Periodic quantum graphs from the Bethe–Sommerfeld perspective

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Abstract. The paper is concerned with the number of open gaps in spectra of periodic quantum graphs. The well-known conjecture by Bethe and Sommerfeld (1933) says that the number of open spectral gaps for a system periodic in more than one direction is finite. To the date its validity is established for numerous systems, however, it is known that quantum graphs do not comply with this law as their spectra have typically infinitely many gaps, or no gaps at all. These facts gave rise to the question about the existence of quantum graphs with the 'Bethe–Sommerfeld property', that is, featuring a nonzero finite number of gaps in the spectrum. In this paper we prove that the said property is impossible for graphs with the vertex couplings which are either scale-invariant or associated to scale-invariant ones in a particular way. On the other hand, we demonstrate that quantum graphs with a finite number of open gaps do indeed exist. We illustrate this phenomenon on an example of a rectangular lattice with a δ coupling at the vertices and a suitable irrational ratio of the edges. Our result allows to find explicitly a quantum graph with any prescribed exact number of gaps, which is the first such example to the date.

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1. Introduction

Quantum graphs are one of the fast developing areas of quantum physics, the interest to them being driven both by their 'practical' use in modeling nanostructures and other physical objects, as well as by theoretical reasons. They allow us to understand better various quantum effects by analyzing them in the situation where the configuration space has nontrivial geometrical and topological properties. The literature concerning quantum graphs is extensive and we limit ourselves to referring the reader to the recent monograph [2] as a guide to further ilumination.

While the quantum graph Hamiltonians describing particles 'living' on a metric graph share many properties with the 'usual' Schrödinger operators, this analogy is far from being complete; a well-known example is the failure of the unique continuation property [2, Sec. 3.4] that makes possible, for instance, the existence of compactly supported eigenfunctions on infinite graphs. This concerns, in particular, *infinite periodic graphs* the spectrum of which may not be purely absolutely continuous containing flat bands, or infinitely degenerate eigenvalues, and it is even possible that the absolutely continuous part is empty as is the case for magnetic chain graphs with a half-of-the-quantum flux through each chain element [10, Thm 2.3].

Our goal in this paper is to investigate Hamiltonians of infinite periodic graphs from another point of view, namely the number of open gaps in their spectra. To begin with we recall the *Bethe–Sommerfeld conjecture* [20] put forward in the early days of the quantum theory, according to which a quantum system periodic in more than one direction — with a slight abuse of terminology one usually speaks of $\mathbb{Z}^\nu$-periodicity with $\nu \geq 2$ — has a finite number of open gaps in the spectrum only. The reasoning behind the conjecture is based on the behavior of the spectral bands identified with the ranges of the dispersion curves or surfaces. Those at most touch for $\mathbb{Z}$-periodic systems while in higher dimensions they typically overlap making opening of gaps more and more difficult as we proceed to higher energies. This looked convincing and the property was taken for granted, although mathematically it proved to be a rather hard problem and it took decades before an affirmative answer was obtained for most cases of the 'ordinary' Schrödinger operators — see, for instance, [6, 11, 14, 18, 19] and references therein.

Discussing this question in the context of quantum graphs, the authors of [2] recall the above mentioned heuristic argument (Sec. 4.7), however, they add immediately that this is not a 'strict law'; in Sec. 5.1 of [2] they illustrate this claim by examples of periodic graphs with an infinite number of resonant gaps created by a graph 'decoration', the effect noticed first in the context of discrete graphs [16] and later verified also for metric graphs. In other words, we have examples of numerous situations in which the claim represented by the BS conjecture is false. The question thus arise whether it is a 'law' at all, that is, whether there *are* infinite periodic graphs having a *finite nonzero* number of open gaps above the threshold of the spectrum. This is the topic we are going to discuss in the present paper; for the brevity of expression we will speak of those graphs as of graphs belonging to the *Bethe–Sommerfeld class*, or simply *Bethe–Sommerfeld graphs.*

We have two main conclusions. The first one concerns the fact that the said property is sensitive to the type of vertex coupling. Recall that the standard coupling conditions

$$(U - I)\Psi + \mathrm{i}(U + I)\Psi' = 0\,, \tag{1.1}$$

where Ψ, Ψ' are vectors of values and derivatives at the vertex, U is an $n \times n$ unitary matrix, where n is the degree of the vertex, can be decomposed into the Dirichlet, Neumann, and Robin parts [2, Thm. 1.4.4] corresponding to the eigenspaces of U referring to eigenvalues -1, 1, and the rest, respectively; if the latter is absent we call such a coupling for obvious reasons *scale-invariant.*

Theorem 1.1. *An infinite periodic quantum graph does not belong to the Bethe–Sommerfeld class if the couplings at its vertices are scale-invariant.*

In fact, one can make a stronger claim. Given a graph with general couplings we consider the same graph with the couplings made scale-invariant by removing the Robin component in the way described in Sec. 2.6. If the latter has at least one gap open, the original one is not of the Bethe–Sommerfeld class, cf. Proposition 2.6 below.

On the other hand, we are going to demonstrate that the said class is nonempty. Our second main result in this paper is expressed in the following claim.

Theorem 1.2. *Bethe–Sommerfeld graphs exist.*

As it is usually the case with existence claims it is sufficient to present an example. With this aim we revisit in the second part of the paper the model introduced in [7] and further discussed in [8, 9] describing a periodic lattice whose basic cell is a rectangle of the side ratio θ and the coupling in the vertices is of the δ-type with a coupling constant $\alpha \in \mathbb{R}$. It was shown in the mentioned papers that the spectral properties of such a quantum graph depend on the number-theoretical properties of the ratio θ. Here we are going to demonstrate that if θ is badly approximable by rationals, there are values of α for which this graph belongs to the Bethe–Sommerfeld class. More than that, our construction makes it possible to find values of α for which the lattice graph in question has any prescribed number of gaps.

Before closing the introduction, let us recall that there are examples of the 'usual' Schrödinger operators where the question about validity of the conjecture remains open, a prominent example being Laplacian in a periodically curved tube or a Schrödinger operator in a straight tube with a $\mathbb{Z}$-periodic potential. These systems are sometimes said to have a 'mixed dimensionality' even if they are obviously periodic in one direction only, however they have a 'two-dimensional' feature, namely that in the absence of potential or the deformation they have intersecting dispersion curves, which could suggest a BS-type behaviour. An analogue of such systems in the present context are $\mathbb{Z}$-periodic graphs with period cells connected by more than a single link for which the question about the Bethe-Sommerfeld property remains also open.

2. Absence of the Bethe–Sommerfeld property

In this section we are going to prove Theorem 1.1 and its generalization.

2.1. The ST-form of the coupling

As it is common in the quantum graph theory the Hamiltonians we consider act as the (negative) second derivative on the graph edges with the domain consisting of functions which belong locally to the second Sobolev space and satisfy suitable coupling conditions at the vertices. For the purposes of the argument it is useful to replace the vertex condition (1.1) by an equivalent form proposed in [4] and referred to as the *ST-form*. Given a vertex of degree n, the vectors Ψ and Ψ' in $\mathbb{C}^n$ will again stand for the boundary values in the vertex,

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

where the limits of the first derivatives are conventionally taken in the outward direction. The coupling condition at the vertex can be then written in the form

$$\begin{pmatrix} I^{(r)} & T \\ 0 & 0 \end{pmatrix} \Psi' = \begin{pmatrix} S & 0 \\ -T^* & I^{(n-r)} \end{pmatrix} \Psi \tag{2.1}$$

for certain r, S, and T, where the symbol $I^{(r)}$ denotes the identity matrix of order r and the matrix S is Hermitian. The condition (2.1) allows us to single out scale-invariant couplings; it is easy to see that the coupling has this property if and only if $S = 0$ [5]. In particular, the on-shell scattering matrix $\mathcal{S}(k)$ for the vertex in question is in the ST-formalism given by

$$\mathcal{S}(k) = -I^{(n)} + 2 \begin{pmatrix} I^{(r)} \\ T^* \end{pmatrix} \left(I^{(r)} + TT^* - \frac{1}{\mathrm{i}k} S \right)^{-1} \begin{pmatrix} I^{(r)} & T \end{pmatrix} \tag{2.2}$$

and it obvious that it is independent of k *iff* $S = 0$.

The spectrum is obtained using the Bloch-Floquet theory [2, Sec. 4.2]. We assume that the graph is locally finite and consider its elementary cell; cutting it out from the original periodic graph we get a finite family of pairs of 'antipodal' vertices related mutually by the action of the corresponding translation group. Each such pair of vertices (v_-, v_+) can be regarded as a single vertex with the boundary conditions

$$\psi(v_+) = \mathrm{e}^{\mathrm{i}\vartheta_l} \psi(v_-), \quad \psi'(v_+) = \mathrm{e}^{\mathrm{i}\vartheta_l} \psi'(v_-) \tag{2.3}$$

for some $\vartheta_l \in (-\pi, \pi]$, where $l = 1, \dots, \nu$, and ν is the dimension of translation group associated with graph periodicity. The pair of edges with the endpoints $v_\pm$ can be turned into a single edge by identifying these endpoints, and the acquired phase ϑ_l coming from the conditions (2.3) can be also regarded as being induced by a magnetic potential. Denoting such a graph Γ and assuming that it has E edges, we consider the $2E \times 2E$ matrices $\mathbf{A}$, $\mathbf{L}$, and $\mathbf{S}$ which are defined in the following way. The diagonal matrix $\mathbf{L}$ is determined by the lengths of the directed edges (bonds) of the graph Γ. The diagonal matrix $\mathbf{A}$ has the entries $\mathrm{e}^{\mathrm{i}\vartheta_l}$ or $\mathrm{e}^{-\mathrm{i}\vartheta_l}$ at the positions corresponding to the edges created by the mentioned vertex identification, all its other entries are zero;

the sign in the exponents depends on the edge orientation. Finally, the matrix $\mathbf{S}$ is the bond scattering matrix, which contains directed edge-to-edge scattering coefficients. In this way, each element of the matrix $\mathbf{S}$ corresponds to a certain entry of the scattering matrix at a certain vertex of the elementary cell, cf. [2, eq. (2.1.15)]. Recall that the bond scattering matrix $\mathbf{S}$ is unitary.

This definitions follow the usual treatment of periodic quantum graphs [1]. Having introduced the matrices $\mathbf{A}$, $\mathbf{L}$, and $\mathbf{S}$, we define the function $F(k;\vec{\vartheta})$ as

$$F(k;\vec{\vartheta}) := \det\left(\mathbf{I} - \mathrm{e}^{\mathrm{i}(\mathbf{A}+k\mathbf{L})}\mathbf{S}(k)\right)\,; \tag{2.4}$$

this allows us to write the spectral condition in the form

$$k^2 \in \sigma(H) \quad \Leftrightarrow \quad (\exists\vec{\vartheta} \in (-\pi,\pi]^\nu)(F(k;\vec{\vartheta}) = 0)\,. \tag{2.5}$$

Note that the function $F(k;\vec{\vartheta})$ is in general complex, however, one can consider a real-valued function instead, dividing $F(k;\vec{\vartheta})$ by $\sqrt{\det(\mathrm{e}^{\mathrm{i}(\mathbf{A}+k\mathbf{L})}\mathbf{S}(k))}$, cf. [2, Rem. 2.1.10].

2.2. Graphs with scale-invariant couplings

Consider first the case of a periodic graph with scale-invariant couplings at all the vertices. The scale-invariance assumption implies that the scattering matrix at each graph vertex is independent of k and the same is naturally true for the matrix $\mathbf{S}$ entering formula (2.4). The function value $F(k;\vec{\vartheta})$ thus depends on the vectors $\vec{\vartheta}$ and $(k\ell_0, k\ell_1, \ldots, k\ell_d)$, where $\{\ell_0, \ell_1, \ldots, \ell_d\}$, $d+1 \leq E$, is the set of mutually different edge lengths of Γ. Moreover, the value $F(k;\vec{\vartheta})$ is 2π-periodic in each of the terms $k\ell_0, k\ell_1, \ldots, k\ell_d$. As a result, $F(k;\vec{\vartheta})$ depends on the vectors $(\{k\ell_0\}_{(2\pi)}, \{k\ell_1\}_{(2\pi)}, \ldots, \{k\ell_d\}_{(2\pi)})$ and $\vec{\vartheta}$ only, where $\{\ell_0, \ell_1, \ldots, \ell_d\}$, $d+1 \leq E$, is the set of mutually different edge lengths of Γ and the symbol $\{x\}_{(2\pi)}$ stands for the difference between x and the nearest integer multiple of 2π, i.e.

$$\{x\}_{(2\pi)} = x - 2\pi m \quad \text{if} \;\; x \in ((2m-1)\pi, (2m+1)\pi]\,. \tag{2.6}$$

The spectral condition (2.5) can be, therefore, written in the form

$$k^2 \in \sigma(H_0) \quad \Leftrightarrow \quad \left(\exists\vec{\vartheta} \in (-\pi,\pi]^\nu\right)\left(F_0(\{k\ell_0\}_{(2\pi)}, \{k\ell_1\}_{(2\pi)}, \ldots, \{k\ell_d\}_{(2\pi)}; \vec{\vartheta}) = 0\right)$$

(for simplicity here and elsewhere in this section the subscript 0 refers to graphs with scale-invariant couplings).

Proposition 2.1. *Let the assumptions given above be satisfied, then the following holds:*

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

(ii) The gaps can be classified into series that have asymptotically constant lengths with respect to k, thus the gap lengths within a series grow linearly with respect to k^2.

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

Proof. The easiest part to prove is (iii). If all the lengths are rationally dependent, there exists an elementary length $L > 0$ and integers $m_j \in \mathbb{N}$ such that $\ell_j = m_j L$ holds for $j = 0, 1, \ldots, d$. Hence $\left(k + \frac{2\pi}{L}\right)\ell_j = k\ell_j + 2\pi m_j$ which implies

$$\left\{\left(k + \frac{2\pi}{L}\right)\ell_j\right\}_{(2\pi)} = \{k\ell_j\}_{(2\pi)}$$

for all $j = 0, 1, \ldots, d$. This means that $F_0(\{k\ell_0\}_{(2\pi)}, \{k\ell_1\}_{(2\pi)}, \ldots, \{k\ell_d\}_{(2\pi)}; \vec{\vartheta})$ as a function of k is periodic with period $2\pi/L$, and consequently, the spectrum has a periodic structure in terms of the momentum.

Next we proceed to the proof of (i). We shall prove that the existence of a $k > 0$ with property $k^2 \notin \sigma(H_0)$ implies

$$(\forall C > 0)(\exists k' > C)((k')^2 \notin \sigma(H_0)) .$$

Since the function $k \mapsto F(k; \vec{\vartheta})$ is continuous, it obviously suffices to check that for any $k > 0$ and $C > 0$ there is a $k' > C$ such that the values $k'\ell_j$ are arbitrarily close to $k\ell_j$ up to an integer multiple of 2π, more explicitly

$$(\forall k > 0)(\forall C > 0)(\forall \delta > 0)(\exists k' > C)(\forall j \in \{0, 1, \ldots, d\})\left(|\,\{k'\ell_j - k\ell_j\}_{(2\pi)}\,| < \delta\right), \tag{2.7}$$

where the symbol $\{\cdot\}_{(2\pi)}$ was defined in (2.6).

We shall prove the claim (2.7) using the simultaneous version of the Dirichlet's approximation theorem. First of all, we set

$$\alpha_j = \frac{\ell_j}{\ell_0} \tag{2.8}$$

for all $j = 1, \ldots, d$. The said theorem guarantees for any $\alpha_1, \ldots, \alpha_d \in \mathbb{R}$ and for any natural number N the existence of integers $p_1, \ldots, p_d,\ q \in \mathbb{Z},\ 1 \leq q \leq N$, such that

$$\left|\alpha_j - \frac{p_j}{q}\right| \leq \frac{1}{qN^{1/d}} . \tag{2.9}$$

Let k, C and δ be given and choose m as an integer with the property that

$$m > \frac{\ell_0 C}{2\pi} . \tag{2.10}$$

Once m is fixed, the number N can be taken as any integer satisfying

$$N > \left(\frac{2\pi}{\delta} m\right)^d . \tag{2.11}$$

Let q be the integer from the simultaneous version of the Dirichlet's approximation theorem corresponding to N chosen according to (2.11). Notice that q depends on N, and therefore also on δ. For this q, we define k'_δ as follows,

$$k'_\delta := k + 2\pi m \frac{q}{\ell_0} .$$

Our aim is to show that k'_δ satisfies the following two conditions:

$$k'_\delta > C \tag{2.12}$$

$$|\{k'_\delta \ell_j - k\ell_j\}_{(2\pi)}| < \delta\,, \quad j = 0, 1, \ldots, d \tag{2.13}$$

Applying the definition of k'_δ, the inequality $q \geq 1$ and the assumption (2.10), we get

$$k'_\delta = k + 2\pi m \frac{q}{\ell_0} > 2\pi m \frac{q}{\ell_0} \geq 2\pi m \frac{1}{\ell_0} > C\,,$$

in other words, condition (2.12) holds true. Let us proceed to condition (2.13). We have

$$k'_\delta \ell_j - k\ell_j = 2\pi m \frac{q}{\ell_0} \ell_j = 2\pi m q \alpha_j\,,$$

where α_j was introduced in equation (2.8). Since $\left|\{x\}_{(2\pi)}\right| \leq |x - 2\pi p|$ holds obviously for all $x \in \mathbb{R}$ and $p \in \mathbb{Z}$, we obtain in particular

$$\left|\{k'_\delta \ell_j - k\ell_j\}_{(2\pi)}\right| \leq |k'_\delta \ell_j - k\ell_j - 2\pi m p_j| = |2\pi m q \alpha_j - 2\pi m p_j| = 2\pi m q \left|\alpha_j - \frac{p_j}{q}\right|$$

for $p_1, \ldots, p_d$ denoting the integers from (2.9). Consequently, the inequality (2.9) and the assumption (2.11) imply

$$\left|\{k'_\delta \ell_j - k\ell_j\}_{(2\pi)}\right| \leq 2\pi m q \frac{1}{q N^{1/d}} = \frac{2\pi m}{N^{1/d}} < \delta\,, \tag{2.14}$$

which proves condition (2.13). The claim (2.7) thus holds true.

Finally, the claim (ii) is a consequence of the argument used to prove (i). It follows trivially from (2.14) that letting $\delta \to 0$ we can always construct a number $k'_\delta > C$ with the property that $\lim_{\delta\to 0} \{(k'_\delta + x)\ell_j - (k + x)\ell_j\}_{(2\pi)} = 0$ holds for any $x \in \mathbb{R}$. This means that $\lim_{\delta\to 0} F(k'_\delta + x; \vec{\vartheta}) = F(k + x; \vec{\vartheta})$ holds for any $x \in \mathbb{R}$ as $\delta \to 0$, and in particular,

$$\lim_{\delta\to 0} F(k'_\delta; \vec{\vartheta}) \begin{cases} = 0 & \text{if } F(k; \vec{\vartheta}) = 0; \\ \neq 0 & \text{if } F(k; \vec{\vartheta}) \neq 0. \end{cases} \tag{2.15}$$

Suppose that the momentum spectrum of H_0 has a gap $(k - \Delta_1, k + \Delta_2)$ of the width $\Delta_1 + \Delta_2$ located around the value k. For any $C > 0$ and $\delta > 0$ we can construct a gap $(k'_\delta - \Delta'_1, k'_\delta + \Delta'_2)$, located around the momentum value $k'_\delta > C$. Relation (2.15) implies that in the limit $\delta \to 0$ we haves $\Delta'_1 \to \Delta_1$ and $\Delta'_2 \to \Delta_2$, hence the width of the gap around k'_δ is $\Delta'_1 + \Delta'_2 \to \Delta_1 + \Delta_2$. In other words, if k'_δ is constructed by the procedure described above by choosing a sufficiently small δ, then the widths of gaps around k and k'_δ can be as close to each other as required. □

Corollary 2.2. *Theorem 1.1 is valid.*

2.3. More general vertex couplings

Our next aim is to show that the Bethe–Sommerfeld property can be excluded also for graphs with vertex couplings from a wider class. We begin with the following definition.

Definition 2.3. *Let a vertex coupling be given by condition (2.1). The* associated scale-invariant vertex coupling *is given by condition*

$$\begin{pmatrix} I^{(r)} & T \\ 0 & 0 \end{pmatrix} \Psi' = \begin{pmatrix} 0 & 0 \\ -T^* & I^{(n-r)} \end{pmatrix} \Psi \,. \tag{2.16}$$

In other words, the coupling associated to a given (2.1) is obtained by removing the Robin part represented by the square matrix S.

In the following proposition we show that the scattering matrix referring to (2.1) decomposes into a constant part and a part that vanishes as $k \to \infty$. This observation is useful for dealing with high momenta values, $k \gg 1$, note that this is the regime crucial from the viewpoint of the Bethe–Sommerfeld property.

Proposition 2.4. *Consider a quantum graph vertex with a general coupling described by the condition (2.1). Its scattering matrix satisfies*

$$\mathcal{S}(k) = \mathcal{S}_0 + \frac{1}{k}\mathcal{S}_1(k)\,, \tag{2.17}$$

where

$$\mathcal{S}_0 = \lim_{k\to\infty} \mathcal{S}(k) = -I^{(n)} + 2 \begin{pmatrix} I^{(r)} \\ T^* \end{pmatrix} \left(I^{(r)} + TT^*\right)^{-1} \begin{pmatrix} I^{(r)} & T \end{pmatrix}$$

is the constant scattering matrix corresponding to the associated scale-invariant vertex coupling (2.16), and

$$\mathcal{S}_1(k) = -2\mathrm{i} \begin{pmatrix} I^{(r)} \\ T^* \end{pmatrix} \left(I^{(r)} + TT^*\right)^{-1} S \left(I^{(r)} + TT^* - \frac{1}{\mathrm{i}k}S\right)^{-1} \begin{pmatrix} I^{(r)} & T \end{pmatrix}.$$

Moreover, the matrix function $k \mapsto \mathcal{S}_1(k)$ is bounded on the interval $[1, \infty)$.

Proof. It is easy to check that the sum $\mathcal{S}_0 + \frac{1}{k}\mathcal{S}_1(k)$ is equal to the right-hand side of equation (2.2). The boundedness of $\mathcal{S}_1(k)$ on $[1, \infty)$ is a straightforward consequence of the continuity of $k \mapsto \mathcal{S}_1(k)$ and the existence of the limit

$$\lim_{k\to\infty} \mathcal{S}_1(k) = -2\mathrm{i} \begin{pmatrix} I^{(r)} \\ T^* \end{pmatrix} \left(I^{(r)} + TT^*\right)^{-1} S \left(I^{(r)} + TT^*\right)^{-1} \begin{pmatrix} I^{(r)} & T \end{pmatrix}.$$

□

Since each entry of the matrix $\mathbf{S}(k)$, appearing in (2.4) and referring to all the vertices of the graph Γ, corresponds to a certain entry of $\mathcal{S}(k)$ for a particular vertex, we can decompose the matrix $\mathbf{S}(k)$ in a way similar to (2.17), writing

$$\mathbf{S}(k) = \mathbf{S}_0 + \frac{1}{k}\mathbf{S}_1(k)\,, \tag{2.18}$$

where $\mathbf{S}_0$ is a constant unitary matrix, corresponding to the same graph with the associated scale-invariant couplings at its vertices, and $\mathbf{S}_1(k)$ is a matrix that is bounded on $[1,\infty)$ as a function of k.

Proposition 2.5. *The quantity $F(k;\vec{\vartheta})$ of (2.4) can be expressed as*

$$F(k;\vec{\vartheta}) = F_0(\{k\ell_0\}_{(2\pi)},\{k\ell_1\}_{(2\pi)},\dots,\{k\ell_d\}_{(2\pi)};\vec{\vartheta}) + \frac{1}{k}F_1(k;\vec{\vartheta})\,, \tag{2.19}$$

where

$$F_0(\{k\ell_0\}_{(2\pi)},\{k\ell_1\}_{(2\pi)},\dots,\{k\ell_d\}_{(2\pi)};\vec{\vartheta}) := \det\left(\mathbf{I} - \mathrm{e}^{\mathrm{i}(\mathbf{A}+k\mathbf{L})}\mathbf{S}_0\right)$$

and the function $k \mapsto F_1(k;\vec{\vartheta})$ is continuous and bounded on $[1,\infty)$.

Proof. According to (2.4) and (2.18) we have

$$F(k;\vec{\vartheta}) = \det\left(\mathbf{I} - \mathrm{e}^{\mathrm{i}(\mathbf{A}+k\mathbf{L})}\mathbf{S}(k)\right) = \det\left(M_0 + \frac{1}{k}M_1\right)$$

with $M_0 := \mathbf{I} - \mathrm{e}^{\mathrm{i}(\mathbf{A}+k\mathbf{L})}\mathbf{S}_0$ and $M_1 := -\mathrm{e}^{\mathrm{i}(\mathbf{A}+k\mathbf{L})}\mathbf{S}_1(k)$. We distinguish two cases.

(i) Let $F_0(k;\vec{\vartheta}) \neq 0$, i.e., $\det M_0 \neq 0$. This assumption means that M_0 is regular, hence

$$F(k;\vec{\vartheta}) = \det\left[M_0\cdot\left(I + \frac{1}{k}M_0^{-1}M_1\right)\right] = \det M_0\cdot\left(1+\mathcal{O}(k^{-1})\right) = \det M_0 + k^{-1}\mathcal{O}(1)\,.$$

(ii) On the contrary, let $F_0(k;\vec{\vartheta}) = 0$, i.e., $\det M_0 = 0$. Then

$$F(k;\vec{\vartheta}) = \det\left(M_0 + \frac{1}{k}M_1\right) = k^{-h}\mathcal{O}(1)\,,$$

where $h \geq 2E - \operatorname{rank}(M_0) \geq 1$.

In both cases the leading term of the component $\mathcal{O}(1)$ is a sum of products of entries of the matrices $\mathbf{S}_0$ and $\mathbf{S}_1(k)$ in (2.17), all of them being continuous and bounded with respect to $k \in [1,\infty)$. Consequently, the terms $k^{-1}\mathcal{O}(1)$ and $k^{-h}\mathcal{O}(1)$ in $F(k;\vec{\vartheta})$ can be written in the form $\frac{1}{k}F_1(k;\vec{\vartheta})$, where the function $k \mapsto F_1(k;\vec{\vartheta})$ is continuous and bounded on $[1,\infty)$. □

For the sake of brevity we would also often employ the symbol $F_0(k;\vec{\vartheta})$ as a shorthand for the expression $F_0(\{k\ell_0\}_{(2\pi)},\{k\ell_1\}_{(2\pi)},\dots,\{k\ell_d\}_{(2\pi)};\vec{\vartheta})$ appearing in (2.19).

Proposition 2.6. *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. Then the following claims hold true:*

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

(ii) If the edge lengths are rationally dependent, then the gaps of $\sigma(H)$ asymptotically coincide with those of $\sigma(H_0)$.

Proof. (i) If $\sigma(H_0)$ has a gap, then there is a $k^2>0$ such that $k^2\notin\sigma(H_0)$. From now on we regard $k>0$ as a fixed number. Let us recall that

$$k^2\notin\sigma(H_0) \quad\Leftrightarrow\quad (\forall\vec\vartheta\in(-\pi,\pi]^\nu)(|F_0(k;\vec\vartheta)|>0)\,.$$

Since $|F_0(k;\cdot)|$ is a continuous function of the quasimomentum $\vec\vartheta$, it attains a minimum on any compact interval, hence

$$\min_{\vec\vartheta\in[-\pi,\pi]^\nu}|F_0(k;\vec\vartheta)|=\gamma\,.$$

Moreover, the Brillouin zone has the structure of a torus, hence the function $|F_0(k;\cdot)|$ is periodic with the period 2π in every component of the vector $\vec\vartheta$, which in particular means that the same value of minimum is attained also at the left-open interval $(-\pi,\pi]^\nu$. Since $k^2\notin\sigma(H_0)$, the value γ must be positive, hence we obtain

$$(\forall\vec\vartheta\in(-\pi,\pi]^\nu)(|F_0(k;\vec\vartheta)|\geq\gamma>0)\,. \tag{2.20}$$

Equation (2.15) implies that for every $C>0$ there is a $k'>C$ such that

$$\left|F_0(k';\vec\vartheta)-F_0(k;\vec\vartheta)\right|<\frac{\gamma}{3}\,. \tag{2.21}$$

Let us limit ourselves to large values C, specifically, to the values C with the property

$$k'>C \quad\Rightarrow\quad \frac{|F_1(k';\vec\vartheta)|}{k'}<\frac{\gamma}{3}\,, \tag{2.22}$$

where $\frac{1}{k}F_1(k;\vec\vartheta)$ is the term appearing in equation (2.19). Now we apply twice the triangle inequality to the decomposition (2.19) and after that we use inequalities (2.20), (2.21), and (2.22). In this way we obtain

$$\begin{aligned}|F(k';\vec\vartheta)| &\geq \left|F_0(\{k'\ell_0\}_{(2\pi)},\{k'\ell_1\}_{(2\pi)},\dots,\{k'\ell_d\}_{(2\pi)};\vec\vartheta)\right|-\frac{|F_1(k';\vec\vartheta)|}{k'}\\ &\geq \left|F_0(k;\vec\vartheta)\right|-\left|F_0(k';\vec\vartheta)-F_0(k;\vec\vartheta)\right|-\frac{|F_1(k';\vec\vartheta)|}{k'}\\ &>\gamma-\frac{\gamma}{3}-\frac{\gamma}{3}=\frac{\gamma}{3}>0\,,\end{aligned}$$

for all $\vec\vartheta\in(-\pi,\pi]^\nu$; hence $k'^2\notin\sigma(H)$. To sum up, for any sufficiently large $C>0$ one can find a $k'>C$ such that $k'^2\notin\sigma(H)$, which proves the existence of infinitely many gaps in $\sigma(H)$ given the fact that the operator in question is unbounded.

(ii) We know from Proposition 2.1(iii) that the momentum spectrum of the graph with scale-invariant couplings is periodic. Every such period contains a finite number of gaps, thus there is a finite number of possible gap widths. Choose $\delta>0$ as a number sufficiently small in the sense that all the gaps are wider than 2δ. Gaps are open intervals of type (a,b); for each of them we consider the closed interval $[a+\delta,b-\delta]$, nonempty by construction, and define their union as follows:

$$M_\delta=\bigcup\{[a+\delta,b-\delta]\;;\;(a,b)\;\text{ is a gap}\}\,.$$

The set M_δ covers the gaps of $\sigma(H_0)$ up to their margins of width δ. Obviously, for all $\vec\vartheta \in [-\pi,\pi]^\nu$ we have

$$k \in M_\delta \quad \Rightarrow \quad F_0(k;\vec\vartheta) \neq 0\,.$$

The function $k \mapsto F_0(k;\vec\vartheta)$ is periodic, the set M_δ is closed, and the set $[-\pi,\pi]^\nu$ is compact. Consequently, there exists the minimum

$$\min\left\{|F_0(k;\vec\vartheta)|\;;\; k \in M_\delta, \vec\vartheta \in [-\pi,\pi]^\nu\right\} = \gamma_\delta > 0\,. \tag{2.23}$$

The quantity $F_1(k;\vec\vartheta)$ appearing in equation (2.19) is bounded with respect to k, hence there is a C_δ such that

$$k > C_\delta \quad \Rightarrow \quad \frac{|F_1(k;\vec\vartheta)|}{k} < \frac{\gamma_\delta}{2}\,. \tag{2.24}$$

Applying the triangle inequality to (2.19) and using inequalities (2.23) with (2.24), we arrive at

$$|F(k;\vec\vartheta)| \geq |F_0(k;\vec\vartheta)| - \frac{|F_1(k;\vec\vartheta)|}{k} > \gamma_\delta - \frac{\gamma_\delta}{2} = \frac{\gamma_\delta}{2} > 0\,,$$

for all $C_\delta < k \in M_\delta$ and $\vec\vartheta \in (-\pi,\pi]^\nu$, i.e. $k^2 \notin \sigma(H)$. At the same time, the value δ can be chosen as small as necessary. To sum up, to any $\delta > 0$ there is a C_δ such that

$$k > C_\delta \;\wedge\; \rho(k,\sigma(H_0)) \geq \delta \quad \Rightarrow \quad k \notin \sigma(H)\,,$$

where $\rho(k,\sigma(H_0))$ is the distance of k from the momentum spectrum of the graph with scale invariant couplings. In other words, as $k \to \infty$, gaps of $\sigma(H_0)$ coincide with gaps of $\sigma(H)$. □

3. Number theoretic preliminaries

Before turning to our second main topic we need to recall some number-theoretic notions on which the analysis of rectangular-lattice graphs will rely substantially. 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 $[c_0, c_1, c_2, c_3, \ldots]$ are bounded [13]. With our goal in mind we observe that according to [8, Thm. 3.2] the badly approximable numbers are the only ratios $\frac{a}{b}$ for which the spectrum of the rectangular lattice described above may have a finite number of gaps.

The so-called *Markov constant* $\mu(\theta)$ of $\theta \in \mathbb{R}$ is defined as

$$\mu(\theta) = \inf\left\{c > 0 \;\middle|\; \left(\exists_\infty (p,q) \in \mathbb{Z}^2\right)\left(\left|\theta - \frac{p}{q}\right| < \frac{c}{q^2}\right)\right\}. \tag{3.1}$$

The Markov constant is sometimes denoted by $\nu(\theta)$, cf. [3]. Notice that $\mu(\theta) > 0$ if and only if θ is badly approximable. Since every $\theta \in \mathbb{Q}$ has trivially $\mu(\theta) = 0$, some authors define $\mu(\theta)$ only for θ being irrational.

Recall that by a theorem of Hurwitz [12] for every irrational number θ there are infinitely many $(p, q) \in \mathbb{Z}^2$ such that $\left|\theta - \frac{p}{q}\right| < \frac{1}{\sqrt{5}q^2}$, in other words, $\mu(\theta) \le \frac{1}{\sqrt{5}}$ holds for any $\theta \in \mathbb{R}$.

We say that $\theta, \theta' \in \mathbb{R}$ are *equivalent* if there are integers r, s, t, u such that

$$\theta = \frac{r\theta' + s}{t\theta' + u} \quad \text{and} \quad ru - ts = \pm 1. \tag{3.2}$$

According to [3, Thm. IV], $\theta, \theta' \in (0, 1)$ are equivalent if and only if their continued fractions take the form

$$\begin{aligned} \theta &= [0; a_1, a_2, \dots, a_l, c_1, c_2, \dots] \\ \theta' &= [0; b_1, b_2, \dots, b_m, c_1, c_2, \dots] \end{aligned} \tag{3.3}$$

for suitable l, m and $a_1, \dots, a_l$, $b_1, \dots, b_m$, and $c_1, c_2, \dots$. One can prove that if θ and θ' are equivalent, then $\mu(\theta) = \mu(\theta')$; cf. [3, p. 11]. The particular choice $r = u = 0$ and $s = t = 1$ in equation (3.2) establishes the equivalence of the numbers θ and θ^{-1}; hence

$$\mu(\theta) = \mu(\theta^{-1}). \tag{3.4}$$

Now we will introduce a function $\upsilon : \mathbb{R} \to \mathbb{R}_+$ the values $\upsilon(\theta)$ of which will play an important role in the analysis of our spectral problem; they can be regarded as a one-sided version of the Markov constant.

Definition 3.1. *For any $\theta > 0$, we set*

$$\upsilon(\theta) := \inf\left\{ c > 0 \;\middle|\; \left(\exists_\infty (p, q) \in \mathbb{Z}^2\right) \left(0 < \theta - \frac{p}{q} < \frac{c}{q^2}\right) \right\}. \tag{3.5}$$

Proposition 3.2. *For every $\theta > 0$, we have*

$$\upsilon(\theta) = \inf\left\{c > 0 \mid (\exists_\infty m \in \mathbb{N})\left(m(m\theta - \lfloor m\theta \rfloor) < c\right)\right\}, \tag{3.6}$$

$$\upsilon(\theta^{-1}) = \inf\left\{c > 0 \mid (\exists_\infty m \in \mathbb{N})\left(m(\lceil m\theta \rceil - m\theta) < c\right)\right\}, \tag{3.7}$$

$$\mu(\theta) = \min\{\upsilon(\theta), \upsilon(\theta^{-1})\}, \tag{3.8}$$

where $\lfloor\cdot\rfloor$ and $\lceil\cdot\rceil$ are the floor and the ceiling function, respectively.

Proof. One can see easily that the right-hand side of (3.5) will remain unchanged if we assume $q > 0$ and p is replaced with $\lfloor q\theta \rfloor$, i.e.,

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

In this way we obtain formula (3.6).

Let us next prove (3.7). It follows from the definition that the left-hand side of (3.7) equals

$$\text{LHS} = \inf\left\{c > 0 \;\middle|\; \left(\exists_\infty (p, q) \in (\mathbb{Z}\backslash\{0\})^2\right) \left(q(q\theta^{-1} - p) < c\right)\right\}. \tag{3.9}$$

At the same time, in analogy with the previous step, it is easy to see that the right-hand side of (3.7) is equal to

$$\mathrm{RHS} = \inf\left\{c > 0 \;\middle|\; \left(\exists_\infty (p,q) \in (\mathbb{Z}\backslash\{0\})^2\right) \left(p(q - p\theta) < c\right)\right\}. \tag{3.10}$$

Our goal is to prove that LHS = RHS. To that end we will use the identity

$$q(q\theta^{-1} - p) = p(q - p\theta) + \frac{[p(q - p\theta)]^2}{p^2\theta}, \tag{3.11}$$

which implies

$$q(q\theta^{-1} - p) \geq p(q - p\theta) \qquad \text{for all } \ (p,q) \in (\mathbb{Z}\backslash\{0\})^2 ;$$

hence LHS $\geq$ RHS. At the same time, for every $c >$ RHS there are infinitely many $(p,q) \in (\mathbb{Z}\backslash\{0\})^2$ such that $p(q - p\theta) < c$. Therefore, due to identity (3.11), there are infinitely many $(p,q) \in (\mathbb{Z}\backslash\{0\})^2$ such that

$$q(q\theta^{-1} - p) < c + \frac{c^2}{p^2\theta}.$$

Choosing p large enough, we can find for any $c >$ RHS and any $\epsilon > 0$ infinitely many pairs $(p,q) \in \mathbb{Z}^2$ with the property

$$q(q\theta^{-1} - p) < c + \epsilon .$$

Consequently, we have also the inequality LHS $\leq$ RHS which completes the proof of the sought relation LHS = RHS.

It remains to prove formula (3.8). We know from the previous step that $\mu(\theta^{-1}) =$ RHS according to (3.10), hence

$$\upsilon(\theta^{-1}) = \inf\left\{c > 0 \;\middle|\; \left(\exists_\infty (p,q) \in \mathbb{Z}^2\right) \left(\frac{q}{p} - \theta < \frac{c}{p^2}\right)\right\}. \tag{3.12}$$

Formula (3.8) follows trivially from equations (3.5), (3.12) (where we have to rename the variables, $p \mapsto q$, $q \mapsto p$) and (3.1). □

Regarding equation (3.8), let us remark that the values $\upsilon(\theta)$ and $\upsilon(\theta^{-1})$ may or may not coincide. For example, for the golden mean, $\phi = (\sqrt{5} + 1)/2$, we have $\upsilon(\phi) = \upsilon(\phi^{-1}) = 1/\sqrt{5}$ (see Section 5 below), on the other hand, the literature on the Markov constant provides hints of the existence of numbers θ with the property $\upsilon(\theta) \neq \upsilon(\theta^{-1})$, see e.g. [15].

Function $\upsilon(\theta)$ is closely related to approximations of θ by rationals. A number $\frac{p}{q} \in \mathbb{Q}$ with $p, q \in \mathbb{Z}$ is called *best Diophantine approximation of the second kind* to a given $\theta \in \mathbb{R}$ if

$$|q\theta - p| < |q'\theta - p'| \tag{3.13}$$

holds for all $\frac{p'}{q'} \neq \frac{p}{q}$ such that $p', q' \in \mathbb{Z}$ and $0 < q' \leq q$. Every best Diophantine approximation of the second kind to a $\theta \in \mathbb{R}$ is a convergent $\frac{p_n}{q_n}$ of the continued fraction corresponding to θ, see e.g. [13]. If the inequality (3.13) is replaced with $\left|\theta - \frac{p}{q}\right| < \left|\theta - \frac{p'}{q'}\right|$, the corresponding fraction $\frac{p}{q}$ is called *best Diophantine approximation of the first kind* to the number θ.

For the discussion of the problem we address in this work, we will need a certain type of one-sided best approximations, which we will call, in analogy to the notions mentioned above, 'best approximation from below (respectively, from above) of the third kind'. They are defined as follows.

Definition 3.3. *Let $\theta \in \mathbb{R}$ and $\frac{p}{q} \in \mathbb{Q}$ for $p, q \in \mathbb{Z}$. We say that the number $\frac{p}{q}$ is a* best approximation from below of the third kind *to θ if*

$$0 \le q(q\theta - p) < q'(q'\theta - p') \tag{3.14}$$

for all $\frac{p'}{q'} \ge \theta$ such that $\frac{p'}{q'} \ne \frac{p}{q}$, $p', q' \in \mathbb{Z}$ and $0 < q' \le q$. Likewise, we call $\frac{p}{q}$ a best approximation from above of the third kind *to θ if*

$$0 \le q(p - q\theta) < q'(p' - q'\theta) \tag{3.15}$$

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

Best approximations from below of the third kind to θ greatly simplify the evaluation of the function $\upsilon(\theta)$. Indeed, we have

$$\upsilon(\theta) = \inf\left\{ q(q\theta - p) \;\middle|\; \frac{p}{q} \text{ is a best approximation from below to } \theta \right\}. \tag{3.16}$$

Formula (3.16) is very efficient providing that one knows best approximations from below of the third kind to θ. Their explicit characterization will be given in Proposition 3.5. To derive the result, we will need the following lemma.

Lemma 3.4. *Let $\theta = [a_0; a_1, a_2, a_3, \ldots]$ and $\frac{p_n}{q_n}$, $n \in \mathbb{N}$, be convergents of θ. If the inequalities*

$$\frac{p_{n-1}}{q_{n-1}} < \frac{p}{q} < \frac{p_{n+1}}{q_{n+1}} \le \theta \qquad \text{or} \qquad \frac{p_{n-1}}{q_{n-1}} > \frac{p}{q} > \frac{p_{n+1}}{q_{n+1}} \ge \theta$$

hold, then we have

$$q|q\theta - p| > \frac{1}{a_n}.$$

Proof. First we estimate the absolute value $\left|\frac{p}{q} - \frac{p_{n-1}}{q_{n-1}}\right|$ from below,

$$\left|\frac{p}{q} - \frac{p_{n-1}}{q_{n-1}}\right| = \frac{|pq_{n-1} - qp_{n-1}|}{q \cdot q_{n-1}} \ge \frac{1}{q \cdot q_{n-1}}, \tag{3.17}$$

where we used a trivial fact that $|pq_{n-1} - qp_{n-1}| \ge 1$ because the expression is by assumption a nonzero integer. In the next step we find an upper estimate of the same quantity, taking advantage of a known formula $\frac{p_{k-2}}{q_{k-2}} - \frac{p_k}{q_k} = \frac{(-1)^{k-1}a_k}{q_k q_{k-2}}$ (cf. [13, Cor. of Thm. 3]) for $[a_0; a_1, a_2, \ldots]$ representing the continued-fraction form of θ,

$$\left|\frac{p}{q} - \frac{p_{n-1}}{q_{n-1}}\right| < \left|\frac{p_{n+1}}{q_{n+1}} - \frac{p_{n-1}}{q_{n-1}}\right| = \frac{a_n}{q_{n+1}q_{n-1}}. \tag{3.18}$$

Combining inequalities (3.17) and (3.18), we obtain

$$q > \frac{q_{n+1}}{a_n}\,. \tag{3.19}$$

Now we use the assumptions of the lemma to estimate $\left|\theta - \frac{p}{q}\right|$:

$$\left|\theta - \frac{p}{q}\right| \geq \left|\frac{p_{n+1}}{q_{n+1}} - \frac{p}{q}\right| = \frac{|qp_{n+1} - pq_{n+1}|}{q\cdot q_{n-1}} \geq \frac{1}{q\cdot q_{n+1}}\,.$$

Hence we obtain, taking advantage of inequality (3.19),

$$q|q\theta - p| \geq \frac{q}{q_{n+1}} > \frac{1}{a_n}\,,$$

which yields the sought claim. □

Proposition 3.5. *Every best approximation of the third kind from below to a number $\theta \in \mathbb{R}$ is a convergent of θ.*

Proof. We will proceed by *reductio ad absurdum.* Suppose that $\frac{p}{q}$ is a best approximation of the third kind from below of θ which is not a convergent of θ. Then either we have $\frac{p}{q} < \frac{p_0}{q_0} = \lfloor\theta\rfloor$, where $\lfloor\cdot\rfloor$ is the floor function, or $\frac{p}{q}$ lies between two convergents that are smaller or equal to θ. First we will disprove the former case. For every $\frac{p}{q} < \lfloor\theta\rfloor$ we have

$$q(q\theta - p) = q^2\left(\theta - \frac{p}{q}\right) \geq \theta - \frac{p}{q} > \theta - \lfloor\theta\rfloor = 1\cdot(1\cdot\theta - \lfloor\theta\rfloor).$$

Comparing this result with condition (3.14) for $p' = \lfloor\theta\rfloor$ and $q' = 1$, we see that $\frac{p}{q}$ cannot be a best approximation from below of the third kind.

In the rest of the proof we will therefore suppose that $\frac{p}{q}$ lies between two convergents that are smaller or equal to θ, i.e.

$$\frac{p_{n-1}}{q_{n-1}} < \frac{p}{q} < \frac{p_{n+1}}{q_{n+1}} \leq \theta \qquad \text{for a certain odd } n\,; \tag{3.20}$$

recall that the parity of n determines whether the convergents are larger or smaller than θ. Our goal is to show that $\frac{p}{q}$ contradicts the requirement (3.14) on a best approximation of the third kind from below, i.e.,

$$q > q_n \quad \wedge \quad q(q\theta - p) \geq q_{n-1}(q_{n-1}\theta - p_{n-1}). \tag{3.21}$$

On one hand, obviously

$$\frac{p}{q} - \frac{p_{n-1}}{q_{n-1}} = \frac{pq_{n-1} - qp_{n-1}}{q\cdot q_{n-1}} \geq \frac{1}{q\cdot q_{n-1}}\,. \tag{3.22}$$

On the other hand, the well-known formula $\frac{p_k}{q_k} - \frac{p_{k-1}}{q_{k-1}} = \frac{(-1)^{k+1}}{q_k q_{k-1}}$ in combination with assumptions (3.20) implies

$$\frac{p}{q} - \frac{p_{n-1}}{q_{n-1}} < \frac{p_{n+1}}{q_{n+1}} - \frac{p_{n-1}}{q_{n-1}} = \frac{p_{n+1}}{q_{n+1}} - \frac{p_n}{q_n} + \frac{p_n}{q_n} - \frac{p_{n-1}}{q_{n-1}} = \frac{(-1)^n}{q_{n+1}q_n} + \frac{(-1)^{n-1}}{q_n q_{n-1}} = \frac{q_{n+1} - q_{n-1}}{q_{n-1}q_n q_{n+1}}. \tag{3.23}$$

Combining inequalities (3.22) and (3.23), we obtain

$$q > \frac{q_n q_{n+1}}{q_{n+1} - q_{n-1}} \,,$$

which, in particular, implies

$$q > q_n \,. \tag{3.24}$$

This verifies the first part of (3.21). In the next step we estimate $q_{n-1}(q_{n-1}\theta - p_{n-1})$. Since $\frac{p_{n-1}}{q_{n-1}}$ is a convergent, we have

$$\theta - \frac{p_{n-1}}{q_{n-1}} < \frac{1}{q_n q_{n-1}}$$

or, in other words

$$q_{n-1}(q_{n-1}\theta - p_{n-1}) < \frac{q_{n-1}}{q_n} \,. \tag{3.25}$$

Now we use Lemma 3.4 to obtain the estimate

$$q(q\theta - p) > \frac{1}{a_n} \,. \tag{3.26}$$

A well-known rule for continued fractions, $q_n = a_n q_{n-1} + q_{n-2}$, implies $q_n > a_n q_{n-1}$, and therefore

$$\frac{1}{a_n} > \frac{q_{n-1}}{q_n} \,. \tag{3.27}$$

Inequalities (3.25), (3.26) and (3.27) together imply $q(q\theta - p) > q_{n-1}(q_{n-1}\theta - p_{n-1})$. Taking into account that $q > q_n$, in view of estimate (3.24), we conclude that $\frac{p}{q}$ is not a best approximation of the third kind from below to θ. □

As for the approximation from above, the situation is slightly different.

Proposition 3.6. *Every best approximation from above of the third kind of a $\theta \in \mathbb{R}$ is either $\lceil\theta\rceil$ or a convergent of θ.*

Proof. We proceed again by contradiction. Let $\frac{p}{q} \neq \lceil\theta\rceil$ be a best approximation of the third kind from above to θ which is not a convergent of θ. Then either $\frac{p}{q}$ lies between two convergents that are smaller than θ, or $\frac{p}{q} > \frac{p_1}{q_1} \wedge \frac{p}{q} \neq \lceil\theta\rceil$. The former case can be treated in the same manner as in the proof of Proposition 3.5; therefore, we will omit it here and proceed directly to the case $\frac{p}{q} > \frac{p_1}{q_1}$, $\frac{p}{q} \neq \lceil\theta\rceil$. Since $\frac{p_1}{q_1} = a_0 + \frac{1}{a_1} = \frac{a_0 a_1 + 1}{a_1}$, every $\frac{p}{q} > \frac{p_1}{q_1}$ satisfies

$$p > q\left(a_0 + \frac{1}{a_1}\right) = q a_0 + \frac{q}{a_1} \,. \tag{3.28}$$

We distinguish two cases.

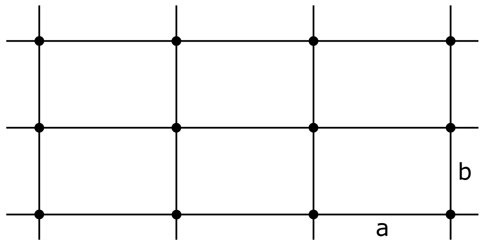

Figure 1. The rectangular-lattice graph

- If $q < a_1$, inequality (3.28) gives $p \geq qa_0 + 1$; hence

$$q(p - q\theta) \geq q(qa_0 + 1 - q\theta) = a_0 + 1 - \theta + (q-1)\left(1 - (q+1)(\theta - a_0)\right)$$

(the last equality can be easily checked). The assumption $q < a_1$ gives $q + 1 \leq a_1$. Taking advantage of the trivial estimate $\theta - a_0 \leq \frac{1}{a_1}$, we get $1 - (q+1)(\theta - a_0) \geq 0$; hence

$$a_0 + 1 - \theta + (q-1)\left(1 - (q+1)(\theta - a_0)\right) \geq a_0 + 1 - \theta.$$

Since $a_0 + 1 \geq \lceil \theta \rceil$, we conclude that

$$q(p - q\theta) \geq 1 \cdot (\lceil \theta \rceil - 1 \cdot \theta),$$

i.e., every $\frac{p}{q} \neq \lceil \theta \rceil$ contradicts the condition (3.15) with the choice $p' = \lceil \theta \rceil$, $q' = 1$.

- If $q \geq a_1$, inequality (3.28) gives

$$q(p - q\theta) > q\left(qa_0 + \frac{q}{a_1} - q\theta\right) = a_1(a_0 a_1 + 1 - a_1\theta) + (q^2 - a_1^2)\left(\frac{1}{a_1} - (\theta - a_0)\right).$$

Using the assumption $q \geq a_1$ together with the trivial estimate $\theta - a_0 \leq \frac{1}{a_1}$, we get

$$q(p - q\theta) > a_1(a_0 a_1 + 1 - a_1\theta);$$

i.e., $\frac{p}{q}$ contradicts the condition (3.15) with the choice $p' = a_0 a_1 + 1$, $q' = a_1$.

To sum up, in both cases we found that $\frac{p}{q} > \frac{p_1}{q_1}$, $\frac{p}{q} \neq \lceil \theta \rceil$ cannot be a best approximation from above of the third kind to θ. □

4. Number of spectral gaps of lattice graphs

Now we can address our second main topic, the existence of graphs with the Bethe-Sommerfeld property. As indicated in the introduction, to this aim we shall revisit the model introduced in [7] and further discussed in [8, 9]. Let us first recall some needed notions. Consider a rectangular lattice graph in the plane with edges of lengths a and b – cf. Fig. 1. In addition, suppose that the graph Hamiltonian H is the Laplacian defined as a self-adjoint operator by imposing at each graph vertex v the δ coupling condition – that is, continuity together with the requirement $\sum_{j=1}^{4} \psi'(v) = \alpha\psi(v)$ –

with a parameter $\alpha \in \mathbb{R}$. According to [8], a number $k^2 > 0$ belongs to a gap if and only if $k > 0$ satisfies the gap condition, which reads

$$\tan\left(\frac{ka}{2} - \frac{\pi}{2}\left\lfloor\frac{ka}{\pi}\right\rfloor\right) + \tan\left(\frac{kb}{2} - \frac{\pi}{2}\left\lfloor\frac{kb}{\pi}\right\rfloor\right) < \frac{\alpha}{2k} \quad \text{for } \alpha > 0 \tag{4.1}$$

and

$$\cot\left(\frac{ka}{2} - \frac{\pi}{2}\left\lfloor\frac{ka}{\pi}\right\rfloor\right) + \cot\left(\frac{kb}{2} - \frac{\pi}{2}\left\lfloor\frac{kb}{\pi}\right\rfloor\right) < \frac{|\alpha|}{2k} \quad \text{for } \alpha < 0\,; \tag{4.2}$$

we neglect the case $\alpha = 0$ where the spectrum is trivial, $\sigma(H) = [0, \infty)$. Note that for $\alpha < 0$ the spectrum extends to the negative part of the real axis and may have a gap there. From the point of view of our present problem this is not that important, though, the reason is that if such a gap exists, it always extends to positive values of the energy – see Proposition 4.7 below and Figure 2 in [9] – hence it is sufficient to analyze solutions to the gap conditions (4.1) and (4.2) only. Since the sign of α plays role here, it is reasonable to discuss the two cases separately.

4.1. The case $\alpha > 0$

Let us first make the gap description more specific.

Proposition 4.1. *Let $\theta = \frac{a}{b}$. The following claims are valid:*

- *Every gap in the spectrum has the left (lower) endpoint equal to $k^2 = \left(\frac{m\pi}{a}\right)^2$ or $k^2 = \left(\frac{m\pi}{b}\right)^2$ for some $m \in \mathbb{N}$.*
- *A gap with the left endpoint at $k^2 = \left(\frac{m\pi}{a}\right)^2$ is present if and only if*

$$\frac{2m\pi}{a} \tan\left(\frac{\pi}{2}(m\theta^{-1} - \lfloor m\theta^{-1}\rfloor)\right) < \alpha. \tag{4.3}$$

- *A gap with the left endpoint at $k^2 = \left(\frac{m\pi}{b}\right)^2$ is present if and only if*

$$\frac{2m\pi}{b} \tan\left(\frac{\pi}{2}(m\theta - \lfloor m\theta\rfloor)\right) < \alpha. \tag{4.4}$$

Proof. The gap condition (4.1) is equivalent to $F(k) < \alpha$, where

$$F(k) = 2k\left(\tan\left(\frac{ka}{2} - \frac{\pi}{2}\left\lfloor\frac{ka}{\pi}\right\rfloor\right) + \tan\left(\frac{kb}{2} - \frac{\pi}{2}\left\lfloor\frac{kb}{\pi}\right\rfloor\right)\right).$$

Function $k \mapsto F(k)$ has discontinuities at points $k = \frac{m\pi}{a}$ and $k = \frac{m\pi}{b}$ for $m \in \mathbb{N}$. It is easy to check that $F(\cdot)$ is strictly increasing in each interval of continuity and has limits

$$\lim_{k \nearrow \frac{m\pi}{a}} F(k) = \lim_{k \nearrow \frac{m\pi}{b}} F(k) = +\infty$$

at the right endpoints of the continuity intervals. Hence there is at most one gap in each interval of continuity of $F(k)$, and moreover, all gaps are adjacent to points k^2 corresponding to k being left endpoints of those intervals. This proves the first part of the proposition.

Furthermore, a gap with the left endpoint equal to $k^2 = \left(\frac{m\pi}{a}\right)^2$ is present if and only if $\lim_{k \searrow \frac{m\pi}{a}} F(k) < \alpha$, and since

$$\lim_{k \searrow \frac{m\pi}{a}} F(k) = \frac{2m\pi}{a} \tan\left(\frac{\pi}{2}\left(m\frac{b}{a} - \left\lfloor m\frac{b}{a}\right\rfloor\right)\right),$$

we arrive at the gap conditions (4.3); the gap condition (4.4) is obtained similarly by considering $\lim_{k \searrow \frac{m\pi}{b}} F(k) < \alpha$. □

Corollary 4.2. *Let $\theta = \frac{a}{b}$. If*

$$\frac{2m\pi}{a} \tan\left(\frac{\pi}{2}(m\theta^{-1} - \lfloor m\theta^{-1}\rfloor)\right) \geq \alpha \quad \wedge \quad \frac{2m\pi}{b} \tan\left(\frac{\pi}{2}(m\theta - \lfloor m\theta\rfloor)\right) \geq \alpha \tag{4.5}$$

holds for all $m \in \mathbb{N}$, then there are no gaps in the spectrum.

Next we relate the number of gaps to values of the function $\upsilon(\theta)$ introduced above.

Proposition 4.3. *Let $\theta = \frac{a}{b}$. If*

$$\alpha < \pi^2 \cdot \min\left\{\frac{\upsilon(\theta)}{b}, \frac{\upsilon(\theta^{-1})}{a}\right\}, \tag{4.6}$$

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

Proof. The expression at the left-hand side of condition (4.4) satisfies

$$\frac{2m\pi}{b} \tan\left(\frac{\pi}{2}\left(\theta m - \lfloor\theta m\rfloor\right)\right) > \frac{2m\pi}{b} \cdot \frac{\pi}{2}\left(\theta m - \lfloor\theta m\rfloor\right) = \frac{m\pi^2}{b} \cdot \left(\theta m - \lfloor\theta m\rfloor\right).$$

At the same time, (3.6) implies that for every $c < \upsilon(\theta)$, the inequality

$$\theta m - \lfloor\theta m\rfloor \geq \frac{c}{m}$$

holds except possibly for finitely many values of m. Therefore, if $c < \upsilon(\theta)$, we have

$$\frac{2m\pi}{b} \tan\left(\frac{\pi}{2}\left(\theta m - \lfloor\theta m\rfloor\right)\right) > \frac{m\pi^2}{b} \cdot \frac{c}{m} = \frac{\pi^2}{b}\, c$$

for all m with at most finitely many exceptions. To sum up, if

$$(\exists c < \upsilon(\theta))\left(\alpha \leq \frac{\pi^2}{b}\, c\right), \tag{4.7}$$

the gap condition (4.4) is satisfied for at most finitely many values m only; note that condition (4.7) is equivalent to

$$\alpha < \frac{\pi^2}{b}\, \upsilon(\theta). \tag{4.8}$$

One can repeat the same considerations for the gap condition (4.3). We get

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

For every $c < \upsilon(\theta^{-1})$ we have in view of (3.6)

$$\theta^{-1}m - \lfloor \theta^{-1}m \rfloor \geq \frac{c}{m}$$

except possibly for finitely many values of m. Hence

$$\frac{2m\pi}{a} \tan\left(\frac{\pi}{2}\left(\theta^{-1}m - \lfloor \theta^{-1}m \rfloor\right)\right) > \frac{m\pi^2}{a} \cdot \frac{c}{m} = \frac{\pi^2}{a}\, c$$

holds for all m with possibly finitely many exceptions. To sum up, if

$$\left(\exists c < \upsilon(\theta^{-1})\right)\left(\alpha \leq \frac{\pi^2}{a}\, c\right), \tag{4.9}$$

then the gap condition (4.3) is satisfied for at most finitely many values m only, and we can again simplify (4.9) to the form

$$\alpha < \frac{\pi^2}{a}\, \upsilon(\theta^{-1})\,. \tag{4.10}$$

The assumption (4.6) guarantees the validity of both (4.8) and (4.10), and thus implies the finiteness of the total number of gaps with regard to Proposition 4.1. □

To see that the condition on the number of gaps stated in Proposition 4.3 is sharp, consider now the opposite situation.

Proposition 4.4. *Let $\theta = \frac{a}{b}$. For all α satisfying*

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

the spectrum has infinitely many gaps.

Proof. If $\min\left\{\frac{\upsilon(\theta)}{b}, \frac{\upsilon(\theta^{-1})}{a}\right\} = \frac{\upsilon(\theta)}{b}$, we set $c = \sqrt{\frac{b\cdot\alpha\cdot\upsilon(\theta)}{\pi^2}}$. Since $\alpha > \pi^2 \cdot \frac{\upsilon(\theta)}{b}$, we have $c > \upsilon(\theta)$. For such c and for any $\delta > 0$, equation (3.6) guarantees that

$$(\exists_\infty m \in \mathbb{N})\left(m\theta - \lfloor m\theta \rfloor < \frac{c}{m} < \frac{2}{\pi}\delta\right), \tag{4.11}$$

where the second inequality can be satisfied by taking values m large enough. Now we use the general fact

$$(\forall \xi > 1)(\exists \delta > 0)(\forall x \in (0,\delta))(\tan x < \xi x)\,. \tag{4.12}$$

Taking $\xi = \frac{c}{\upsilon(\theta)}$ and the corresponding δ, we use (4.11) to estimate the left-hand side of the gap condition (4.4) as follows:

$$\frac{2m\pi}{b} \tan\left(\frac{\pi}{2}(m\theta - \lfloor m\theta \rfloor)\right) < \frac{2m\pi}{b} \cdot \frac{c}{\upsilon(\theta)} \cdot \frac{\pi}{2}(m\theta - \lfloor m\theta \rfloor) = \frac{\pi^2 c^2}{b \cdot \upsilon(\theta)}\,. \tag{4.13}$$

Since $\frac{\pi^2 c^2}{b\cdot\upsilon(\theta)} = \alpha$, we have established the existence of infinitely many $m \in \mathbb{N}$ satisfying the gap condition (4.4). Consequently, the total number of spectral gaps is infinite due to Proposition 4.1.

If $\min\left\{\frac{\upsilon(\theta)}{b}, \frac{\upsilon(\theta^{-1})}{a}\right\} = \frac{\upsilon(\theta^{-1})}{a}$, we set $c = \sqrt{\frac{a\cdot\alpha\cdot\upsilon(\theta^{-1})}{\pi^2}}$ and proceed similarly as above. Using function $\upsilon(\theta^{-1})$, we establish the existence of infinitely many $m \in \mathbb{N}$ satisfying the gap condition (4.3). $\square$

As an immediate consequence of Propositions 4.1 and 4.3, we obtain a sufficient condition for the graph in question to have the Bethe–Sommerfeld property:

Theorem 4.5. *Let* $\theta = \frac{a}{b}$ *and*

$$\gamma := \min\left\{\inf_{m\in\mathbb{N}}\left\{\frac{2m\pi}{a}\tan\left(\frac{\pi}{2}(m\theta^{-1} - \lfloor m\theta^{-1}\rfloor)\right)\right\}, \inf_{m\in\mathbb{N}}\left\{\frac{2m\pi}{b}\tan\left(\frac{\pi}{2}(m\theta - \lfloor m\theta\rfloor)\right)\right\}\right\}. \tag{4.14}$$

If the coupling constant α *satifies*

$$\gamma < \alpha < \pi^2\cdot\min\left\{\frac{\upsilon(\theta)}{b}, \frac{\upsilon(\theta^{-1})}{a}\right\}, \tag{4.15}$$

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

Remark 4.6. Using equation (3.8), we can estimate the quantity $\min\left\{\frac{\upsilon(\theta)}{b}, \frac{\upsilon(\theta^{-1})}{a}\right\}$ in terms of the Markov constant of θ; namely:

$$\frac{\mu(\theta)}{\max\{a,b\}} \le \min\left\{\frac{\upsilon(\theta)}{b}, \frac{\upsilon(\theta^{-1})}{a}\right\} \le \frac{\mu(\theta)}{\min\{a,b\}}.$$

Propositions 4.3, 4.4 and Theorem 4.5 can be thus formulated in a weaker way as follows:

- If $\alpha > \frac{\pi^2\mu(\theta)}{\min\{a,b\}}$, the spectrum has infinitely many gaps.
- If $\alpha < \frac{\pi^2\mu(\theta)}{\max\{a,b\}}$, the spectrum has at most finitely many gaps.
- If $\gamma < \alpha < \frac{\pi^2\mu(\theta)}{\max\{a,b\}}$ for γ given by (4.14), there is a nonzero and finite number of gaps in the spectrum.

4.2. The case $\alpha < 0$

In this situation, the gap condition is of the form $G(k) < |\alpha|$, where

$$G(k) := 2k\left(\cot\left(\frac{ka}{2} - \frac{\pi}{2}\left\lfloor\frac{ka}{\pi}\right\rfloor\right) + \cot\left(\frac{kb}{2} - \frac{\pi}{2}\left\lfloor\frac{kb}{\pi}\right\rfloor\right)\right).$$

Using the identity

$$\cot\left(\frac{\pi}{2}(x - \lfloor x\rfloor)\right) = \tan\left(\frac{\pi}{2}(\lceil x\rceil - x)\right) \qquad \text{for all } x \notin \mathbb{Z},$$

we can rewrite $G(k)$ for all k except for the points of discontinuity in the form

$$G(k) = 2k\left(\tan\left(\frac{\pi}{2}\left(\left\lceil\frac{ka}{\pi}\right\rceil - \frac{ka}{\pi}\right)\right) + \tan\left(\frac{\pi}{2}\left(\left\lceil\frac{kb}{\pi}\right\rceil - \frac{kb}{\pi}\right)\right)\right),$$

which allows to write the condition in the form more similar to the case $\alpha > 0$, the main difference being the swap between the floor and ceiling functions in the arguments. Since the reasoning is completely analogous to the previous case, we limit ourselves to presenting the results omitting the proofs.

Proposition 4.7. *Let $\alpha < 0$ and $\theta = \frac{a}{b}$, then the following claims are valid:*

- *Every gap in the spectrum has the right (upper) endpoint equal to $k^2 = \left(\frac{m\pi}{a}\right)^2$ or $k^2 = \left(\frac{m\pi}{b}\right)^2$ for some $m \in \mathbb{N}$.*
- *A gap with the right endpoint at $k^2 = \left(\frac{m\pi}{a}\right)^2$ is present if and only if*
$$\frac{2m\pi}{a} \tan\left(\frac{\pi}{2}\left(\lceil m\theta^{-1}\rceil - m\theta^{-1}\right)\right) < |\alpha|. \tag{4.16}$$
- *A gap with the right endpoint at $k^2 = \left(\frac{m\pi}{b}\right)^2$ is present if and only if*
$$\frac{2m\pi}{b} \tan\left(\frac{\pi}{2}\left(\lceil m\theta\rceil - m\theta\right)\right) < |\alpha|. \tag{4.17}$$
- *In particular, if*
$$\frac{2m\pi}{a} \tan\left(\frac{\pi}{2}\left(\lceil m\theta^{-1}\rceil - m\theta^{-1}\right)\right) \geq |\alpha| \quad\wedge\quad \frac{2m\pi}{b} \tan\left(\frac{\pi}{2}\left(\lceil m\theta\rceil - m\theta\right)\right) \geq |\alpha| \tag{4.18}$$
for all $m \in \mathbb{N}$, then there are no gaps in the spectrum.

Proposition 4.8. *Let $\alpha < 0$ and $\theta = \frac{a}{b}$. If*
$$|\alpha| < \pi^2 \cdot \min\left\{\frac{\upsilon(\theta^{-1})}{b}, \frac{\upsilon(\theta)}{a}\right\},$$
the number of gaps in the spectrum is at most finite. On the other hand, for $|\alpha|$ greater than the right-hand side of the above inequality, there are infinitely many spectral gaps.

Note that in case of attractive potential $\alpha < 0$, the bound on $|\alpha|$ in Proposition 4.8 (i.e., $\min\{\upsilon(\theta^{-1})/b, \upsilon(\theta)/a\}$) is different from the bound in case of a repulsive potential, which is equal to $\min\{\upsilon(\theta^{-1})/a, \upsilon(\theta)/b\}$ (cf. Propositions 4.3 and 4.4). However, the estimates of the bounds in terms of the Markov constant for $\alpha < 0$ are the same as for $\alpha > 0$, cf. Remark 4.6, namely
$$\frac{\mu(\theta)}{\max\{a,b\}} \leq \min\left\{\frac{\upsilon(\theta^{-1})}{b}, \frac{\upsilon(\theta)}{a}\right\} \leq \frac{\mu(\theta)}{\min\{a,b\}}\,. \tag{4.19}$$

Theorem 4.9. *Let $\alpha < 0$, $\theta = \frac{a}{b}$, and*
$$\gamma := \min\left\{\inf_{m\in\mathbb{N}}\left\{\frac{2m\pi}{a} \tan\left(\frac{\pi}{2}\left(\lceil m\theta^{-1}\rceil - m\theta^{-1}\right)\right)\right\}, \inf_{m\in\mathbb{N}}\left\{\frac{2m\pi}{b} \tan\left(\frac{\pi}{2}\left(\lceil m\theta\rceil - m\theta\right)\right)\right\}\right\}.$$
If the coupling constant α satisfies
$$\gamma < |\alpha| < \pi^2 \cdot \min\left\{\frac{\upsilon(\theta^{-1})}{b}, \frac{\upsilon(\theta)}{a}\right\}, \tag{4.20}$$
there is a nonzero and finite number of gaps in the spectrum.

5. Example: golden-mean lattice

The sufficient conditions in Theorems 4.5 and 4.9 do not yet solve our problem because we do not know whether these statements are not empty. Let us now examine a particular case discussed already in [8, 9] in which we choose the golden mean, $\phi = \frac{\sqrt{5}+1}{2}$, for the rectangle side ratio θ.

For proving Theorem 5.1 below, we will employ the convergents of ϕ. The continued fraction representation of ϕ is $[1; 1, 1, 1, \ldots]$, and therefore the convergents are of the form

$$\frac{F_{n+1}}{F_n} = \frac{p_{n-1}}{q_{n-1}}\,, \tag{5.1}$$

where F_n are Fibonacci numbers; recall that

$$F_n = \frac{\phi^n - (-\phi)^{-n}}{\sqrt{5}}\,.$$

We will also need the values of $\upsilon(\phi)$ and $\upsilon(\phi^{-1})$. It is possible to find them using formula (3.16) and Proposition 3.5, but we instead take advantage of known results on the Markov constant. Since $\phi^{-1} = \phi - 1$, we have, due to (3.6),

$$\begin{aligned} \upsilon(\phi^{-1}) = &\ \inf\{c > 0 \mid (\exists_\infty m \in \mathbb{N})\,(m(m(\phi-1) - \lfloor m(\phi-1)\rfloor) < c)\} \\ = &\ \inf\{c > 0 \mid (\exists_\infty m \in \mathbb{N})\,(m(m\phi - \lfloor m\phi\rfloor) < c)\} = \upsilon(\phi)\,. \end{aligned}$$

Consequently, equation (3.8) implies $\upsilon(\phi) = \upsilon(\phi^{-1}) = \mu(\phi)$, where the value of $\mu(\phi)$ is known to be equal to $1/\sqrt{5}$, cf. [3, Chapter I, Thm. V]. To sum up,

$$\upsilon(\phi) = \upsilon(\phi^{-1}) = \frac{1}{\sqrt{5}}\,. \tag{5.2}$$

Theorem 5.1. *Let* $\frac{a}{b} = \phi = \frac{\sqrt{5}+1}{2}$, *then the following claims are valid:*

(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 spectrum.

(iii) If

$$-\frac{\pi^2}{\sqrt{5}a} < \alpha < -\frac{2\pi}{a}\tan\left(\frac{3-\sqrt{5}}{4}\pi\right), \tag{5.3}$$

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

Proof. (i) With regard to (5.2), the existence of an infinite number of spectral gaps for $\alpha > \frac{\pi^2}{\sqrt{5}a}$ follows immediately from Proposition 4.4, for $\alpha < -\frac{\pi^2}{\sqrt{5}a}$ we similarly employ Proposition 4.8.

The case $\alpha = -\frac{\pi^2}{\sqrt{5}a}$. We shall demonstrate that there are infinitely many $m \in \mathbb{N}$ such that the gap condition (4.16) which reads

$$\frac{2m\pi}{a} \tan\left(\frac{\pi}{2}\left(\lceil m\phi^{-1}\rceil - m\phi^{-1}\right)\right) < \frac{\pi^2}{\sqrt{5}a}$$

is satisfied. Choosing $m = F_n$ for even n and using the identity $\phi^{-1} = \phi - 1$, we can rewrite the gap condition in the form

$$F_n \tan\left(\frac{\pi}{2}\left(\lceil F_n\phi\rceil - F_n\phi\right)\right) < \frac{\pi}{2\sqrt{5}}. \tag{5.4}$$

For even n, we have

$$\begin{aligned} F_n\phi &= \frac{\phi^n - \phi^{-n}}{\sqrt{5}}\phi = \frac{\phi^{n+1} - \phi^{-n+1}}{\sqrt{5}} = \frac{\phi^{n+1} + \phi^{-n-1}}{\sqrt{5}} + \frac{-\phi^{-n-1} - \phi^{-n+1}}{\sqrt{5}} \\ &= \frac{\phi^{n+1} - (-\phi)^{-(n+1)}}{\sqrt{5}} - \frac{\phi + \phi^{-1}}{\sqrt{5}}\phi^{-n} = F_{n+1} - \phi^{-n} \in (F_{n+1} - 1, F_{n+1}), \end{aligned}$$

which means that

$$\lceil F_n\phi\rceil - F_n\phi = F_{n+1} - F_n\phi = \phi^{-n} \qquad \text{for even } n. \tag{5.5}$$

Hence we get, using the Taylor series of $\tan(x)$,

$$\begin{aligned} F_n \tan\left(\frac{\pi}{2}\left(\lceil F_n\phi\rceil - F_n\phi\right)\right) &= \frac{\phi^n - \phi^{-n}}{\sqrt{5}} \tan\left(\frac{\pi}{2}\phi^{-n}\right) \\ &= \frac{1}{\sqrt{5}}\left(\phi^n - \phi^{-n}\right)\left(\frac{\pi}{2}\phi^{-n} + \frac{1}{3}\left(\frac{\pi}{2}\right)^3\phi^{-3n} + \frac{2}{15}\left(\frac{\pi}{2}\right)^5\phi^{-5n} + \cdots\right) \\ &= \frac{\pi}{2\sqrt{5}}\left(1 - \left(1 - \frac{1}{3}\cdot\frac{\pi^2}{4}\right)\phi^{-2n} - \left(\frac{1}{3}\cdot\frac{\pi^2}{4} - \frac{2}{15}\cdot\frac{\pi^4}{16}\right)\phi^{-4n}\cdots\right). \end{aligned}$$

That is, taking n even leads to the expansion

$$F_n \tan\left(\frac{\pi}{2}\left(\lceil F_n\phi\rceil - F_n\phi\right)\right) = \frac{\pi}{2\sqrt{5}}\left(1 + \left(\frac{\pi^2}{12} - 1\right)\phi^{-2n} + \mathcal{O}(\phi^{-4n})\right). \tag{5.6}$$

Since the coefficient $\frac{\pi^2}{12} - 1$ at ϕ^{-2n} in (5.6) is negative, condition (5.4) is satisfied for all sufficiently large even n. The gap condition (4.16) with $\alpha = -\frac{\pi^2}{\sqrt{5}a}$ is thus satisfied for infinitely many numbers $m = F_n$ with n being even; then Proposition 4.7 implies the existence of infinitely many gaps.

(ii) We divide the argument into several parts referring to different values of α: *The case* $\alpha \in (0, \frac{\pi^2}{\sqrt{5}a}]$. Using the identity $\phi^{-1} = \phi - 1$, we obtain

$$\begin{aligned} \frac{2m\pi}{a} \tan\left(\frac{\pi}{2}(m\phi^{-1} - \lfloor m\phi^{-1}\rfloor)\right) &\geq \frac{2m\pi}{a}\left(\frac{\pi}{2}(m\phi^{-1} - \lfloor m\phi^{-1}\rfloor)\right) \\ &= \frac{\pi^2}{a}m\left(m(\phi - 1) - \lfloor m(\phi - 1)\rfloor\right) = \frac{\pi^2}{a}m\left(m\phi - \lfloor m\phi\rfloor\right), \end{aligned}$$

and similarly,

$$\frac{2m\pi}{b} \tan\left(\frac{\pi}{2}(m\phi - \lfloor m\phi\rfloor)\right) \geq \frac{2m\pi}{b}\left(\frac{\pi}{2}(m\phi - \lfloor m\phi\rfloor)\right) = \frac{\pi^2}{b}m\left(m\phi - \lfloor m\phi\rfloor\right). \tag{5.7}$$

In order to disprove the existence of gaps using Corollary 4.2, we shall demonstrate that

$$\frac{\pi^2}{a} m\,(m\phi - \lfloor m\phi \rfloor) \geq \frac{\pi^2}{\sqrt{5}a} \quad \wedge \quad \frac{\pi^2}{b} m\,(m\phi - \lfloor m\phi \rfloor) \geq \frac{\pi^2}{\sqrt{5}a} \quad \text{for all } \ m \in \mathbb{N}\,. \tag{5.8}$$

With regard to the assumption $a > b$, condition (5.8) is equivalent to

$$m\,(m\phi - \lfloor m\phi \rfloor) \geq \frac{1}{\sqrt{5}} \quad \text{for all } \ m \in \mathbb{N}\,, \tag{5.9}$$

which we are about to prove. We will verify that $m\,(m\phi - p) \geq \frac{1}{\sqrt{5}}$ for any $m \in \mathbb{N}$ and $p \in \mathbb{N}_0$. In view of Definition 3.3, it suffices to consider pairs (p, m) such that $\frac{p}{m}$ is a best approximation from below of the third kind to ϕ. Such approximations are convergents of ϕ, cf. Proposition 3.5. Convergents of ϕ that are smaller than ϕ are known to be of the form $\frac{F_{n+1}}{F_n}$, where n is odd. We obtain

$$\begin{aligned} F_n\,(F_n\phi - F_{n+1}) &= \frac{\phi^n + \phi^{-n}}{\sqrt{5}} \left(\frac{\phi^n + \phi^{-n}}{\sqrt{5}}\phi - \frac{\phi^{n+1} - \phi^{-(n+1)}}{\sqrt{5}} \right) \\ &= \frac{1}{5}(\phi + \phi^{-1})(1 + \phi^{-2n}) = \frac{1 + \phi^{-2n}}{\sqrt{5}} > \frac{1}{\sqrt{5}}\,, \end{aligned}$$

i.e., the inequality $m\,(m\phi - p) \geq \frac{1}{\sqrt{5}}$ holds true for each best approximation from below of the third kind to ϕ. Consequently, it holds true for all $\frac{p}{q} < \theta$, in particular, for $p/q = \lfloor m\phi \rfloor / m$. This proves condition (5.9), hence there are no spectral gaps for $\alpha \in (0, \frac{\pi^2}{\sqrt{5}a}]$.

The case $\alpha = 0$. Kirchhoff couplings obviously generate no gaps‡, see also [9].

The case $\alpha \in [-\frac{2\pi}{a} \tan(\frac{3-\sqrt{5}}{4}\pi), 0)$. We are going to show that for all $m \in \mathbb{N}$, condition (4.18) holds true; then the claim would follow from Proposition 4.7. If $m = 1$, we have

$$\frac{2 \cdot 1 \cdot \pi}{a} \tan\left(\frac{\pi}{2} \left(\lceil 1 \cdot \phi^{-1} \rceil - 1 \cdot \phi^{-1} \right) \right) = \frac{2\pi}{a} \tan\left(\frac{\pi}{2} \cdot \frac{3 - \sqrt{5}}{2} \right) \geq |\alpha|$$

and

$$\frac{2 \cdot 1 \cdot \pi}{b} \tan\left(\frac{\pi}{2} \left(\lceil 1 \cdot \phi \rceil - 1 \cdot \phi \right) \right) = \frac{2\pi}{b} \tan\left(\frac{\pi}{2} \cdot \frac{3 - \sqrt{5}}{2} \right) \geq |\alpha|\,.$$

If $m \geq 2$, we use the identity $\phi^{-1} = \phi - 1$ to get

$$\begin{aligned} \frac{2m\pi}{a} \tan\left(\frac{\pi}{2} \left(\lceil m\phi^{-1} \rceil - m\phi^{-1} \right) \right) &= \frac{2m\pi}{a} \tan\left(\frac{\pi}{2} \left(\lceil m\phi \rceil - m\phi \right) \right) \\ &> \frac{2m\pi}{a} \left(\frac{\pi}{2} \left(\lceil m\phi \rceil - m\phi \right) \right) = \frac{\pi^2}{a} m \left(\lceil m\phi \rceil - m\phi \right), \end{aligned}$$

and

$$\frac{2m\pi}{b} \tan\left(\frac{\pi}{2} \left(\lceil m\phi \rceil - m\phi \right) \right) > \frac{\pi^2}{b} m \left(\lceil m\phi \rceil - m\phi \right)\,.$$

‡ Note that this also means that Proposition 2.6 has no implications for the present case, because Kirchhoff condition is scale-invariant and associated with the δ-coupling of the considered model.

According to condition (4.18), we have to check that

$$\min\left\{\frac{\pi^2}{a}m\left(\lceil m\phi\rceil - m\phi\right)\,,\ \frac{\pi^2}{b}m\left(\lceil m\phi\rceil - m\phi\right)\right\} \geq \frac{2\pi}{a}\tan\left(\frac{3-\sqrt{5}}{4}\pi\right)$$

holds for all $m \geq 2$, which is equivalent, due to $a > b$, to

$$m\left(\lceil m\phi\rceil - m\phi\right) \geq \frac{2}{\pi}\tan\left(\frac{3-\sqrt{5}}{4}\pi\right) \approx 0.4355 \quad \text{for all } \ m \geq 2. \tag{5.10}$$

Again, in view of Definition 3.3, it is sufficient to verify that $m\,(p - m\phi) \geq \frac{2}{\pi}\tan\left(\frac{3-\sqrt{5}}{4}\pi\right)$ holds for $\frac{p}{m}$ (with $m \geq 2$) being best approximations from above of the third kind to ϕ. According to Proposition 3.6, such approximations are convergents of ϕ, i.e., we have to consider $\frac{p}{q}$ taking the form $\frac{F_{n+1}}{F_n}$, where n is even. For this choice we obtain

$$\begin{aligned} F_n\left(F_{n+1} - F_n\phi\right) &= \frac{\phi^n - \phi^{-n}}{\sqrt{5}}\left(\frac{\phi^{n+1} + \phi^{-(n+1)}}{\sqrt{5}} - \frac{\phi^n - \phi^{-n}}{\sqrt{5}}\phi\right) \\ &= \frac{1}{5}(\phi + \phi^{-1})(1 - \phi^{-2n}) = \frac{1 - \phi^{-2n}}{\sqrt{5}}\,. \end{aligned}$$

Moreover, we may assume $n \geq 4$, because $F_4 = 3$ is the smallest Fibonacci number F_n obeying our conditions (having an even index n and satisfying $m = F_n \geq 2$). Hence

$$F_n\left(F_{n+1} - F_n\phi\right) \geq \frac{1 - \phi^{-8}}{\sqrt{5}}\,,$$

and consequently,

$$m\,(p - m\phi) \geq \frac{1 - \phi^{-8}}{\sqrt{5}} \approx 0.4377$$

for all $\frac{p}{m} > \phi$; in particular, for $p = \lceil m\phi\rceil$. This verifies condition (5.10), hence there are no gaps in the spectrum.

(iii) It remains to deal with the case when $-\frac{\pi^2}{\sqrt{5}a} < \alpha < -\frac{2\pi}{a}\tan\left(\frac{3-\sqrt{5}}{4}\pi\right)$. The claim follows from Theorem 4.9 in combination with equation (5.2) and the estimate

$$\begin{aligned} &\inf_{m\in\mathbb{N}}\left\{\frac{2m\pi}{a}\tan\left(\frac{\pi}{2}\left(\lceil m\phi^{-1}\rceil - m\phi^{-1}\right)\right)\right\} \leq \frac{2\cdot 1\cdot \pi}{a}\tan\left(\frac{\pi}{2}\left(\lceil 1\cdot\phi^{-1}\rceil - 1\cdot\phi^{-1}\right)\right) \\ &= \frac{2\pi}{a}\tan\left(\frac{\pi}{2}\cdot\frac{3-\sqrt{5}}{2}\right). \end{aligned}$$

This concludes the proof of the theorem. □

In particular, the claim (iii) of the theorem provides and affirmative answer to the question we have posed in the introduction.

Corollary 5.2. *Theorem 1.2 is valid.*

Remark 5.3. Note that a finite nonzero number of gaps in the spectrum 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 the numerical observation made in [9]. In addition, the window in which the golden-mean lattice has the Bethe–Sommerfeld property is narrow, roughly can be characterized as $4.298 \lesssim -\alpha a \lesssim 4.414$.

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

Theorem 5.4. *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*

$$-\frac{2\pi\left(\phi^{2(N+1)}-\phi^{-2(N+1)}\right)}{\sqrt{5}a}\tan\left(\frac{\pi}{2}\phi^{-2(N+1)}\right) \leq \alpha < -\frac{2\pi\left(\phi^{2N}-\phi^{-2N}\right)}{\sqrt{5}a}\tan\left(\frac{\pi}{2}\phi^{-2N}\right). \quad (5.11)$$

Proof. The bounds on α can be concisely written as $-A_{N+1} \leq \alpha < -A_N$, where

$$A_j := \frac{2\pi\left(\phi^{2j}-\phi^{-2j}\right)}{\sqrt{5}}\tan\left(\frac{\pi}{2}\phi^{-2j}\right).$$

One can easily check that $\{A_j\}_{j=1}^{\infty}$ is an increasing sequence with the property

$$A_1 = \frac{2\pi\left(\phi^{2}-\phi^{-2}\right)}{\sqrt{5}}\tan\left(\frac{\pi}{2}\phi^{-2}\right) = 2\pi\tan\left(\frac{3-\sqrt{5}}{4}\pi\right)$$

and

$$A_j < \frac{\pi^2}{\sqrt{5}} \quad \text{for all } \ j \in \mathbb{N}. \quad (5.12)$$

Let us examine validity of the conditions (4.16) and (4.17) for $m \in \mathbb{N}$. Using the identity $\phi^{-1} = \phi - 1$, we can rewrite them in the form

$$\frac{2m\pi}{a}\tan\left(\frac{\pi}{2}\left(\lceil m\phi\rceil - m\phi\right)\right) < |\alpha| \quad (5.13)$$

and

$$\frac{2m\pi}{b}\tan\left(\frac{\pi}{2}\left(\lceil m\phi\rceil - m\phi\right)\right) < |\alpha|, \quad (5.14)$$

respectively.

We start with the situation where $m = F_n$ for an even n. In this case we have $\lceil F_n\phi\rceil - F_n\phi = \phi^{-n}$, cf. (5.5). The gap condition (5.13) for $m = F_n$ with n even thus acquires the form

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

in other words, $\frac{1}{a}A_{\frac{n}{2}} < |\alpha|$. Since $|\alpha| \in [\frac{A_N}{a}, \frac{A_{N+1}}{a})$ in view of the assumptions (5.11), the gap condition (5.13) is obviously satisfied with $m = F_n$ for all even values $n = 2, 4, \ldots, 2N$, and violated for even values $n \geq 2(N+1)$. Similarly, the gap condition (5.14) acquires the form

$$\frac{1}{b}A_{\frac{n}{2}} < |\alpha|.$$

Since

$$\frac{1}{b}A_{\frac{n}{2}} = \frac{\phi}{a}A_{\frac{n}{2}} \geq \frac{\phi}{a}A_1 = \phi\frac{2\pi}{a}\tan\left(\frac{3-\sqrt{5}}{4}\pi\right) \approx \frac{6.955}{a}$$

and

$$|\alpha| \leq \frac{\pi^2}{\sqrt{5}a} \approx \frac{4.414}{a}\,,$$

we have $\frac{1}{b}A_{\frac{n}{2}} \not< |\alpha|$. Consequently, the gap condition (5.14) cannot be satisfied for the special choice $m = F_n$ with n even.

Let us proceed to the situation when m is different from the values F_n with even indices n. In this case we will show that none of the gap conditions (5.13) and (5.14) is satisfied. First, we estimate an expression appearing on the left-hand side of conditions (5.13) and (5.14) as follows:

$$2\pi m\tan\left(\frac{\pi}{2}\left(\lceil m\phi\rceil - m\phi\right)\right) \geq 2\pi m\frac{\pi}{2}\left(\lceil m\phi\rceil - m\phi\right) = \pi^2 m\left(\lceil m\phi\rceil - m\phi\right)\,.$$

The bounds (5.11) together with the estimate (5.12) imply that $|\alpha| < \frac{\pi^2}{\sqrt{5}a}$. Therefore, conditions (5.13) and (5.14) can be disproved for a given m by showing that

$$\frac{\pi^2}{a}m\left(\lceil m\phi\rceil - m\phi\right) \geq \frac{\pi^2}{\sqrt{5}a} \quad \wedge \quad \frac{\pi^2}{b}m\left(\lceil m\phi\rceil - m\phi\right) \geq \frac{\pi^2}{\sqrt{5}a}\,. \tag{5.15}$$

Since $a > b$ holds by assumption, condition (5.15) is equivalent to

$$m\left(\lceil m\phi\rceil - m\phi\right) \geq \frac{1}{\sqrt{5}}\,, \tag{5.16}$$

which we are now about to prove. We distinguish the following three possibilities:

(i) $\frac{\lceil m\phi\rceil}{m}$ lies between two convergents greater than θ, that is, $\frac{\lceil m\phi\rceil}{m} \in \left(\frac{F_{n+2}}{F_{n+1}}, \frac{F_n}{F_{n-1}}\right)$ for a certain odd n;

(ii) $\frac{\lceil m\phi\rceil}{m}$ lies above the greatest convergent $\frac{F_3}{F_2} = \frac{2}{1}$;

(iii) $m = r\cdot F_n$ and $\lceil m\phi\rceil = r\cdot F_{n+1}$ holds for a certain $r \geq 2$ and even $n \in \mathbb{N}$.

In case (i) we use Lemma 3.4 to obtain the estimate

$$m\left(\lceil m\phi\rceil - m\phi\right) > \frac{1}{a_n} = 1\,,$$

which means that (5.16) holds true. Case (ii) is actually impossible. Indeed, one can easily check that $\frac{\lceil m\phi\rceil}{m} \leq 2$ for all $m \in \mathbb{N}$. Finally, in case (iii) we get

$$m\left(\lceil m\phi\rceil - m\phi\right) = r^2\cdot F_n(F_{n+1} - F_n\phi) = r^2\cdot\frac{1-\phi^{-2n}}{\sqrt{5}}\,.$$

Since $r \geq 2$ and $n \in \mathbb{N}$ is even, we have

$$m(\lceil m\phi\rceil - m\phi) \geq 4\cdot\frac{1-\phi^{-4}}{\sqrt{5}} \approx \frac{3.42}{\sqrt{5}}\,,$$

and therefore (5.16) holds true. Consequently, the gap conditions (5.13) and (5.14) cannot be satisfied in any of the cases (i)–(iii).

To sum up, the assumption (5.11) allows the gap condition (5.13) to be satisfied for $m = F_n$ with $n = 2, 4, 6, \ldots, 2N$, while the gap condition (5.14) is never satisfied. This implies the existence of exactly N gaps in view of Proposition 4.7. □

6. Concluding remarks

As we have seen in the example discussed in Section 5, the Bethe–Sommerfeld property for the special case of golden-mean ratio required an attractive δ coupling. One may ask whether the Bethe–Sommerfeld behaviour is possible for some other ratios, and whether it can occur for repulsive couplings. In this section we give an affirmative answer to both these questions. First, we present an example of an edge ratio θ for which the Bethe–Sommerfeld property is valid within a certain range of α for both signs of α. Then we introduce an explicit method to construct ratios θ for which the Bethe–Sommerfeld property of the graph is guaranteed.

Let $\theta = \frac{a}{b}$. Without loss of generality, we may assume $\theta < 1$, i.e., $a < b$. If $\alpha > 0$, then Theorem 4.5 and Remark 4.6 imply that the rectangular-lattice Hamiltonian has a nonzero and finite number of gaps in its spectrum whenever there exists an $m_+ \in \mathbb{N}$ such that

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

Similarly, if $\alpha < 0$, Theorem 4.9 together with the estimate (4.19) implies that the Hamiltonian has a nonzero and finite number of gaps in the spectrum whenever there exists an $m_- \in \mathbb{N}$ such that

$$\frac{2m_+\pi}{b}\tan\left(\frac{\pi}{2}(\lceil m_-\theta \rceil - m_-\theta)\right) < |\alpha| < \frac{\pi^2\mu(\theta)}{b}.$$

Therefore, the Hamiltonian has a nonzero and finite number of gaps in the spectrum for some repulsive and attractive potentials whenever conditions (6.1) and (6.2) below are satisfied, respectively:

$$(\exists m_+ \in \mathbb{N}) \left(\frac{2m_+}{\pi}\tan\left(\frac{\pi}{2}(m_+\theta - \lfloor m_+\theta \rfloor)\right) < \mu(\theta)\right), \tag{6.1}$$

$$(\exists m_- \in \mathbb{N}) \left(\frac{2m_-}{\pi}\tan\left(\frac{\pi}{2}(\lceil m_-\theta \rceil - m_-\theta)\right) < \mu(\theta)\right). \tag{6.2}$$

As the following Theorem explicitly shows, there exists a θ such that both conditions (6.1) and (6.2) are satisfied at the same time.

Theorem 6.1. *Let the edge ratio be*

$$\theta = \frac{2t^3 - 2t^2 - 1 + \sqrt{5}}{2(t^4 - t^3 + t^2 - t + 1)} \quad \text{for } t \in \mathbb{N},\ t \geq 3; \tag{6.3}$$

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

Proof. The number θ defined in (6.3) can be written as $\theta = \frac{t\phi+1}{(t^2+1)\phi+t}$ for $\phi = \frac{1+\sqrt{5}}{2}$ being the golden mean. Since θ is equivalent to ϕ, cf. (3.2), the Markov constant of θ is $\mu(\theta) = \mu(\phi) = \frac{1}{\sqrt{5}} \approx 0.4472$.

It is easy to check that conditions (6.1) and (6.2) are satisfied for the choice $m_+ = 1$ and $m_- = t$ with $t \geq 3$, respectively. Indeed,

$$\frac{2\cdot 1}{\pi}\tan\left(\frac{\pi}{2}(1\cdot\theta - \lfloor 1\cdot\theta\rfloor)\right) = \frac{2}{\pi}\tan\left(\frac{\pi}{2}\cdot\frac{2t^3-2t^2-1+\sqrt{5}}{2(t^4-t^3+t^2-t+1)}\right)$$

is a decreasing function of t that has an approximate value $0.3310 < \mu(\theta)$ at $t = 3$. Similarly, for $m_- = t$, we get

$$\frac{2t}{\pi}\tan\left(\frac{\pi}{2}(\lceil t\theta\rceil - t\theta)\right) = \frac{2t}{\pi}\tan\left(\frac{\pi}{2}\cdot\frac{2t^2-t-t\sqrt{5}+2}{2(t^4-t^3+t^2-t+1)}\right),$$

which is again a decreasing function of t being approximately equal to $0.2546 < \mu(\theta)$ at the point $t = 3$. □

To conclude the paper, we present a general method to construct ratios θ that give rise to graphs with the Bethe–Sommerfeld property. We start from any badly approximable irrational number $\beta \in (0,1)$ with a continued-fraction representation

$$\beta = [0; c_1, c_2, c_3, \ldots];$$

recall that β is badly approximable if and only if the terms $c_1, c_2, c_3, \ldots$ are bounded. Then we define numbers ρ, ς and τ with continued-fraction representations

$$\rho = [0; t, c_1, c_2, c_3, \ldots]; \tag{6.4}$$

$$\varsigma = [0; 1, t, c_1, c_2, c_3, \ldots]; \tag{6.5}$$

$$\tau = [0; t, t, c_1, c_2, c_3, \ldots] \tag{6.6}$$

for $t \in \mathbb{N}$ being a parameter to be specified. Since the numbers ρ, ς, τ are equivalent to β, cf. (3.3), we have

$$\mu(\rho) = \mu(\varsigma) = \mu(\tau) = \mu(\beta),$$

where $\mu(\beta) > 0$, because β is badly approximable. Now we examine conditions (6.1) and (6.2). At first we prove that ρ and τ with a large enough parameter t satisfy condition (6.1) for $m_+ = 1$. Indeed, since $\rho < 1/t$ and $\tau < 1/t$, we have

$$\frac{2\cdot 1}{\pi}\tan\left(\frac{\pi}{2}(1\cdot\rho - \lfloor 1\cdot\rho\rfloor)\right) = \frac{2}{\pi}\tan\left(\frac{\pi}{2}\rho\right) < \frac{2}{\pi}\tan\left(\frac{\pi}{2t}\right) \to 0 \quad \text{as } t\to\infty \tag{6.7}$$

and

$$\frac{2\cdot 1}{\pi}\tan\left(\frac{\pi}{2}(1\cdot\tau - \lfloor 1\cdot\tau\rfloor)\right) = \frac{2}{\pi}\tan\left(\frac{\pi}{2}\tau\right) < \frac{2}{\pi}\tan\left(\frac{\pi}{2t}\right) \to 0 \quad \text{as } t\to\infty. \tag{6.8}$$

Similarly we can show that the number ς for a large enough t satisfies condition (6.2) with $m_- = 1$. Since $1/(1+1/t) < \varsigma < 1$, we have $\lceil\varsigma\rceil = 1$ and $1-\varsigma < 1/t$; therefore,

$$\frac{2\cdot 1}{\pi}\tan\left(\frac{\pi}{2}(\lceil 1\cdot\varsigma\rceil - 1\cdot\varsigma)\right) = \frac{2}{\pi}\tan\left(\frac{\pi}{2}(1-\varsigma)\right) < \frac{2}{\pi}\tan\left(\frac{\pi}{2t}\right) \to 0 \text{ as } t\to\infty. \tag{6.9}$$

Finally we prove that τ with a large enough t obeys condition (6.2) with the choice $m_- = t$. Since $t/(t+1/t) < t\tau < 1$, we have $\lceil t\tau \rceil = 1$ and $1 - t\tau < 1/(t^2+1)$; hence

$$\frac{2t}{\pi}\tan\left(\frac{\pi}{2}(\lceil t\tau\rceil - t\tau)\right) = \frac{2t}{\pi}\tan\left(\frac{\pi}{2}(1-t\tau)\right) < \frac{2t}{\pi}\tan\frac{\pi}{2(t^2+1)} < \frac{2}{\pi}\tan\left(\frac{\pi}{2t}\right). \quad (6.10)$$

To sum up, we see from equations (6.7)–(6.10) that choosing t such that

$$\frac{2}{\pi}\tan\left(\frac{\pi}{2t}\right) < \mu(\beta) \quad (6.11)$$

guarantees the Bethe–Sommerfeld property of the graph as follows:

- 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.

Example 6.2. *Let β be a root of a quadratic irreducible polynomial over $\mathbb{Z}$ with discriminant D. For such β we have the estimate $\mu(\beta) \geq \frac{1}{\sqrt{D}}$, which follows from [17, Sect. I, Lem. 2E]. Consequently, with regard to (6.11), we can define the numbers ρ, ς, τ by (6.4)–(6.6) for any t such that $\frac{2}{\pi}\tan\frac{\pi}{2t} < \frac{1}{\sqrt{D}}$.*

The idea was applied to construct the number θ from Theorem 6.1. The continued-fraction representation of θ from equation (6.3) is $[0; t, t, 1, 1, 1, 1, \ldots]$, i.e., θ was obtained from $\beta = [0; 1, 1, 1, \ldots] = (\sqrt{5}-1)/2$ using scheme (6.6). Since $\mu(\beta) = 1/\sqrt{5}$ (because $\beta = \phi^{-1}$, see also Section 5 and (3.4)), condition (6.11) gives $t \geq 3$.

As a final remark, recall the observation made in the introduction, namely that the question of validity of Bethe–Sommerfeld property remains open for $\mathbb{Z}$-periodic graphs with the period cells linked by more than a single edge.

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