. Representation (11) is usually written in a compact way as $\theta = [a_0; a_1, a_2, a_3, \ldots]$.

Example 4.1. For $\theta = [1; 1, 1, 1, \ldots] = [1; \bar{1}]$, we have

$$\theta = 1 + \cfrac{1}{1 + \cfrac{1}{1 + \cfrac{1}{1 + \cfrac{1}{\cdots}}}} = 1 + \frac{1}{\theta}\,,$$

hence $\theta^2 = \theta + 1$, which has the unique positive solution $\theta = \frac{1+\sqrt{5}}{2}$. This constant is notoriously known under the name *golden mean* and usually denoted by ϕ.

The continued fraction expansion of θ is finite if and only if θ is rational. Infinite expansions $[a_0; a_1, a_2, a_3, \ldots]$ always converge [Kh64]. Consequently, every continued fraction defines a unique real number θ.

Terminating the expansion $[a_0; a_1, a_2, a_3, \ldots]$ at the n-th position, one gets a rational number

$$\frac{p_n}{q_n} = [a_0; a_1, a_2, \ldots, a_n],$$

which is called the *n-th convergent* of the number $\theta = [a_0; a_1, a_2, a_3, \ldots]$. Even-order convergents approach θ from below, odd-order convergents approach θ from above; that is,

$$\frac{p_0}{q_0} < \frac{p_2}{q_2} < \frac{p_4}{q_4} < \frac{p_6}{q_6} < \cdots \leq \theta \leq \cdots < \frac{p_7}{q_7} < \frac{p_5}{q_5} < \frac{p_3}{q_3} < \frac{p_1}{q_1}\,.$$

Example 4.2. If $\theta = [1; 1, 1, 1, \ldots]$ (the golden mean), we obtain

$$\frac{p_0}{q_0} = [1] = 1 = \frac{1}{1}, \qquad \frac{p_1}{q_1} = [1; 1] = 1 + \frac{1}{1} = \frac{2}{1}, \qquad \frac{p_2}{q_2} = [1; 1, 1] = 1 + \frac{1}{1 + \frac{1}{1}} = \frac{3}{2},$$

and similarly $\frac{p_3}{q_3} = \frac{5}{3}$, $\frac{p_4}{q_4} = \frac{8}{5}$, $\frac{p_5}{q_5} = \frac{13}{8}$ etc.

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 $q \neq 0$. An irrational number θ is badly approximable if and only if the elements of its continued fraction representation $[a_0; a_1, a_2, a_3, \ldots]$ are bounded [Sch80].

4.2 The existence of a Bethe–Sommerfeld quantum graph

Earlier results [Ex96a, EG96] suggest that the considered rectangular graph can be of Bethe–Sommerfeld type only if the rectangle side ratio $\theta = a/b$ is a badly approximable irrational number. That is, the coefficients of the continued fraction representation of θ must be bounded. Let us focus on the simplest case when all the coefficients are equal to 1,

$$\theta = [1; 1, 1, 1, \ldots];$$

that is, θ is chosen to be the golden mean $\phi = \frac{\sqrt{5}+1}{2}$ (cf. Example 4.1). Analyzing inequalities (9) and (10) for the particular ratio $\frac{a}{b} = \phi$, we get the following description of the spectrum:

Theorem 4.3 ([ET17])**.** *Consider a rectangular lattice graph with edge lengths a and b such that $\frac{a}{b} = \phi = \frac{\sqrt{5}+1}{2}$. Assume that there are the δ couplings with parameter α in the vertices.*

(i) If $\alpha > \frac{\pi^2}{\sqrt{5}a}$ or $\alpha \leq -\frac{\pi^2}{\sqrt{5}a}$, the graph has infinitely many spectral gaps.

(ii) If

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

there are no gaps in the spectrum.

(iii) If

$$-\frac{\pi^2}{\sqrt{5}a} < \alpha < -\frac{2\pi}{a}\tan\left(\frac{3-\sqrt{5}}{4}\pi\right), \tag{12}$$

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

Part (iii) of Theorem 4.3 is the most important one: it gives the affirmative answer to the longstanding open problem regarding the existence of Bethe–Sommerfeld quantum graphs.

At the same time Theorem 4.3 indicates that the Bethe–Sommerfeld behaviour is special. By inequalities (12), a nonzero finite number of gaps in the spectrum occurs only for the value αa lying in a narrow window, roughly $-4.414 \lesssim \alpha a \lesssim -4.298$. The strictness of these conditions intuitively explains the rarity of Bethe–Sommerfeld quantum graphs.

4.3 Periodic graphs with a given number of spectral gaps

As the next step, we will count the exact number of spectral gaps in the Bethe–Sommerfeld case (iii) of Theorem 4.3. As a by-product we obtain Result 3.3 announced earlier.

Theorem 4.4 ([ET17])**.** *Consider a rectangular lattice graph with edge lengths a and b such that $\frac{a}{b} = \phi = \frac{\sqrt{5}+1}{2}$ and with the δ couplings with parameter α in the vertices. For a given $N \in \mathbb{N}$, there are exactly N gaps in the spectrum if and only if α is chosen within the bounds*

$$-\frac{A_{N+1}}{a} \le \alpha < -\frac{A_N}{a}\,, \tag{13}$$

where

$$A_j := \frac{2\pi\left(\phi^{2j} - \phi^{-2j}\right)}{\sqrt{5}} \tan\left(\frac{\pi}{2}\phi^{-2j}\right) \quad \textit{for every } j \in \mathbb{N}. \tag{14}$$

Since the numbers A_j given by (14) form an increasing sequence, inequalities (13) give a nonempty interval for every N. This fact immediately implies the claim of Result 3.3: *For any prescribed number $N \in \mathbb{N}$, there exists a periodic quantum graph having exactly N gaps in its spectrum.*

5 A control of the arrangement of gaps

Finally we will establish a connection between the spectral properties of the graph and the number-theoretical properties of its edge lengths ratio. For the rectangular lattice with edge lengths a and b and with the δ couplings with parameter α in the vertices, we will reveal an explicit relation between the terms in the continued fraction representation of the value $\theta = a/b$ and the number and positions of gaps in the spectrum of the graph.

In order to keep the presentation as straightforward as possible, we will focus on the case $\alpha > 0$ (repulsive coupling) and restrict our attention on edge lengths ratios $\theta = a/b$ with continued fraction representations of type

$$\theta = [1; 1, c_2, 1, c_4, 1, c_6, 1, c_8, 1, \ldots] \quad \text{such that } c_{2n} \in \{1,2\} \text{ for all } n \in \mathbb{N}. \tag{15}$$

In other words, θ is obtained from the golden mean $\phi = [1; 1, 1, 1, 1, 1, \ldots]$ by replacing some of the even-order terms with 2's.

Then the values $c_2, c_4, c_6, \ldots$ determine the positions of spectral gaps in accordance with the following theorem, which is a special case of [Tu19, Theorem 3].

Theorem 5.1. *Consider a rectangular lattice graph with edge lengths a and $b = a/\theta$ having a δ coupling with parameter $\alpha \in \left[\frac{4\pi(2-\sqrt{3})}{a}, \frac{2\pi^2}{5a}\right]$ in each vertex. If θ takes the form* (15)*, then k^2 is a lower endpoint of a spectral gap if and only if*

$$k^2 = \left(\frac{p_{2n-1}\pi}{a}\right)^2$$

for p_{2n-1} denoting the numerator of the $(2n-1)$-th convergent of θ such that $c_{2n} = 2$.

The theorem says that under the assumptions, the number of spectral gaps is equal to the number of 2's in the continued fraction representation (15), and the locations of the gaps are directly governed by the arrangement of 2's. Let us illustrate the result with an example.

Example 5.2. Let $a > 0$ and $\alpha \in \left[\frac{4\pi(2-\sqrt{3})}{a}, \frac{2\pi^2}{5a}\right]$.

- If $\theta = [1; 1, 2, \bar{1}] = (15+\sqrt{5})/10$, the spectrum has only one gap, whose lower endpoint is located at $(p_1\pi/a)^2$. Since the first convergent of θ is

  $$\frac{p_1}{q_1} = [1; 1] = 1 + \frac{1}{1} = \frac{2}{1},$$

  the lower endpoint of the gap is $k^2 = (p_1\pi/a)^2 = 4\pi^2/a^2$.

- If $\theta = [1; 1, 2, 1, 2, \bar{1}] = (209 + \sqrt{5})/122$, the spectrum has exactly 2 gaps, whose lower endpoints are located at $(p_1\pi/a)^2$ and $(p_3\pi/a)^2$. Since the 1st and the 3rd convergent of θ are

  $$\frac{p_1}{q_1} = [1; 1] = 1 + \frac{1}{1} = \frac{2}{1} \qquad \text{and} \qquad \frac{p_3}{q_3} = [1; 1, 2, 1] = 1 + \frac{1}{1 + \frac{1}{2 + \frac{1}{1}}} = \frac{7}{4},$$

  the lower endpoints of the gaps are $(2\pi/a)^2 = 4\pi^2/a^2$ and $(7\pi/a)^2 = 49\pi^2/a^2$.

Conclusions

The results presented in the lecture can be summarized as follows.

- We proved the existence of a periodic quantum graph having a nonzero finite number of gaps in its spectrum. This achievement solves a longstanding open problem – not a single example of such a graph had been known for two decades until 2017.
- The proof is constructive and shows even more: For any chosen number $N \in \mathbb{N}$, there is a periodic quantum graph having exactly N gaps in its spectrum.
- In addition, we demonstrated that the positions of the gaps can be directly controlled by varying the terms in the continued fraction expansion of the edge lengths ratio. This result confirms a deep connection between the number-theoretical properties and the arrangement of the gaps. It also contributes to the study of the problem of controlling the number and positions of gaps in spectra of periodic quantum graphs, which is known to be extremely hard [BK13].

References

[BB13] R. Band, G. Berkolaiko: Universality of the momentum band density of periodic networks, *Phys. Rev. Lett.* **111** (2013), 130404.

[BG00] F. Barra, P. Gaspard: On the level spacing distribution in quantum graphs, *J. Stat. Phys.* **101** (2000), 283–319.

[BK13] G. Berkolaiko, P. Kuchment: *Introduction to Quantum Graphs*, Amer. Math. Soc., Providence, R.I., 2013.

[CET10a] T. Cheon, P. Exner, O. Turek: Approximation of a general singular vertex coupling in quantum graphs, *Ann. Phys. (NY)* **325** (2010), 548–578.

[CET10b] T. Cheon, P. Exner, O. Turek: Tripartite connection condition for a quantum graph vertex, *Phys. Lett. A* **375** (2010), 113–118.

[CS98] T. Cheon and T. Shigehara: Realizing discontinuous wave functions with renormalized short-range potentials, *Phys. Lett. A* **243** (1998), 111–116.

[CT10] T. Cheon, O. Turek: Fulop-Tsutsui interactions on quantum graphs, *Phys. Lett. A* **374** (2010), 4212–4221.

[DT82] J. Dahlberg, E. Trubowitz: A remark on two dimensional periodic potentials, *Comment. Math. Helvetici* **57** (1982), 130–134.

[Ex95a] P. Exner: Lattice Kronig-Penney models, *Phys. Rev. Lett.* **74** (1995), 3503–3506.

[Ex96a] P. Exner: Contact interactions on graph superlattices, *J. Phys. A: Math. Gen.* **29** (1996), 87–102.

[Ex96b] P. Exner: Weakly coupled states on branching graphs, *Lett. Math. Phys.* **38** (1996), 313–320.

[EG96] P. Exner, R. Gawlista: Band spectra of rectangular graph superlattices, *Phys. Rev. B* **53** (1996), 7275–7286.

[EKST08] P. Exner, J. P. Keating, P. Kuchment, T. Sunada, A. Teplyaev, eds.: *Analysis on Graphs and Applications*, Proceedings of a Isaac Newton Institute programme, January 8–June 29, 2007; 670 p.; AMS "Proceedings of Symposia in Pure Mathematics" Series, vol. 77, Providence, R.I., (2008).

[EP09] P. Exner, O. Post: Approximation of quantum graph vertex couplings by scaled Schrödinger operators on thin branched manifolds, *J. Phys. A: Math. Theor.* **42** (2009), 415305.

[EŠ89] P. Exner and P. Šeba: Free quantum motion on a branching graph, *Rep. Math. Phys.* **28** (1989), 7–26.

[ET15] P. Exner, O. Turek: Spectrum of a dilated honeycomb network, *Integr. Equat. Oper. Th.* **81** (2015), 535–557.

[ET17] P. Exner, O. Turek: Periodic quantum graphs from the Bethe–Sommerfeld perspective, *J. Phys. A: Math. Theor.* **50** (2017), 455201.

[FT00] T. Fülőp, I. Tsutsui: A free particle on a circle with point interaction, *Phys. Lett. A* **264** (2000), 366–374.

[GP88] N. I. Gerasimenko and B. S. Pavlov: Scattering problem on noncompact graphs, *Teor. Mat. Fiz.* **74** (1988), 345–359.

[Ha00] M. Harmer: Hermitian symplectic geometry and extension theory, *J. Phys. A: Math. Gen.* **33** (2000), 9193–9203.

[HM98] B. Helffer, A. Mohamed: Asymptotic of the density of states for the Schrödinger operator with periodic electric potential, *Duke Math. J.* **92** (1998), 1–60.

[Kh64] A. Ya. Khinchin: *Continued Fractions*, University of Chicago Press, 1964.

[KS99] V. Kostrykin, R. Schrader: Kirchhoff's rule for quantum wires, *J. Phys. A: Math. Gen.* **32** (1999), 595–630.

[KS00] V. Kostrykin, R. Schrader: Kirchhoff's rule for quantum wires. II: The Inverse Problem with Possible Applications to Quantum Computers, *Fortschr. Phys.* **48** (2000), 703–716.

[KP07] P. Kuchment, O. Post: On the spectra of carbon nano-structures, *Comm. Math. Phys.* **275** (2007), no. 3, 805–826.

[NS00] K. Naimark, M. Solomyak, *Eigenvalue estimates for the weighted Laplacian on metric trees*, Proc. London Math. Soc. **80** (2000) 690–724.

[Pa08] L. Parnovski: Bethe-Sommerfeld conjecture, *Ann. Henri Poincaré* **9** (2008), 457–508.

[RS53] K. Ruedenberg and C. W. Scherr: Free-electron network model for conjugated systems, I. Theory, *J. Chem. Phys.* **21** (1953), 1565–1581.

[Sch80] W. M. Schmidt: *Diophantine Approximation*, Lecture Notes in Mathematics, vol. 785, Springer Verlag, Berlin 1980.

[SA00] J. H. Schenker, M. Aizenman: The creation of spectral gaps by graph decoration, *Lett. Math. Phys.* **53** (2000), 253–262.

[Sk79] M. M. Skriganov: Proof of the Bethe-Sommerfeld conjecture in dimension two, *Soviet Math. Dokl.* **20** (1979), 956–959.

[Sk85] M. M. Skriganov: The spectrum band structure of the threedimensional Schrödinger operator with periodic potential, *Invent. Math.* **80** (1985), 107–121.

[SB33] A. Sommerfeld, H. Bethe: *Electronentheorie der Metalle.* 2nd edition, Handbuch der Physik, Springer Verlag 1933.

[Tu19] O. Turek: Gaps in the spectrum of a cuboidal periodic lattice graph, *Rep. Math. Phys.* **83** (2019), 107–127.

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