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Katedra fyziky
Obor: Matematická fyzika

Spektrum periodických kvantových grafů v závislosti na vrcholové vazbě

The spectrum of periodic quantum graphs in dependence of the vertex coupling

DIPLOMOVÁ PRÁCE

Vypracoval: Bc. Pavel Lokvenc
Vedoucí práce: Prof. RNDr. Pavel Exner, DrSc.
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ČESKÉ VYSOKÉ UČENÍ TECHNICKÉ V PRAZE
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ZADÁNÍ DIPLOMOVÉ PRÁCE

Student: Bc. Pavel Lokvenc

Studijní program: Aplikace přírodních věd

Obor: Matematická fyzika

Název práce: (česky) Spektrum periodických kvantových grafů v závislosti na vrcholové vazbě

Název práce: (anglicky) The spectrum of periodic quantum graphs in dependence of the vertex coupling

Pokyny pro vypracování:

Využívaje zkušeností z výzkumného úkolu, student vyšetří nejprve kvantové grafy tvaru periodické mřížky a vrcholovou vazbou, jež je interpolací mezi delta vazbou a vazbou neinvariantní vůči časové inversi, jak je zavedena v práci [4]. Cílem je nalezení spektra takových systémů, v prvé řadě zjištění, zda výsledky o počtu lakun z prací [2,3] přestávají platit v důsledku narušení časové invariance. Zbude-li čas, bude úkolem vyšetřit jiné periodické kvantové grafy, zejména s ohledem na výsledky práce [5].

Doporučená literatura:

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[5] G. Berkolaiko, Y. Latushkin, S. Sukhtaiev: Limits of quantum graph operators with shrinking edges, Advances in Mathematics 352 (2019), 632-669.

Jméno a pracoviště vedoucího diplomové práce:

Prof, RNDr. Pavel Exner, DrSc.

Ústav jaderé fyziky AV ČR, v.v.i.

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Doba platnosti zadání je dva roky od data zadání.

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vedoucí katedry

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V Praze dne 25.10.2019

Prohlášení

Prohlašuji, že jsem svoji diplomovou práci vypracoval samostatně a použil jsem pouze podklady (literaturu, projekty, SW atd.) uvedené v přiloženém seznamu.

Nemám závažný důvod proti použití tohoto školního díla ve smyslu § 60 Zákona č. 121/2000 Sb., o právu autorském, o právech souvisejících s právem autorským a o změně některých zákonů (autorský zákon).

V Praze dne ....

podpis

Poděkování

Rád bych poděkoval vedoucímu diplomové práce Prof. RNDr. Pavlovi Exnerovi, DrSc. za odborné vedení, vstřícnost při konzultacích a především za cenné rady, které mi vypracování práce velice usnadnily.

Bc. Pavel Lokvenc

Název práce:
Spektrum periodických kvantových grafů v závislosti na vrcholové vazbě

Autor: Bc. Pavel Lokvenc

Studijní program: Aplikace přírodních věd
Obor: Matematická fyzika
Druh práce: Diplomová práce

Vedoucí práce: Prof. RNDr. Pavel Exner, DrSc.
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Abstract: V této práci zkoumáme kvantový graf, který má tvar nekonečné periodické obdélníkové mřížky a je vybaven novou parametrickou množinou vrcholových vazeb. Tato množina tvoří interpolaci mezi časově invariantní δ-vazbou a nově zkoumanou časově neinvariantní vazbou. Cílem práce je určit vlastnosti spektra v závislosti na parametrech systému.

Klíčová slova: Kvantový graf, parametrická množina vrcholových vazeb, symetrie vazeb, obdelníková mřížka, spektrum.

Title:
The spectrum of periodic quantum graphs in dependence of the vertex coupling

Author: Bc. Pavel Lokvenc

Abstract: This thesis studies an infinite rectangular lattice quantum graph with a new parametric class of couplings. This couplings interpolates between time-reversal δ-coupling and a new time non-invariant coupling. The main aim of this thesis is to identify spectral properties in dependence on the parameters of the model.

Key words: Quantum graph, parametric class of vertex coupling, coupling symmetries, rectangular lattice, band-gap spectrum.

Contents

Introduction

Quantum graphs were first studied in the 1930s but they gained importance only in the last three decades. There are multiple reasons for it. Quantum graphs can be used as simple, yet not trivial, models for complicated structures appearing in many fields, such as chemistry, mathematics and engineering. For example, rapid development in fabrication techniques allows us to produce plenty of graph like structures of pure semiconductor material, for which quantum graphs represent a natural model. There are plenty of other applications worth mentioning, for instance, photonic crystals, free-electron theory, conjugated molecules, number theory, etc., more examples can be found in the monograph [1].

The article [6] which aimed at modeling of the anomalous Hall effect has been published in 2015. The authors of this article created an elegant mathematical model which described the motion of electrons in atomic orbitals using network of rings with the δ-coupling at their junctions. This model had a drawback, though, as electrons involved in the effect can appear only in orbitals with particular angular momentum. If we want to model this situation using quantum graph theory, we would have to assume that the electrons have a preferred direction of motion. How would such a time non-invariant quantum graph look like? It turns out that this property can be ensured by choosing a suitable vertex coupling. In the paper [3] a new kind of coupling was proposed which is not time-reversal, unlike other, more commonly used couplings, such as Kirchhoff's, δ-coupling or δ'-coupling. One of the aims of this thesis will be to examine this coupling on a simple graph having the form of infinite rectangular lattice shape and to identify spectral properties.

These properties can be compared with those of a rectangular lattice graph with δ-coupling at the vertices. This problem was treated in [2, 7] and we present a summary of the results without proofs. Note that these results will be important in our further research.

It is well known that the choice of vertex coupling has a significant impact on spectral properties; recall that any self-adjoint coupling may be given a reasonable physical meaning. From the point of view of applications, it is useful to have wide parametric class of vertex coupling, which allows us to tune quantum graph properties according to the situation. This motivates the main topic of this thesis, which is an investigation of a new parametric set of interactions introduced in [4] interpolating between δ-interaction and time non-invariant coupling introduced in [3]. It is known, that the spectrum of infinite periodic system has generically the band-gap character. The number of gaps in a rectangular lattice with a δ-coupling has an interesting property, namely that in case of incommensurate rectangle sides it may depend on the type of the irrationality: it may contain an infinite number of gaps, no gaps or, in some cases, finite number of gaps (see [7]). Our main goal is to study these spectral properties for the whole parametric class of couplings.

Let us take a look at the thesis' structure.

The first chapter is dedicated to the introduction of quantum graphs, including the basic concepts with which we will work with throughout the entire thesis. In this part, we summarize only the information necessary in the following research. We refer to the monograph [1] for more detailed information about the quantum graph concept.

The second chapter is devoted to properties of an infinite rectangular lattice with the indicated non-invariant coupling extending the result obtained in the paper [3] for the particular case of a square lattice. We derive here the condition that determines the spectrum. By analyzing this condition, we identify some properties of the spectrum. We also present numerical results of the spectrum at the end of this chapter.

The third chapter recapitulates the results of articles [2] and [7] about rectangular lattice quantum graph with δ-coupling at the vertices. These results will be needed in the final chapter.

The final chapter contain the main results of the thesis examining the rectangular lattice again, now with the new parametric family of couplings. We again derive the spectral condition and use it to find some properties of the spectrum in dependence on the parameters of the model.

Chapter 1

Introduction to Quantum Graphs

This chapter deals with basic notions of the theory of quantum graphs. We point out that most of definitions and theorems are taken from monograph [1].

1.1 Graphs

Definition 1.1. A **graph** Γ consists of a two parts:

1. Set of vertices $\mathcal{V} := \{v_i\}_{i\in I}$.

2. Set of edges $\mathcal{E} := \{e_j\}_{j\in J}$.

The sets I, J are finite or countably infinite. With the convention described below, the graph is fully determined by its **adjacency matrix** A_Γ. The elements of the adjacency matrix indicate if pairs of vertices are connected with an edge or not.

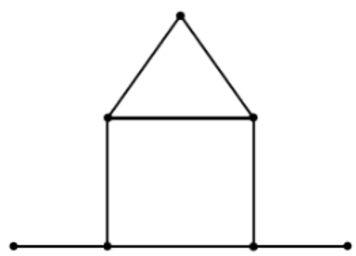

Figure 1.1: A Graph.

We denote by $|\mathcal{V}|$ the number of vertices and by $|\mathcal{E}|$ the number of edges. The **degree** d_v of a vertex v is the number of edges emanating from it.

The characterization of a graphs by its adjacency matrix makes sense because we may assume without loss of generality that it is free of (a) single-edge loops connecting a vertex to itself and (b) multiple edges connecting two vertices. Should any of these situations occur, we can eliminate it by adding "dummy" vertices of degree two as shown in Fig. 1.2.

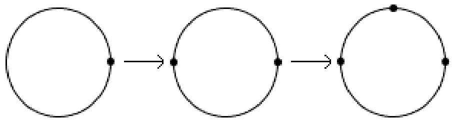

Figure 1.2: Eliminating single-edge loops and multiple edges.

With this convention taken into account the $|\mathcal{V}| \times |\mathcal{V}|$ adjacency matrix has a simple form:

$$\begin{array}{rcll} A_{\Gamma_{u,v}} & = & 1 & \text{if there exists edge connecting vertices } u \text{ and } v, \\ A_{\Gamma_{u,v}} & = & 0 & \text{otherwise.} \end{array}$$

1.2 Metric graphs

Definition 1.2. A graph is said to be a **metric graph**, if:

1. Each edge is assigned a positive length $L_e \in (0, \infty)$.

2. A coordinate $x_e \in [0, L_e]$ increasing in one direction of the edge is associated with each edge. If the opposite direction is chosen then the corresponding coordinate $x_{\bar{e}}$ satisfies $x_{\bar{e}} = L_e - x_e$.

Definition 1.3. We will call a graph **infinite** if it has infinitely many vertices (equivalently, infinitely many edges). Otherwise the graph will be called **finite**. A finite graph, whose edges all have finite lengths will be called **compact**.

If the sequence of edges $\{e_i\}_{i=1}^N$, $N \in \mathbb{N}$ forms a path we can define the length of the path as $\sum_{i=1}^N L_{e_i}$. Any graph can be naturally equipped with metric in following way. The distance $\rho(v, w)$ between two vertices is defined as minimal length of the path connecting them. In the same way also the distance $\rho(x, y)$ between arbitrary two points x, y of the graph which are not necessarily vertices may be defined.

Now we can easily introduce other useful structures on a metric graph. Every edge of a metric graph has its coordinate x_b. Hence a function $f(x_b)$ can be defined on every edge and thus on the whole graph Γ. Using the metric structure one can speak about continuous functions and also define the standard space of continuous functions $C(\Gamma)$ on the metric graph Γ. Moreover, the Lebesgue measure dx_b can be introduced in natural way on every edge. Having this measure, one can define other standard function spaces on Γ, e.g. $L_2(e)$ space and Sobolev spaces $W^{n,p}(e)$.

Let us recall the definition of the Sobolev space $W^{n,p}$ in the one-dimensional situation before we proceed to its definition on a metric graph.

Definition 1.4. Let a function f be locally integrable on an open interval $(a, b) \subset \mathbb{R}$, i.e. $f \in L^1_{\text{loc}}((a, b))$. We say that f has weak derivative of order $k \in \mathbb{N}$ if there exist a $g \in L^1_{\text{loc}}((a, b))$ such that

$$\int_a^b f(x)\partial^k \phi(x)dx = (-1)^n \int_a^b g(x)\phi(x)dx$$

for every ϕ from the space of test functions $\mathcal{D}((a,b))$. We put $\partial^k f := g$.

Remark 1.1. For $p \in \langle 1, \infty \rangle$ the Hölder inequality immediately implies that $L^p_{\text{loc}}((a,b)) \subset L^1((a,b))$. Hence the weak derivative is also well defined on $L^p_{\text{loc}}((a,b))$.

Definition 1.5. The **Sobolev space** $W^{n,p}((a,b))$ consists of equivalence classes of functions from $L^p((a,b))$ which have weak derivatives to the order n in $L^p((a,b))$, i.e. $W^{n,p}((a,b)) = \{f \in L^p((a,b))|$ weak derivative $\partial^k f \in L^p((a,b)),\ \forall k \in \mathbb{N},\ k \leq n\}$. The norm is defined as:

$$\begin{aligned} \|f\|_{W^{n,p}(a,b)} &:= \Big(\sum_{k=1}^{n} \|\partial^k f\|_p^p\Big)^{\frac{1}{p}}, \quad p \in (1, +\infty), \\ \|f\|_{W^{n,p}(a,b)} &:= \sum_{k=1}^{n} \|\partial^k f\|_\infty, \quad p = \infty. \end{aligned}$$

Remark 1.2. The notation $W^{n,2}((a,b)) = H^n((a,b))$ is usually used.

Definition 1.6. 1. The **space** $L_2(\Gamma)$ on Γ consists of functions that are measurable, square integrable on each edge e and satisfy

$$\|f\|^2_{L_2(\Gamma)} := \sum_{e \in \mathcal{E}} \|f\|^2_{L_2(e)} < \infty.$$

2. The **Sobolev space** $H^1(\Gamma)$ on Γ consists of all continuous functions that belong to $H^1(e)$ for each edge e and satisfy

$$\|f\|^2_{H^1(\Gamma)} := \sum_{e \in \mathcal{E}} \|f\|^2_{H^1(e)} < \infty.$$

The continuity condition is a natural vertex condition for functions from the Sobolev space $H^1(\Gamma)$. On the other hand there are no such natural junction conditions for functions from Sobolev space $H^k(\Gamma)$ for $k > 1$. As we will see further there is a certain freedom in choosing those junction conditions and our quantum system will have different properties in dependence how we choose them. In other words, an appropriate junction conditions will have to be imposed in definition of the quantum graph.

These considerations make the definition of Sobolev space $H^k(\Gamma)$ complicated for $k > 1$. Hence we start with the definition without junction conditions and we just require smoothness along the edges.

Definition 1.7. By $\tilde{H}^k(\Gamma)$ will be denoted the space

$$\tilde{H}^k(\Gamma) := \bigoplus_{e \in \mathcal{E}} H^k(e)$$

which consist of functions f on Γ that on each edge e belong to the Sobolev space $\tilde{H}^k(e)$ and they are

$$\|f\|^2_{\tilde{H}^k(\Gamma)} := \sum_{e \in \mathcal{E}} \|f\|^2_{H^k(e)} < \infty$$

1.3 Quantum graph

A metric graph equipped by a suitable differential operator is called **quantum graph**. The differential operator will be called **Hamiltonian** and it is required to be self-adjoint in the following text.

Example 1. Let us introduce some of the differential operators which are frequently used as quantum graphs Hamiltonians.

1. The negative second order derivative:

$$f(x_e) \mapsto -\frac{d^2 f(x_e)}{dx_e^2}, \tag{1.1}$$

where x_e is the coordinate along an edge e.

2. The Schrödinger operator:

$$f(x_e) \mapsto -\frac{d^2 f(x_e)}{dx_e^2} + V(x_e)f(x_e), \tag{1.2}$$

where $V(x_e)$ is an electric potential.

3. The magnetic Schrödinger operator:

$$f(x_b) \mapsto (\frac{1}{i}\frac{d}{dx_b} - A_b(x_b))^2 f(x_b) + V(x_b)f(x_b), \tag{1.3}$$

where $V(x)$ is an eletric potential and $A(x)$ is an magnetic potential.

We will be using only the first one.

We know that a differential operator is not completely defined until its domain is described. If we take an inspiration in the one dimensional case we find out that the domain description should include a smoothness requirement along the edges and some junction conditions at the vertices. The junction conditions or **vertex conditions** are an analogy to boundary conditions for a single interval. We have already mentioned those junction condition and we will study them in more detail later.

Definition 1.8. ([1], Def. 1.4.1.) **Quantum graph** is a metric graph equipped with a differential operator $\mathcal{H}$ (**Hamiltonian**), accompanied by "appropriate" vertex conditions. That is, a quantum graph is triple **{metric graph Γ, Hamiltonian $\mathcal{H}$, vertex conditions}**.

Looking for suitable domains of the second-order differential operator on $L^2(\Gamma)$ we begin with $\bigoplus_{e\in\mathcal{E}} H_0^2(e)$ where $H_0^2(e)$ is the subspace of the Sobolev space $H^2(e)$ with the functions and their derivatives vanishing at the vertices (i.e. at the end of the edges). Using the standard Sturm-Liouville theory, it can be checked that such an operator is symmetric, and our aim is to find proper vertex conditions which produce a self-adjoint extension of this operator. Obviously, a natural candidate for this extension is a subset of the space $\widetilde{H}^2(\Gamma)$ specified by suitable vertex conditions.

Example 2. **Kirchhoff** vertex conditions, sometimes also called **Neumann** (because at a vertex of degree one it reduces to Neumann boundary condition), **standard**, or **free** conditions.

$$f(x) \text{ is continuous on } \Gamma, \tag{1.4}$$

$$\sum_{e\in\mathcal{E}_v} \frac{df}{dx_e}(v) = 0 \text{ at each vertex v.} \tag{1.5}$$

E_v is a set of all edges incident at the vertex v. The derivatives are taken in the directions away from the vertex (**outgoing directions**).

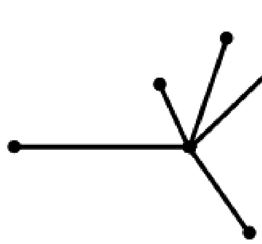

Figure 1.3: A compact star graph.

Example 3 (Spectrum of compact star graph with Kirhhoff vertex conditions). Let us find the spectrum of a compact star graph (Figure 1.3) with Kirhhoff vertex conditions where the Hamiltonian is of the form (1.1) acting as the negative second order derivative. We propose that the Hamiltonian is self-adjoint and has only discrete spectrum (see Theorem 1.1).

Taking this into account, we have to solve the following spectral equation:

$$-\frac{d^2f(x_e)}{dx_e^2} = k^2 f(x_e), \quad k \in \mathbb{R}. \tag{1.6}$$

The well known general solution and its first derivative have the form:

$$f(x_b) = A_e \sin(kx_e) + B_e \cos(kx_e), \tag{1.7}$$

$$\frac{df(x_e)}{dx_e} = kA_e \cos(kx_e) - kB_b \sin(kx_e), \tag{1.8}$$

where A, B are real constants.

Now we use the Kirchhoff condition at the "peripheral" vertices, i.e. $f'(0_e) = 0$. Plugging the first derivative into this conditions we get

$$f'(0_e) = 0 = kA_e \cos(k \cdot 0_e) - kB_e \sin(k \cdot 0_e) = kA \Rightarrow A = 0.$$

Thus the eigenfunction f on the edge e is equal to

$$f(x_b) = B_e \cos(kx_e).$$

The outgoing derivative at the central vertex $x_e = L_e$ is equal to

$$f'(L_e) = kB_e \sin(kL_e).$$

Note that the sign has changed because the derivatives at the vertex are conventionally taken in the *outgoing direction*.

We see that the Kirchhoff vertex conditions at the central vertex have the form

$$A_1 \cos(kL_1) = A_2 \cos(kL_2) = ... = A_{|\mathcal{E}|} \cos(kL_{|\mathcal{E}|}) = C,$$
$$\sum_{e=1}^{|\mathcal{E}|} kA_e \cos(kL_e) = 0.$$

For $C \neq 0$ we can divide the second equation by C and we get that k^2 is an eigenvalue if

$$F(k) := \sum_{e=1}^{|\mathcal{E}|} \tan(kL_e) = 0. \tag{1.9}$$

1.4 Vertex conditions

Suppose that we have the negative second order differential operator (i.e. Hamiltonian (1.1)) on a metric graph Γ with the "maximum" domain $\tilde{H}^2(\Gamma)$ (see Definition 1.7). The main task of this section is to establish appropriate vertex conditions which determine subsets of $\tilde{H}^2(\Gamma)$ such that the corresponding Hamiltonians are self-adjoint.

For our purposes it is completely sufficient to consider only *finite graphs*, i.e. the number of edges $|\mathcal{E}|$ and the number of vertices $|\mathcal{V}|$ is finite. True, the main object of this thesis are infinite graphs, but we will deal with periodic ones the investigation of which can be reduced to analysis of finite sub-graphs. We also consider only the so-called **local vertex conditions**, i.e. those that involve the values of functions and their derivatives at a single vertex at a time.

To describe local vertex conditions it is sufficient to consider graphs with a single vertex, in other words, star-shaped ones; keeping in mind that an arbitrary graph locally (i.e. close to a vertex) looks like a **star graph**.

The Hamiltonian $\mathcal{H}$ acts on a star graph Γ and its domain is subset of $\tilde{H}^2(\Gamma)$. If we choose functions $f_1, ..., f_d$ from this domain we can introduce notations:

1. The column vector $F(v)$ of the values at the vertex v:

$$F(v) := \begin{pmatrix} f_1(v) \\ \cdots \\ \cdots \\ f_d(v) \end{pmatrix}. \tag{1.10}$$

2. The column vector $F'(v)$ of values at vertex v of derivatives of f taken in the outgoing directions

$$F'(v) := \begin{pmatrix} f_1'(v) \\ \cdots \\ \cdots \\ f_d'(v) \end{pmatrix}. \tag{1.11}$$

The Hamiltonian acts as negative second order derivative on each edge. We know from ODE theory that two boundary values has to be given, i.e. the values $f_e(v)$ and $f_e'(v)$. At every vertex the number of conditions is equal to number of edges incident to this vertex, i.e. equal to the degree d_v of the vertex v. Thus the most general *homogeneous* (linear) condition has a form

$$\mathbb{A}_v F(v) + \mathbb{B}_v F'(v) = 0, \tag{1.12}$$

where $\mathbb{A}_v$ and $\mathbb{B}_v$ are $(d_v \times d_v)$-matrices.

Finally, the next theorem gives us an answer how to choose a vertex condition (i.e. how to choose matrices in (1.12)) in order to get a self-adjoint Hamiltonian.

Theorem 1.1 (cf. [1], Thm. 1.4.4.)**.** *Let Γ be a metric graph with finitely many edges. Consider the operator $\mathcal{H}$ acting as $-\frac{d^2}{dx_e^2}$ on each edge e, with the domain consisting of functions that belong to $\tilde{H}^2(\Gamma)$ and satisfying some local vertex conditions involving vertex values of functions and their derivatives. The operator is self-adjoint if and only if the vertex conditions can be written in one (and thus any) of the following three forms:*

A: For every vertex v of degree d_v there exist $d_v \times d_v$ matrices $\mathbb{A}_v$ and $\mathbb{B}_v$ such that

$$\text{the } d_v \times 2d_v \text{ matrix } (\mathbb{A}_v, \mathbb{B}_v) \text{ has the maximal rank,}$$

$$\text{the matrix } \mathbb{A}_v \mathbb{B}_v^* \text{ is self-adjoint,}$$

and the boundary values of f satisfy

$$\mathbb{A}_v F(v) + \mathbb{B}_v F'(v) = 0. \tag{1.13}$$

B: For every vertex v of degree d_v, there exists a unitary $d_v \times d_v$ matrix $\mathbb{U}_v$ such that the boundary values of f satisfy

$$i(\mathbb{U}_v - \mathbb{I})F(v) + (\mathbb{U}_v + \mathbb{I})F'(v) = 0, \tag{1.14}$$

where $\mathbb{I}$ is the $d_v \times d_v$ identity matrix.

C: For every vertex v of degree d_v, there are three orthogonal (and mutually orthogonal) projectors $P_{D,v}$, $P_{N,v}$ and $P_{R,v} := \mathbb{I} - P_{D,v} - P_{N,v}$ (one or two projectors can be zero) acting in $\mathbb{C}^{d_v}$ and an invertible self-adjoint operator Λ_v acting in the subspace $P_{R,v}\mathbb{C}^{d_v}$, such that the boundary values of f satisfy

$$\begin{aligned} P_{D,v}F(v) &= 0 && \text{"Dirichlet part"}, \\ P_{N,v}F'(v) &= 0 && \text{"Neumann part"}, \\ P_{R,v}F'(v) &= \Lambda_v P_{R,v} F(v) && \text{"Robin part"}. \end{aligned} \tag{1.15}$$

Remark 1.3. The operator Λ_v and projectors $P_{D,v}$, $P_{N,v}$ and $P_{R,v}$ satisfies

$$\text{Ran}P_{D,v} = \text{Ker}B, \quad \text{Ran}P_{N,v} = \text{Ker}A, \quad \Lambda_v B^{-1} A P_{D,v}, \tag{1.16}$$

and by definition $P_{R,v} = \mathbb{I} - P_{R,v} - P_{D,v}$.

It is often useful to know the quadratic form of the operator $\mathcal{H}$. The following theorem describes how quadratic form looks like.

Theorem 1.2 ([1], Thm. 1.4.11.)**.** *The quadratic form h of $\mathcal{H}$ is given as*

$$h[f,f] = \sum_{e\in\mathcal{E}} \int_e \left|\frac{df}{dx}\right| + \sum_{v\in\mathcal{V}} \langle \Lambda_v P_{R,v} F, P_{R,v} F\rangle, \tag{1.17}$$

where $\langle,\rangle$ denotes the standard hermitian inner product in $\mathbb{C}^{\dim P_{R,v}}$. The domain of this form consists of all functions f that belong to $H^1(e)$ on each edge e and satisfy at each vertex v the condition $P_{R,v}F = 0$.

Example 4. Vertex conditions:

The δ**-type condition**:

$$f(x) \text{ is continuous at vertex } v,$$
$$\sum_{e\in\mathcal{E}_v} \frac{df}{dx_e}(v) = \alpha_v f(v),$$
$$\mathbb{U} = \frac{2i}{4i+a}\begin{pmatrix} -1+\frac{\alpha_v}{2}i & 1 & 1 & \dots & 1 & 1 \\ 1 & -1+\frac{\alpha_v}{2}i & 1 & & 1 & 1 \\ \vdots & & & \ddots & & \vdots \\ 1 & 1 & 1 & & -1+\frac{\alpha_v}{2}i & 1 \\ 1 & 1 & 1 & \dots & 1 & -1+\frac{\alpha_v}{2}i \end{pmatrix},$$

where α_v is a real number.

The **Dirichlet condition**:

$$\begin{aligned} f(v) &= 0. \\ \mathbb{U} &= \mathbb{I}, \end{aligned} \tag{1.18}$$

where $\mathbb{I}$ is identity matrix.

The δ'_s**-type condition**:

$$\text{The values } \frac{df}{dx_e}(v) \text{ are independent of } e \text{ at the vertex } v,$$
$$\sum_{e\in\mathcal{E}_v} f_e(v) = \alpha_v \frac{df}{dx_e}(v),$$
$$\mathbb{U} = \frac{2}{4+ai}\begin{pmatrix} -1+\frac{\alpha_v}{2}i & 1 & 1 & \dots & 1 & 1 \\ 1 & -1+\frac{\alpha_v}{2}i & 1 & & 1 & 1 \\ \vdots & & & \ddots & & \vdots \\ 1 & 1 & 1 & & -1+\frac{\alpha_v}{2}i & 1 \\ 1 & 1 & 1 & \dots & 1 & -1+\frac{\alpha_v}{2}i \end{pmatrix},$$

where α_v is a real number.

The *Neumann*-**type condition**:

$$\begin{aligned} f(v) &= 0. \\ \mathbb{U} &= i\mathbb{I}, \end{aligned} \tag{1.19}$$

where $\mathbb{I}$ is identity matrix.

Definition 1.9. Let any function $f(x)$ satisfies vertex conditions at v. We say that the vertex conditions are **scale invariant** if also function $f(rx)$ satisfies those conditions for any $r > 0$.

Proposition 1.1 ([1], Thm. 1.4.10.)**.** *Vertex conditions written in the form (1.15) are scale invariant if and only if they do not contain any Robin part, i.e.* $P_{R,v} = 0$.

Remark 1.4. In [1] are all vertex conditions from the Example 4 rewritten in the form (1.15). This allow us use the foregoing theorem and sum up results:

1. δ-type condition:
   - $\alpha_v = 0$: scale invariant
   - $\alpha_v \neq 0$: not scale invariant
2. δ_s'-type condition:
   - $\alpha_v = 0$: scale invariant
   - $\alpha_v \neq 0$: not scale invariant
3. Dirichlet condition: scale invariant

1.5 Periodic graphs

Definition 1.10 ([1], Def. 4.1.1.)**.** An infinite **quantum graph** Γ is called $\mathbb{Z}^n$-periodic if an action of the free abelian group $G = \mathbb{Z}^n$ is defined on it. The action $(g, x) \in G \times \Gamma \mapsto gx \in \Gamma$ has to satisfy following properties:

1. **Group action:**

- The mapping $x \mapsto gx$ is a bijection of Γ for every $g \in G$.
- $0 \cdot x = x$ for every $x \in \Gamma$, where 0 is the neutral element of G.
- $(g_1 \cdot g_2)x = g_1(g_2x)$ for every $g_1, g_2 \in G$.

2. **Continuity:**

- The mapping $x \mapsto gx$ of Γ into itself is continuous for every $g \in G$.

3. **Faithfulness:**

- If $gx = x$ for some $x \in \Gamma$, then $g = 0$.

4. **Discreteness:**

- For every $x \in \Gamma$, there exists a neighbourhood U of x such that $gx \notin U$ for $g = 0$.

5. **Co-compactness:**

- The space of orbits Γ/G is compact. Hence the G-shifts of compact subset produce the whole graph.

6. **Structure preservation:**

- $gu \sim gv \Leftrightarrow u \sim v$. In particular, G acts bijectively on the set of edges.
- The group action preserves edges lengths: $L_{ge} = L_e$.
- The group action commutes with Hamiltonian and preserves the vertex conditions.

Remark 1.5. So called **dual lattice** $G^\star := 2\pi\mathbb{Z}^n$ to $G = \mathbb{Z}^n$ is often used.

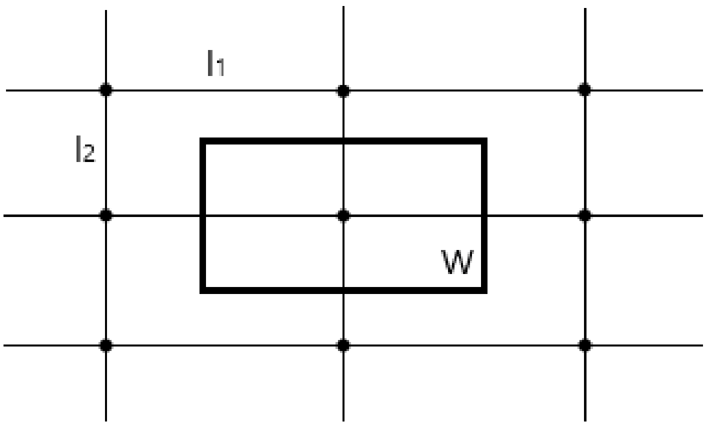

Figure 1.4: A periodic graph with the fundamental domain W.

Definition 1.11 (cf. [1], Def. 4.1.2.)**.** A **fundamental domain** for the action of G on Γ is compact subset W of Γ with following two properties:

1. G-shifts of W covers Γ, i.e.

$$\bigcup_{g\in G} gW = \Gamma.$$

2. For $g_1 \neq g_2$ an intersection $g_1W \cap g_2W$ consists of finitely many points and there are no vertices included.

Remark 1.6. The fundamental domain is not determined uniquely.

1.6 Floquet-Bloch theory

Definition 1.12 ([1], Def. 4.2.1.)**.** A **character** of the group G is a homomorphism $\gamma : G \mapsto \mathbb{C}\backslash\{0\}$, i.e. γ satisfies:

1. $\gamma(e) = 1,\ e$ is neutral element of G.
2. $\gamma(g_1 g_2) = \gamma(g_1)\gamma(g_2)$ for every$g_1, g_2 \in G$.

Lemma 1.1 ([1], Lem. 4.2.2.)**.** *Every character of $g = \mathbb{Z}^n$ can be (unitary) represented by a vector $\theta \in \mathbb{R}^n$ in the following way:*

$$\gamma(g) = \gamma_\theta(g) := e^{i\theta \cdot g},\ \ g \in G,$$

where $k \cdot g = \sum_j \theta_j g_j$.

The vector θ is called **quasi-momenta** and the corresponding vectors

$$\omega := e^{i\theta} := (e^{i\Theta_1}, ..., e^{i\Theta_1}) \in (\mathbb{C}\backslash\{0\})^n$$

are called **Floquet multipliers**. It can be clearly seen that the character γ_k is 2π-periodic with respect to components of the vector θ. Thus the values of θ may be restricted to the fundamental domain B of $G^\star = 2\pi G$ which is called **Brillouin zone** and it is often chosen as

$$B = [-\pi, \pi]^n.$$

Definition 1.13 ([1], Def. 4.2.6.)**.** Let f be function on periodic graph $(\Gamma, \mathbb{Z}^n)$. The **Floquet transformation** of f is formally defined as

$$f \mapsto \tilde{f}(x, \omega) := \sum_{g \in \mathbb{Z}^n} f(gx)\omega^{-g},\ \ x \in \Gamma,\ \ g \in B,$$

where B is the Brillouin zone.

One can see that the Floquet transformation is much similar to the Fourier transformation with respect to abelian group $\mathbb{Z}^n$.

The Floquet transformation of a periodic operator $\mathcal{H}$ on $(\Gamma, \mathbb{Z}^n)$ may be defined by using Definition 1.13 (see in [1], Section 4.2.4.). This transformation reduces the Hamiltonian $\mathcal{H}$ to the parametric set of operators $\mathcal{H}(\omega)$ (resp. $\mathcal{H}(\theta)$) which act on the fundamental domain. The vertex conditions are preserved after the transformation but there also appear new vertices of degree one at the fundamental domain boundary.

Example 5. Let us have the rectangular lattice graph (Figure 1.4), the Hamiltonian $\mathcal{H} = -\frac{d^2}{dx^2}$ and some vertex conditions. The transformed Hamiltonian $\mathcal{H}(\omega) \equiv \mathcal{H}(\omega_1, \omega_2)$ act on W in same way but its domain consists of functions which also have to satisfy conditions

$$f(a) = e^{i\theta_1} f(b), \quad f(c) = e^{i\theta_2} f(d), \tag{1.20}$$

$$f'(a) = -e^{i\theta_1} f'(b), \quad f'(c) = -e^{i\theta_2} f'(d). \tag{1.21}$$

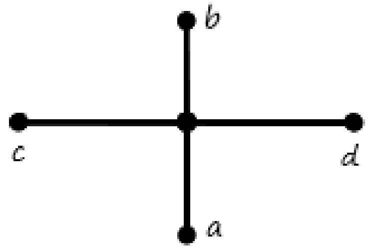

Figure 1.5: The fundamental domain W with the peripheral vertices.

1.7 Spectral properties

Theorem 1.3 ([1], Thm. 4.3.1.). *Let* Γ *be a* $\mathbb{Z}^n$*-periodic quantum graph with a periodic self-adjoint Hamiltonian* $\mathcal{H}$*. The spectrum* $\sigma(\mathcal{H})$ *of the operator* $\mathcal{H}$ *in* $L^2(\Gamma)$ *is equal to the union of the closed intervals* I_j *called the* **spectral bands***:*

$$I_j := \{k : k = k(\omega), \text{ where } \omega \text{ are the Floquet multipliers}\}.$$

These eigenvalues are continuous and piece-wise analytic with respect to ω*.*

Definition 1.14 ([1], Def. 4.3.2.). The representation

$$\sigma(\mathcal{H}) = \bigcup_{j=1}^{\infty} I_j$$

is called the **band-gap structure** of $\sigma(\mathcal{H})$.

Theorem 1.4 ([1], Thm. 4.3.1.). *The spectrum of a periodic self-adjoint Hamiltonian* $\mathcal{H}$ *on a quantum graph* Γ *has no singular continuous part.*

As a consequence of previous theorem the spectrum of a periodic self-adjoint Hamiltonian $\mathcal{H}$ on a quantum graph Γ can contain only absolute continuous and pure point parts. The bound states and also compactly supported eigenfunctions ("scars") may exist for periodic operators due to the failure of the uniqueness of continuation property for quantum graphs (see [1, Section 3.4])

Chapter 2

Rectangular lattice with a preferred orientation

Before we proceed to the following chapters we need to introduce some notions. The momentum scale k instead of the energy scale k^2 is used in the following text. Concretely, if we solve the spectral problem for a Hamiltonian $\mathcal{H}$ we use k^2 instead of k, i.e.

$$\mathcal{H}\psi = k^2\psi, \tag{2.1}$$

thus k has physical meaning of momentum and k^2 has physical meaning of energy. Consequently, if we talk about spectrum it is meant **spectrum in the momentum scale** k. Occasionally we also use the energy scale but every time we are using the energy scale there is, in order to prevent misunderstanding, explicitly written which scale is being used.

A periodic rectangular lattice quantum graph with time-reversal non-invariant coupling is rigorously defined in this chapter. A spectral condition which completely determines the spectrum of this system is found. Some spectral properties of the system are established. Numeric solutions are shown at the end of the chapter.

2.1 Spectral condition

Consider a quantum graph with a periodic rectangular lattice structure (Figure 1.4) where the edges are $l_1, l_2 > 0$ long and its Hamiltonian is given as the negative second order derivative (1.1).

The boundary conditions which we study in this chapter are given by $\mathbb{A} = \mathbb{U} - \mathbb{I}$,

$\mathbb{B} = i(\mathbb{U} - \mathbb{I})$ where $\mathbb{I}$ is the unit matrix and the matrix $\mathbb{U}$ has the form

$$\mathbb{U} = \begin{pmatrix} 0 & 1 & 0 & \dots & 0 & 0 \\ 0 & 0 & 1 & & 0 & 0 \\ \vdots & & & \ddots & & \\ 0 & 0 & 0 & & 1 & 0 \\ 0 & 0 & 0 & & 0 & 1 \\ 1 & 0 & 0 & \dots & 0 & 0 \end{pmatrix}. \tag{2.2}$$

This conditions can be written in the matrix form as

$$(\mathbb{U} - \mathbb{I})\Psi(0_+) + i(\mathbb{U} + \mathbb{I})\Psi'(0_+). \tag{2.3}$$

It holds that $\mathbb{U}\mathbb{U}^\star = \mathbb{U}^\star\mathbb{U} = \mathbb{I}$. Thus the matrix $\mathbb{U}$ is unitary. Using Theorem 1.1 we see that the Hamiltonian is self-adjoint.

Remark 2.1. If we solve the spectral problem $\det(\mathbb{U} - \lambda\mathbb{I})$ then we find out that eigenvalues are determined by equation

$$\lambda^N - 1 = 0, \quad N \geq 3. \tag{2.4}$$

In our case $N = 4$. This imply that the eigenvalues are

$$\sigma(\mathbb{U}(4)) = \{\pm 1, \pm i\}. \tag{2.5}$$

We know that the vertex conditions are scale invariant if and only if the Robin part is missing (see Theorem 1.1) but absence of the Robin part is equivalent to absence of values other than ± 1 in the spectrum of $\mathbb{U}$. In other words, vertex conditions are scale invariant if and only if the matrix $\mathbb{U}$ has only eigenvalues ± 1. Our matrix $\mathbb{U}$ does not satisfy this property thus we conclude that the vertex conditions are not scale invariant.

The vertex condition can be rewritten in the component form as

$$(\psi_{j+1} - \psi_j) + i(\psi'_{j+1} + \psi'_j) = 0, \quad j \in \mathbb{Z} \pmod N, \tag{2.6}$$

where $\psi_j(x) \in \oplus_{j=1}^N H^2(e)$ and $\psi_j := \psi_j(0_+)$, $\psi'_j := \psi'_j(0_+)$. The time-reversion corresponds to the complex conjugate in the quantum mechanic. If we make complex conjugation of the expression (2.6) we get

$$(-\psi_{j+1} + \psi_j) + i(\psi'_{j+1} + \psi'_j) = 0, \quad j \in \mathbb{Z} \pmod N. \tag{2.7}$$

We can see that coupling is not time-reversal. Now we illustrate how the time-reversion is connected with the orientation of the quantum graph. Let us introduce the reversion operator

$$R\psi_j(x) := \psi_{N+1-j}(x), \quad j \in \mathbb{N}. \tag{2.8}$$

If we use this operator on the (2.6) we get (2.7). This brings us to the fact that the time-reversal is equivalent to the change of orientation of our quantum graph.

Now we try to establish spectrum of our quantum graph. In order to do that we have to solve the spectral equation

$$-\frac{d^2\psi(x)}{dx^2} = k^2\psi(x), \quad k \in \mathbb{R}. \tag{2.9}$$

The fundamental domain is the star-shaped graph sketched on Figure 1.5. The general solution and its derivative have the form

$$\psi_j(x) = a_j e^{ikx} + b_j e^{-ikx}, \tag{2.10}$$
$$\psi_j'(x) = ika_j e^{ikx} - ikb_j e^{-ikx}, \tag{2.11}$$

for $j \in \{1,2,3,4\}$. Moreover, the Floquet-Bloch theory establishes additional conditions at the peripheral vertices (see conditions (1.20) and (1.21)). If we use those results and we choose coordinates increasing in the direction up and right we find that

$$\psi_3(a) \equiv a_3 e^{ika} + b_3 e^{-ika} = \omega_1(a_1 e^{ikb} + b_1 e^{-ikb}) \equiv \psi_1(b), \tag{2.12}$$
$$\psi_3'(a) \equiv -(ika_3 e^{ika} - ikb_3 e^{-ika}) = -\omega_1(ika_1 e^{ikb} - ikb_1 e^{-ikb}) \equiv -\psi_1'(b). \tag{2.13}$$

We remind that $\omega_j = e^{i\theta_j}$ are the Floquet multipliers for quasi-momenta θ_j from the Brillouin zone $(-\pi, \pi]$, $j \in \{1,2\}$. Note that derivatives are taken in the direction away from the vertex. By adding and subtracting these equations we get

$$a_3 = a_1\omega_1 e^{ik(b-a)}, \quad b_3 = b_1\omega_1 e^{-ik(b-a)}, \tag{2.14}$$

and similarly we obtain

$$a_4 = a_2\omega_2 e^{ik(d-c)}, \quad b_4 = b_2\omega_2 e^{-ik(d-c)}. \tag{2.15}$$

Finally, we write an Ansatz:

$$\begin{aligned} \psi_1(x) &= a_1 e^{ikx} + b_1 e^{-ikx}, \\ \psi_2(x) &= a_2 e^{ikx} + b_2 e^{-ikx}, \\ \psi_3(x) &= \omega_1(a_1 e^{ik(x+l_1)} + b_1 e^{-ik(x+l_1)}), \\ \psi_4(x) &= \omega_2(a_2 e^{ik(x+l_2)} + b_2 e^{-ik(x+l_2)}). \end{aligned} \tag{2.16}$$

If we enumerate those functions at zero we get

$$\begin{aligned} \psi_1(0_+) &= a_1 + b_1, & \psi_1'(0+) &= ik(a_1 + b_1), \\ \psi_2(0_+) &= a_2 - b_2, & \psi_2'(0_+) &= ik(a_2 - b_2), \\ \psi_3(0_+) &= \omega_1(a_1 e^{ikl_1} + b_1 e^{-ikl_1}), & \psi_3'(0_+) &= ik\omega_1(a_1 e^{ikl_1} + b_1 e^{-ikl_1}), \\ \psi_4(0_+) &= \omega_2(a_2 e^{ikl_2} - b_2 e^{-ikl_2}), & \psi_4'(0_+) &= ik\omega_2(a_2 e^{ikl_2} - b_2 e^{-ikl_2}). \end{aligned} \tag{2.17}$$

By plugging these values into the boundary conditions we get a system of linear equations for coefficients a_j and b_j, $j \in \{1,2\}$. Once again we point out that derivatives are taken in the direction away from the vertex. The system has the form

$$\begin{aligned} a_1(-1-k) + a_2(1-k) + b_1(-1+k) + b_2(1+k) &= 0, \\ a_1\omega_1 e^{ikl_1}(1+k) + a_2(-1+k) + b_1\omega_1 e^{-ikl_1}(1-k) + b_2(-1+k) &= 0, \\ a_1\omega_1 e^{ikl_1}(-1+k) + a_2\omega_2 e^{ikl_2}(1+k) + b_1\omega_1 e^{-ikl_1}(-1-k) + b_2\omega_2 e^{-ikl_2}(1-k) &= 0, \\ a_1(1-k)a_2\omega_2 e^{ikl_2}(-1+k) + b_1(1+k)b_2\omega_2 e^{-ikl_2}(-1-k) &= 0, \end{aligned}$$

and it is solvable if the determinant

$$D(k,l_1,l_2,\omega_1,\omega_2)=\begin{vmatrix} -1 & -\eta & \eta & 1\\ \omega_1 L_1^+ & \omega_1 L_1^-\eta & -1 & -\eta\\ -\omega_1 L_1^+\eta & -\omega_1 L_1^- & \omega_2 L_2^+ & \omega_2 L_2^-\eta\\ \eta & 1 & -\omega_2 L_2^+\eta & -\omega_2 L_2^- \end{vmatrix} \tag{2.18}$$

is equal to zero. There the abbreviations $\eta=\frac{1-k}{1+k}$, $L_1^\pm=e^{\pm ikl_1}$, $L_2^\pm=e^{\pm ikl_2}$ are used. By subtracting the first row from the others rows the determinant takes the form

$$D=\begin{vmatrix} -1 & 0 & 0 & 0\\ \omega_1 L_1^+ & \omega_1 L_1^-\eta-\omega_1 L_1^+\eta & -1+\omega_1 L_1^+\eta & -\eta+\omega_1 L_1^+\\ -\omega_1 L_1^+\eta & -\omega_1 L_1^- - \omega_1 L_1^+\eta^2 & \omega_2 L_2^+ - \omega_1 L_1^+\eta^2 & \omega_2 L_2^-\eta-\omega_1 L_1^+\eta\\ \eta & 1-\eta^2 & -\omega_2 L_2^+\eta+\eta^2 & -\omega_2 L_2^- + \eta \end{vmatrix}.$$

Finally we can use the Sarus rule to get

$$D=\frac{k}{(1+k)^4}16ie^{i(\theta_1+\theta_2)}\Big\{\Big(k^2-1\Big)\Big(\sin(kl_2)\ \cos(\theta_1)+\sin(kl_1)\ \cos(\theta_2)\Big)+ \\ +\Big(k^2+1\Big)\sin(k(l_1+l_2))\Big\}. \tag{2.19}$$

Using a goniometric identity for $\cos(k(l_1+l_2))$ we get spectral condition in the following form

$$\Phi_1\big(k,\theta_1,\theta_2\big):=\sin(kl_2)\Big[\frac{(k^2-1)}{(k^2+1)}\cos(\theta_1)+\cos(kl_1)\Big] \\ +\sin(kl_1)\Big[\frac{(k^2-1)}{(k^2+1)}\cos(\theta_2)+\cos(kl_2)\Big]. \tag{2.20}$$

However, this condition does not describe all the spectrum. The star graph with the vertex condition (2.6) has also negative spectrum. This spectrum is obtained by substituting $k=i\kappa$ with $\kappa>0$ (see [3]). If we do this substitution for our periodic quantum graph we get

$$\tilde{\Phi}_2(\kappa,\theta_1,\theta_2):=\sinh(\kappa l_2)\Big[(\kappa^2+1)\cos(\theta_1)+(\kappa^2-1)\cosh(\kappa l_1)\Big] \\ +\sinh(\kappa l_1)\Big[(\kappa^2+1)\cos(\theta_2)+(\kappa^2-1)\cosh(\kappa l_2)\Big]. \tag{2.21}$$

In other words, the foregoing two conditions completely determine the spectrum of our quantum graph.

Proposition 2.1. *Let us have the periodic rectangular lattice quantum graph (Figure 1.4) with the Hamiltonian $\mathcal{H}:=-\frac{d^2}{dx^2}$ and with the vertex conditions determined by the matrix*

$$\mathbb{U}=\begin{pmatrix}0&1&0&0\\0&0&1&0\\0&0&0&1\\1&0&0&0\end{pmatrix}. \tag{2.22}$$

Then its spectrum has following properties:

Positive spectrum

- *For every* $l_1, l_2 > 0$ *there are infinitely many gaps. The gaps are located in the vicinity of the points* $\{\frac{m\pi}{l_1}, \frac{n\pi}{l_2}\}$, $m, n \in \mathbb{N}$.

- *If* $\frac{l_1}{l_2}$ *is rational number then there are infinitely many infinitely degenerate eigenvalues.*

- *If* $l_1 \geq 2 \wedge l_2 \geq 2$ *then the first positive band starts at zero.*

- *If* $l_1 < 2 \wedge l_2 < 2$ *then the first positive band is separated from zero.*

Negative spectrum

- *Energy -1 always belongs to the spectrum, thus inf* $\sigma(H) < -1$.

- *If* $l_1 > 2 \wedge l_2 > 2$ *then negative spectrum is separated from zero.*

- *If* $l_1 \leq 2 \wedge l_2 \leq 2$ *then the spectrum extends to zero.*

2.2 Analytic solution - illustrated by plots

Let us demonstrate figures which could provide us a better understanding to the spectrum structure. The figures consists of two parts: the positive one and the negative one. The momentum k is taken as the variable on the positive part of the horizontal axis. Similarly, $-i\kappa$ is taken as the variable on the negative part of the horizontal axis. In other words, the horizontal axis shows positive and negative part of the spectrum if the edges lengths are fixed. The vertical axis shows values of functions which depends on k and κ, respectively. Those values have no physical meaning.

Positive part

Functions $k \mapsto \cos(kl_1)$ and $k \mapsto \cos(kl_2)$ are shown in red and blue color, respectively. We also plot the region bordered from below and above by the curves $k \mapsto \pm\frac{k^2-1}{k^2+1}$ for fixed values of $t \in [0,1]$ in the grey colour.

The cosine functions are plotted with a solid line if they both intersect the grey region, i.e. if the conditions

$$|\cos(kl_1)| < \left|\frac{k^2-1}{k^2+1}\right| \wedge |\cos(kl_2)| < \left|\frac{k^2-1}{k^2+1}\right|.$$

are fulfilled. In other words, the *cosine* functions are solid if we can certainly establish that k belongs to the positive spectrum. Otherwise they are plotted with a dotted line.

Negative part

The negative part is similar the positive one if we swap functions: $\cos(kl_1) \to \cosh(\kappa l_1)$, $\cos(kl_2) \to \cosh(\kappa l_2)$, $k \mapsto \pm\frac{k^2-1}{k^2+1} \to \kappa \mapsto \pm\frac{\kappa^2+1}{\kappa^2-1}$.

On the vertical axis are also shown: the spectrum (black color), the gaps (no color) and in blue color are drawn cases where we are not able to analytically establish if k belongs to the spectrum or not.

We also point out that the last picture illustrates the case $l_1 = l_2$ (i.e. square lattice graph) which was discussed in [3, Chapter 2].

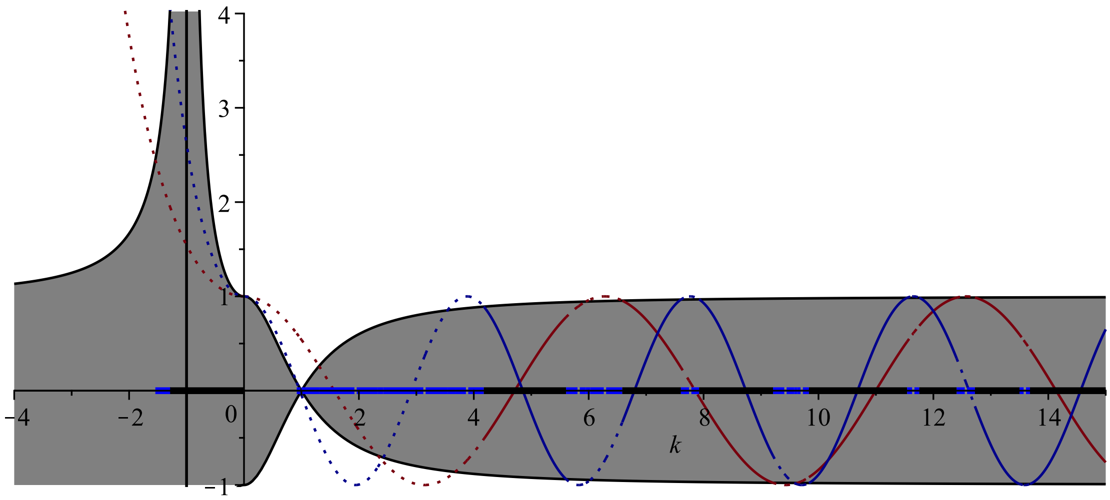

Figure 2.1: The situation for edge lengths $l_1 = 1$ and $l_2 = \frac{1+\sqrt{5}}{2}$.

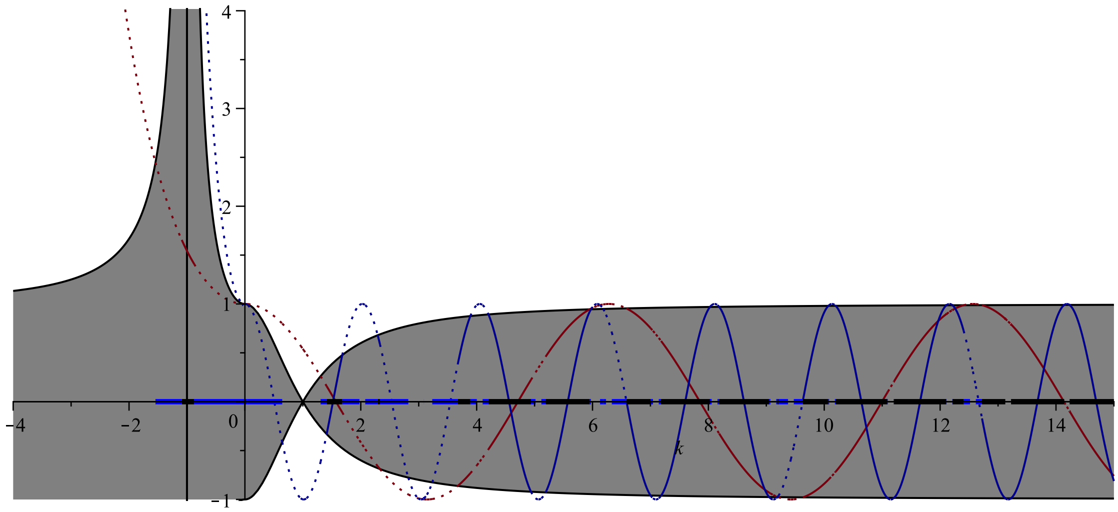

Figure 2.2: The situation for edge lengths $l_1 = 1$ and $l_2 = 3.1$.

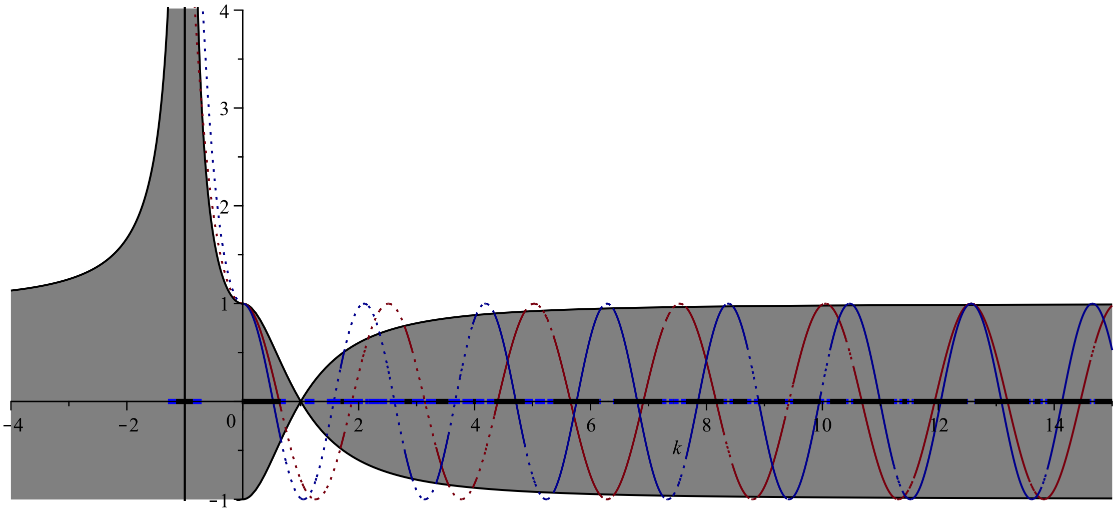

Figure 2.3: The situation for edge lengths $l_1 = 2.5$ and $l_2 = 3$.

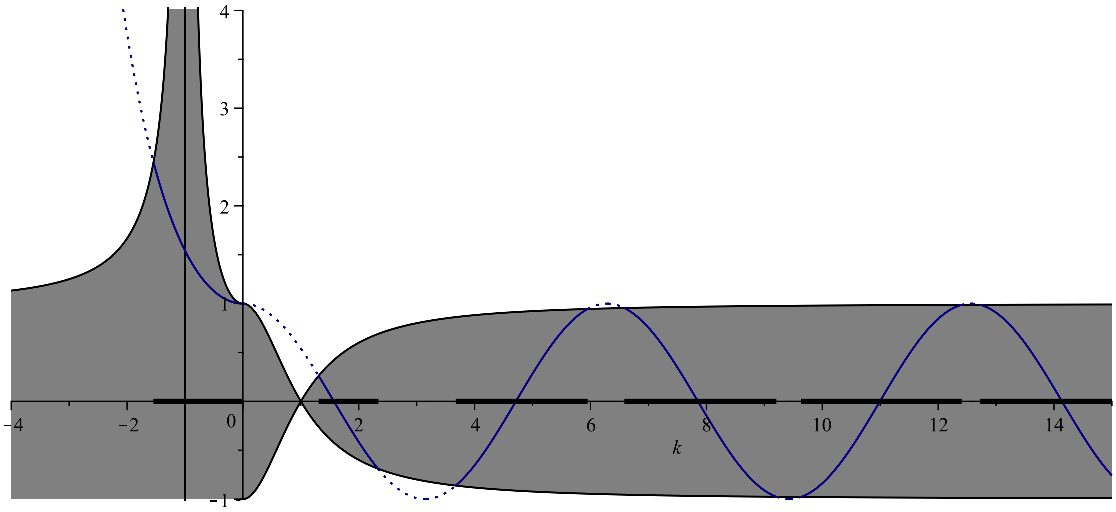

Figure 2.4: The situation for edge lengths $l_1 = 1$ and $l_2 = 1$. The $l_1 = l_2$ case was discussed in [3].

2.3 Numerical solutions

The numerical solutions show how the spectrum depends on edge length. For this purpose we fixed one edge and the second one is taken as variable. Both the momentum scale and the energy scale are displayed in these figures.

One can see gaps in the vicinity of points $\{\frac{m\pi}{l_1}\}_{m\in\mathbb{N}}$ as expected due to the Theorem 4.1. Moreover, it can be seen that the gap width decreases as the momentum k grows in accordance with Proposition 4.3.

We also point out that the figures in the logarithmic scale nicely illustrate that our vertex condition is not scale invariant.

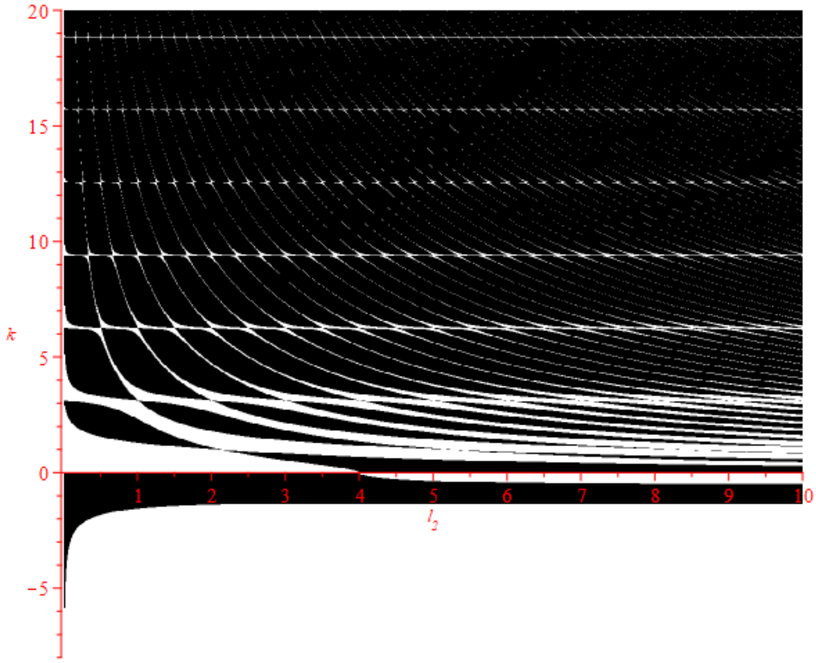

Figure 2.5: The momentum scale solution for $l_1 = 1$.

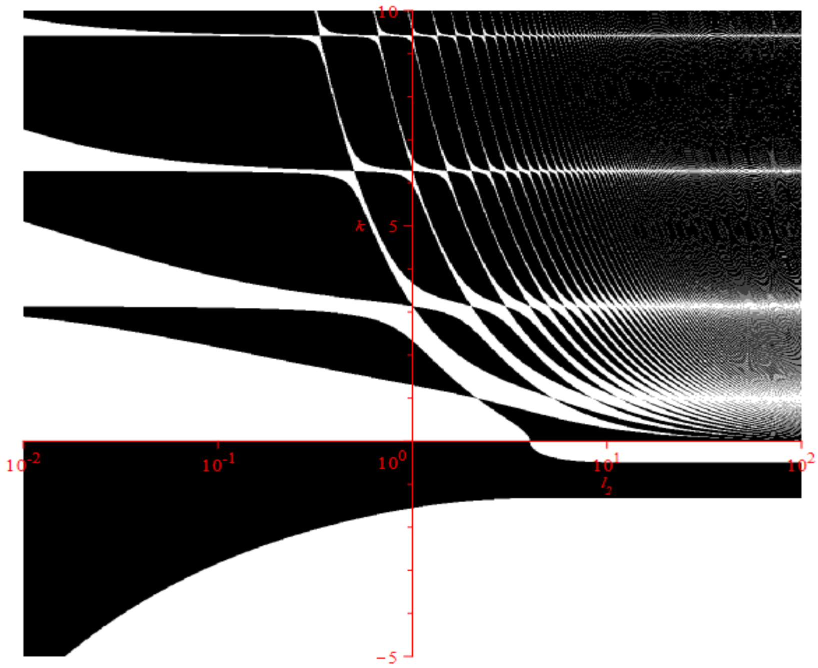

Figure 2.6: The momentum scale solution for $l_1 = 1$ in the logarithmic scale on the horizontal axis.

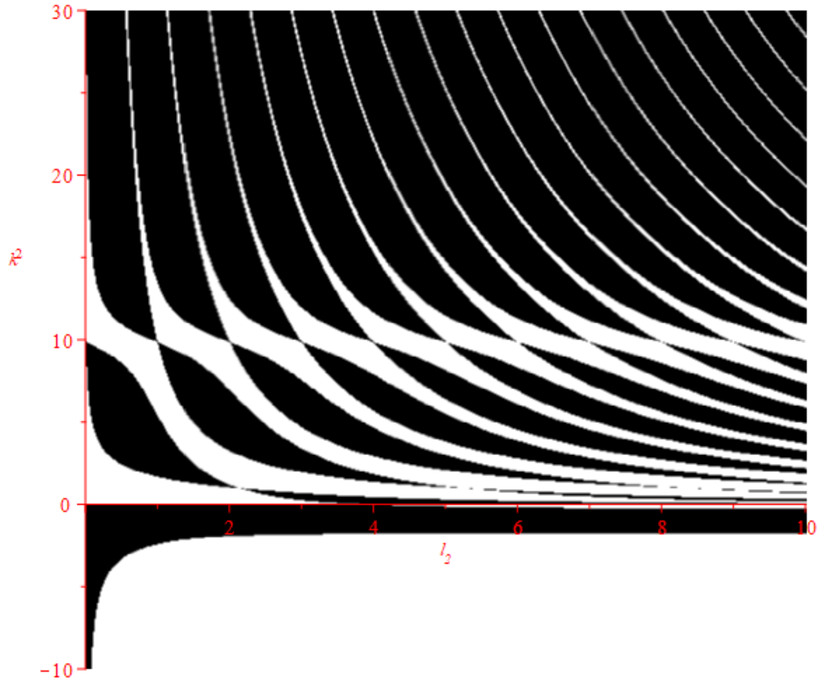

Figure 2.7: The energy scale solution for $l_1 = 1$.

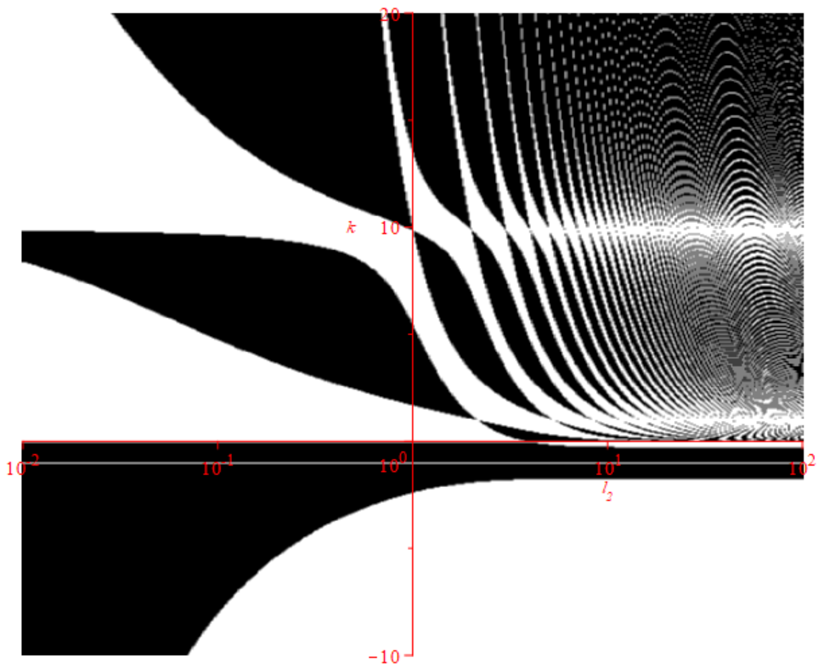

Figure 2.8: The energy scale solution for $l_1 = 1$ in the logarithmic scale on the horizontal axis.

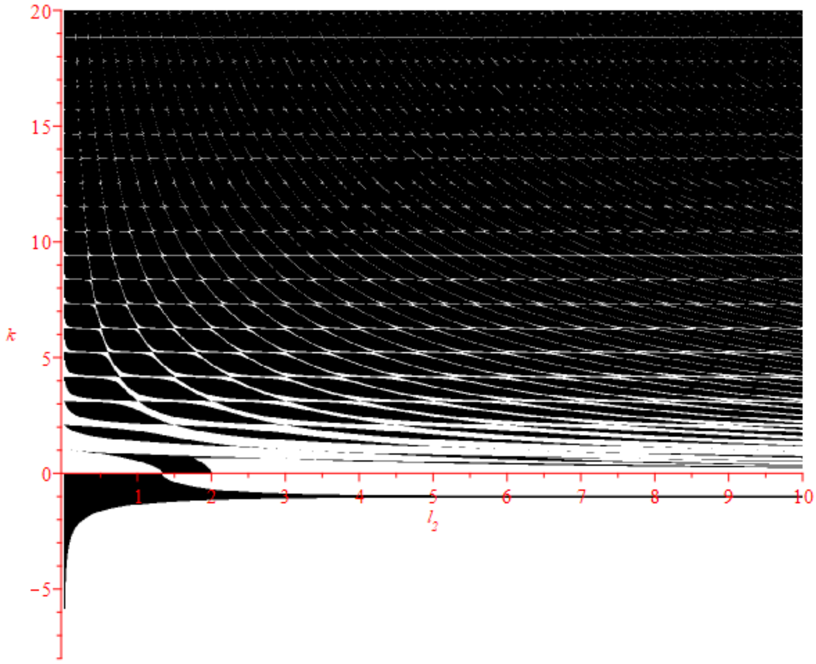

Figure 2.9: The momentum scale solution for $l_1 = 3$.

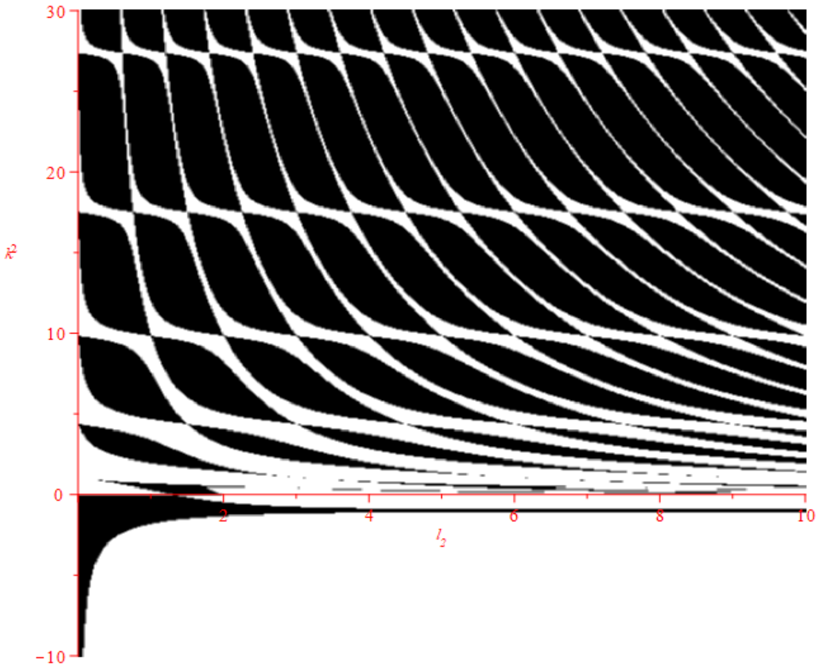

Figure 2.10: The energy scale solution for $l_1 = 3$.

Chapter 3

Rectangular lattice quantum graph - δ-coupling

3.1 Spectral condition

We recapitulate the existing results about rectangular lattice quantum graph with δ-coupling in this chapter. Those results will play important role in the following research where we will study a new parametric class of coupling which interpolates between δ-coupling and time-reversal non-invariant coupling which was introduced in the previous chapter. It is important to study the couplings between which the interpolation takes place in order to properly understand to the whole interpolation class of couplings.

The δ-coupling was widely examined in [2] and [7]. The results introduced here are mostly taken from those two articles and we recapitulate them here without proofs and further details. In order to get better insight about the problem we recommend to reader to study those articles.

The δ-coupling is, particularly for the rectangular lattice quantum graph, defined as follows

$$\psi(v) \text{ is continuous at vertex } v,$$
$$\sum_{i=1}^{4} \psi'(v) = \alpha\psi(v), \quad \alpha \in \mathbb{R},$$

or this coupling can be described by unitary matrix

$$\mathbb{U} = -\mathbb{I} + \frac{2}{n+i\alpha}\mathbb{J}, \quad \alpha \in \mathbb{R}. \tag{3.1}$$

where I is unit matrix and J denotes the matrix with all the elements equal to one.

The spectral condition is given as

$$\frac{\cos\theta_2 - \cos kl_2}{\sin kl_1} + \frac{\cos\theta_1 - \cos kl_1}{\sin kl_2} - \frac{\alpha}{2k} = 0. \tag{3.2}$$

According to [2] the number $k^2 > 0$ does not belong to the spectrum if and only if

$$\tan\left(\frac{kl_1}{2} - \frac{\pi}{2}\left\lfloor\frac{kl_1}{\pi}\right\rfloor\right) + \tan\left(\frac{kl_2}{2} - \frac{\pi}{2}\left\lfloor\frac{kl_2}{\pi}\right\rfloor\right) < \frac{\alpha}{2k}, \quad \text{for } \alpha > 0 \tag{3.3}$$

and

$$\cot\left(\frac{kl_1}{2} - \frac{\pi}{2}\left\lfloor\frac{kl_1}{\pi}\right\rfloor\right) + \cot\left(\frac{kl_2}{2} - \frac{\pi}{2}\left\lfloor\frac{kl_2}{\pi}\right\rfloor\right) < \frac{|\alpha|}{2k}, \quad \text{for } \alpha < 0 \tag{3.4}$$

where $\lfloor\cdot\rfloor$ is the floor function. Note that for $\alpha = 0$ is spectrum the positive half-line, i.e. $\sigma(\mathcal{H}) = [0, \infty]$.

3.2 Number theory notions

Before we step further let us introduce some notions from the number theory. A number $\theta \in \mathbb{R}$ is called **badly approximable** if there exist a $c > 0$ such that

$$\left|\theta - \frac{p}{q}\right| > \frac{c}{q^2} \tag{3.5}$$

for all $p, q \in \mathbb{Z}$ with $q \neq 0$. A counterpart to badly approximable numbers are so-called **Last admissible** numbers. A number $\theta \in \mathbb{R}$ is Last admissible if there are sequences $\{q_r\}_{r=1}^{\infty}, \{p_r\}_{r=1}^{\infty}$ of pairwise relatively prime integers such that

$$\lim_{r\to\infty} q_r^2 \left|\theta - \frac{p_r}{q_r}\right| = 0. \tag{3.6}$$

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

$$\mu(\theta) = \inf\left\{c > 0 \;\middle|\; (\exists_\infty (p,q) \in \mathbb{Z}^2) \;\middle|\left(|\theta - \frac{p}{q}| < \frac{c}{q^2}.\right)\right\}. \tag{3.7}$$

where $\exists_\infty$ means "there exist infinitely many". The Markov constant is positive if and only if θ is badly approximable. Moreover, the Hurwitz theorem states that for every $\theta \in \mathbb{R}$ there are infinitely many integers p, q such that

$$\left|\theta - \frac{p}{q}\right| < \frac{c}{\sqrt{5}q^2}. \tag{3.8}$$

As consequence we see that $\mu(\theta) \in [0, \frac{1}{\sqrt{5}}]$ for all $\theta \in \mathbb{R}$. Note that if θ is rational or Last admissible then Markov constant is equal to zero, i.e. $\mu(\theta) = 0$.

The following definition may be considered as one-side version of the Markov constant.

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

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

Proposition 3.1 ([7], Proposition 3.2.)**.**

$$\begin{aligned} &\nu(\theta) := \inf\{c > 0 \mid (\exists_\infty m \in \mathbb{N}) \;|(m(m\theta - \lfloor m\theta\rfloor) < c.)\}. \\ &\nu(\theta^{-1}) := \inf\{c > 0 \mid (\exists_\infty m \in \mathbb{N}) \;|(m(\lceil m\theta\rceil - m\theta) < c.)\}. \\ &\mu(\theta) = \min\{\nu(\theta), \nu(\theta^{-1})\} \end{aligned} \tag{3.10}$$

3.3 Spectral properties

Following the notation from [7] we denote $\theta = \frac{l_1}{l_2}$. Note that we omit the case $\alpha = 0$ since in this case the spectrum is trivial. Now we can collect some spectral properties:

Proposition 3.2 ([2], Proposition 3.1.)**.** *1. The spectrum has band-gap structure, $\sigma(\mathcal{H}) = \bigcup_{k=1}^{N}[\alpha_k, \beta_k]$ for some $N \geq 1$, where $\alpha_k < \beta_k < \alpha_{k+1}$.*

2. Let $\alpha > 0$. Every gap in the spectrum has the left (lower) endpoint equal to $k^2 = \left(\frac{m\pi}{l_1}\right)^2$ or $k^2 = \left(\frac{m\pi}{l_2}\right)^2$ for some $m \in \mathbb{N}$.
A gap with the left endpoint at $k^2 = \left(\frac{m\pi}{l_1}\right)^2$ is present if and only if

$$\frac{2m\pi}{l_1}\tan\left(\frac{\pi}{2}(m\theta^{-1} - \lfloor m\theta^{-1}\rfloor)\right) < \alpha. \tag{3.11}$$

A gap with the left endpoint at $k^2 = \left(\frac{m\pi}{l_2}\right)^2$ is present if and only if

$$\frac{2m\pi}{l_2}\tan\left(\frac{\pi}{2}(m\theta - \lfloor m\theta\rfloor)\right) < \alpha. \tag{3.12}$$

In particular, if

$$\frac{2m\pi}{l_1}\tan\left(\frac{\pi}{2}(m\theta^{-1} - \lfloor m\theta^{-1}\rfloor)\right) \geq \alpha \wedge \frac{2m\pi}{l_2}\tan\left(\frac{\pi}{2}(m\theta - \lfloor m\theta\rfloor)\right) \geq \alpha. \tag{3.13}$$

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

3. Let $\alpha < 0$. Every gap in the spectrum has the right (lower) endpoint equal to $k^2 = \left(\frac{m\pi}{l_1}\right)^2$ or $k^2 = \left(\frac{m\pi}{l_2}\right)^2$ for some $m \in \mathbb{N}$.
A gap with the left endpoint at $k^2 = \left(\frac{m\pi}{l_2}\right)^2$ is present if and only if

$$\frac{2m\pi}{l_1}\tan\left(\frac{\pi}{2}(\lceil m\theta^{-1}\rceil - m\theta^{-1})\right) < |\alpha|. \tag{3.14}$$

A gap with the left endpoint at $k^2 = \left(\frac{m\pi}{l_1}\right)^2$ is present if and only if

$$\frac{2m\pi}{l_2}\tan\left(\frac{\pi}{2}(\lceil m\theta\rceil - m\theta)\right) < |\alpha|. \tag{3.15}$$

In particular, if

$$\frac{2m\pi}{l_1}\tan\left(\frac{\pi}{2}(\lceil m\theta^{-1}\rceil - m\theta^{-1})\right) \geq |\alpha|. \wedge \frac{2m\pi}{l_2}\tan\left(\frac{\pi}{2}(\lceil m\theta\rceil - m\theta)\right) \geq |\alpha|. \tag{3.16}$$

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

4. $\pm\alpha_1 > 0$ holds if and only if $\pm\alpha > 0$.

5. If $\alpha < -4\frac{\sqrt{\frac{l_1}{l_2}}+\sqrt{\frac{l_2}{l_1}}}{\sqrt{l_1 l_2}}$ then $\beta_1 < 0$ and $\alpha_2 = \left(\frac{\pi}{\max(l_1,l_2)}\right)^2$

6. $\sigma(\mathcal{H})(\alpha') \cap \mathbb{R}_+ \subset \sigma(\mathcal{H})(\alpha) \cap \mathbb{R}_+$ *for* $|\alpha'| > |\alpha|$

7. *All gaps above the threshold are finite. If there is an infinite number of them, their widths are asymptotically bounded,*

$$\alpha_{k+1} - \beta_k < 2|\alpha| \frac{1}{l_1 + l_2} + \mathcal{O}\Big(\frac{1}{k}\Big) \tag{3.17}$$

The following theorems describe the number of gaps it the spectrum. Those theorems can be found in [7, Chapter 2].

Let $\alpha > 0$:

Proposition 3.3. *1. If*

$$\alpha < \pi^2 \cdot \min\Big\{\frac{\nu(\theta)}{l_2}, \frac{\nu(\theta)^{-1}}{l_1}\Big\}, \tag{3.18}$$

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

2. If

$$\alpha > \pi^2 \cdot \min\Big\{\frac{\nu(\theta)}{l_2}, \frac{\nu(\theta)^{-1}}{l_1}\Big\} \tag{3.19}$$

then the spectrum has infinitely many gaps.

Theorem 3.1. *Let*

$$\gamma := \min\Big\{\inf_{m\in\mathbb{N}} \Big\{\frac{2m\pi}{l_1} \tan\Big(\frac{\pi}{2}(m\theta^{-1} - \lfloor m\theta^{-1}\rfloor)\Big)\Big\}, \min_{m\in\mathbb{N}} \Big\{\frac{2m\pi}{l_2} \tan\Big(\frac{\pi}{2}(m\theta - \lfloor m\theta\rfloor)\Big)\Big\}\Big\}. \tag{3.20}$$

If the coupling constant α *satisfies*

$$\gamma < \alpha < \pi^2 \cdot \min\Big\{\frac{\nu(\theta)}{l_2}, \frac{\nu(\theta)^{-1}}{l_1}\Big\}, \tag{3.21}$$

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

Let $\alpha < 0$:

Proposition 3.4. *1. If*

$$|\alpha| < \pi^2 \cdot \min\Big\{\frac{\nu(\theta)}{l_1}, \frac{\nu(\theta)^{-1}}{l_2}\Big\}, \tag{3.22}$$

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

2. If

$$|\alpha| > \pi^2 \cdot \min\Big\{\frac{\nu(\theta)}{l_1}, \frac{\nu(\theta)^{-1}}{l_2}\Big\} \tag{3.23}$$

then the spectrum has infinitely many gaps.

Theorem 3.2. *Let*

$$\gamma := \min\Big\{ \inf_{m\in\mathbb{N}} \Big\{ \frac{2m\pi}{l_1} \tan\Big(\frac{\pi}{2}(\lceil m\theta^{-1}\rceil - m\theta^{-1})\Big)\Big\}, \min_{m\in\mathbb{N}} \Big\{ \frac{2m\pi}{l_2} \tan\Big(\frac{\pi}{2}(\lceil m\theta\rceil - m\theta)\Big)\Big\}\Big\}. \tag{3.24}$$

If the coupling constant α satisfies

$$\gamma < \alpha < \pi^2 \cdot \min\Big\{\frac{\nu(\theta)}{l_1}, \frac{\nu(\theta)^{-1}}{l_2}\Big\}, \tag{3.25}$$

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

Remark 3.1. At the first sight the foregoing theorems looks similar for $\alpha > 0$ and $\alpha < 0$ but there are slight differences. Of course there is taken the absolute value of α in case of $\alpha < 0$ but also $\min\Big\{\frac{\nu(\theta)}{l_2}, \frac{\nu(\theta)^{-1}}{l_1}\Big\}$ and $\min\Big\{\frac{\nu(\theta)}{l_1}, \frac{\nu(\theta)^{-1}}{l_2}\Big\}$ are different expressions.

Corollary 3.1.

1. *If θ id rational number or Last admissible then the spectrum has infinitely many gaps for $\alpha \neq 0$.*
2. *For badly approximable θ there exist $\gamma > 0$ such that $\gamma < \alpha < \pi^2 \cdot \min\Big\{\frac{\nu(\theta)}{l_2}, \frac{\nu(\theta)^{-1}}{l_1}\Big\}$ for $\alpha > 0$, resp. $\gamma < |\alpha| < \pi^2 \cdot \min\Big\{\frac{\nu(\theta)}{l_1}, \frac{\nu(\theta)^{-1}}{l_2}\Big\}$ for $\alpha < 0$ the spectrum has no gaps above the threshold.*
3. *For all $\theta \in \mathbb{R}$ the spectrum has infinitely many gaps if $\alpha > \pi^2 \cdot \min\Big\{\frac{\nu(\theta)}{l_2}, \frac{\nu(\theta)^{-1}}{l_1}\Big\}$ for $\alpha > 0$, resp. $|\alpha| > \pi^2 \cdot \min\Big\{\frac{\nu(\theta)}{l_1}, \frac{\nu(\theta)^{-1}}{l_2}\Big\}$ for $\alpha < 0$*

The following theorem illustrates how the spectrum changes when $\frac{l_1}{l_2}$ is equal to the golden ration. The golden ratio is the "worst" approximable number in sense that $\mu(\theta) = \nu(\theta) = \nu(\theta^{-1}) = \frac{1}{\sqrt{5}}$. Particularly, this case illustrates that there can occur situations when infinite periodic quantum graphs have no-zero finitely many gaps in the spectrum. Those quantum graphs are sometimes called **Bethe-Sommerfeld** graphs or we say that a quantum graph has **Bethe-Sommerfeld** property.

Theorem 3.3. *Let $\theta = \frac{l_1}{l_2} = \frac{\sqrt{5}+1}{2}$, then the following claims are valid:*

1. *If $\alpha > \frac{\pi^2}{\sqrt{5}a}$ or $\alpha \leq -\frac{\pi^2}{\sqrt{5}a}$, there are infinitely many spectral gaps.*
2. *If*
$$-\frac{2\pi}{a} \tan\Big(\frac{3-\sqrt{5}}{4}\pi\Big) \leq \alpha \leq \frac{\pi^2}{\sqrt{5}a} \tag{3.26}$$
there are no gaps in the spectrum.
3. *If*
$$-\frac{\pi^2}{\sqrt{5}a} < \alpha < -\frac{2\pi}{a} \tan\Big(\frac{3-\sqrt{5}}{a}\pi\Big) \tag{3.27}$$
there is a nonzero and finite number of gaps in the spectrum.

Chapter 4

Rectangular lattice quantum graph - interpolating couplings

We follow idea of the paper [4] where a new parametric family of vertex coupling have been introduced. This parametric coupling interpolates between δ-coupling introduced in Chapter 3 and the coupling introduced in Chapter 2.

Similarly to the previous chapters we will be interested in infinite rectangular lattice quantum graphs. The goal of this chapter is to find the spectral condition and establish spectral properties of this graph.

4.1 Vertex coupling - symmetries

One way how to classify vertex coupling is to use symmetries.

Definition 4.1. Symmetry is an invertible map in the space of boundary values, $\mu : \mathbb{C}^n \mapsto \mathbb{C}^n$, or a family of such maps. A vertex coupling is symmetric with respect to μ if the condition (1.14) is equivalent to

$$(\mathbb{U} - \mathbb{I})\mu\Psi(0_+) + i(\mathbb{U} + \mathbb{I})\mu\Psi'(0_+) \tag{4.1}$$

or in other words, if $\mathbb{U}$ obeys the identity

$$\mu^{-1}\mathbb{U}\mu = \mathbb{U}. \tag{4.2}$$

Symmetries examples:

- *Mirror symmetric* coupling has the conditions (1.14) invariant to the simultaneous permutation $(1, ..., n) \mapsto (n, ..., 1)$ of the indexes of $\Psi(0_+)$ and $\Psi'(0_+)$, i.e.

$$\mu = \begin{pmatrix} 0 & 0 & \dots & 0 & 1 \\ 0 & 0 & \dots & 1 & 0 \\ \vdots & \vdots & & \ddots & \vdots \\ 0 & 1 & \ddots & 0 & 0 \\ 1 & 0 & \dots & 0 & 0 \end{pmatrix}. \tag{4.3}$$

is anti-diagonal matrix.

- *Permutation-invariant* couplings is invariant to any simultaneous permutation of the entries of $\Psi(0_+)$ and $\Psi'(0_+)$ in (1.14). In other words, the matrices μ form a representation of the symmetry group S_n.
- *Time-reversal-invariant* coupling: the μ is the anti-linear operator describing the switch in the time direction. In our case it will just be complex conjugation. Using relations $U^T\bar{\mathbb{U}} = \bar{\mathbb{U}}\mathbb{U}^T = \mathbb{I}$ we find out that the coupling must be invariant with respect to transposition, i.e. $\mathbb{U} = \mathbb{U}^T$.
- *Rotationally symmetric* couplings is invariant to cyclic permutation of the entries of $\Psi(0_+)$ and $\Psi'(0_+)$ in (1.14). The map μ has the following form,

$$R := \mu = \begin{pmatrix} 0 & 1 & 0 & \dots & 0 & 0 \\ 0 & 0 & 1 & & 0 & 0 \\ \vdots & & & \ddots & & \\ 0 & 0 & 0 & & 1 & 0 \\ 0 & 0 & 0 & & 0 & 1 \\ 1 & 0 & 0 & \dots & 0 & 0 \end{pmatrix}. \tag{4.4}$$

Proposition 4.1 ([4], Proposition 2.1.)**.** *A rotationally symmetric vertex coupling is mirror symmetric if and only if it is time-reversal-invariant.*

Remark 4.1. Let us point out that the δ-coupling introduced in Chapter 3 posses all the symmetries. On the other hand the coupling introduced in Chapter 2 associated with the choice

$$\mathbb{U} = R \tag{4.5}$$

is rotationally symmetric but is not mirror symmetric and thus also is not time-reversal-invariant.

4.2 Circulant matrix

Let us proceed to definition of parametric family of vertex coupling. First we introduce what the *circulant matrix* is.

Any matrix which have the form

$$C = \begin{pmatrix} c_0 & c_1 & \dots & c_{n-2} & c_{n-1} \\ c_{n-1} & c_0 & c_1 & & c_{n-2} \\ \vdots & c_{n-1} & c_0 & \ddots & \vdots \\ c_2 & & \ddots & \ddots & c_1 \\ c_1 & c_2 & \dots & c_{n-1} & c_0 \end{pmatrix}. \tag{4.6}$$

is called *circulant matrix*. Its normalized eigenvectors have the form

$$\nu_k = \frac{1}{\sqrt{n}}(1, \omega^k, \omega^{2k}, ..., \omega^{(n-1)k})^T, \quad k = 0, 1, ..., n-1,$$

where $\omega := e^{(\frac{2\pi i}{n})}$. The corresponding eigenvalues are

$$\lambda_k = c_0 + c_1\omega^k + c_2\omega^{2k} + ... + c_{n-1}\omega^{(n-1)k}. \tag{4.7}$$

Moreover, every circulant matrix can be diagonalized using the discrete Fourier transform matrix

$$F = \begin{pmatrix} 1 & 1 & 1 & 1 & \dots & 1 \\ 1 & \omega & \omega^2 & \omega^3 & \dots & \omega^{(n-1)} \\ 1 & \omega^2 & \omega^4 & \omega^6 & \dots & \omega^{2(n-1)} \\ \vdots & \vdots & \vdots & \vdots & & \vdots \\ 1 & \omega^{(n-1)} & \omega^{2(n-1)} & \omega^{3(n-1)} & \ddots & \omega^{(n-1)^2} \end{pmatrix}.$$

Using this we can write following identities

$$D = \frac{1}{n}F^*CF \quad \text{and} \quad C = \frac{1}{n}FDF^* \tag{4.8}$$

where D is diagonal matrix with $\lambda_0, \lambda_1, ..., \lambda_{n-1}$ on the diagonal.

4.3 Class of interpolating couplings

The class of interpolating couplings introduced in [4] is given by family of unitary matrices $U(t) : t \in [0, 1]$ such that

$$U(0) = -I + \frac{2}{n + i\alpha}J \quad \text{and} \quad U(1) = R,$$
$$\text{the map } t \mapsto U(t) \text{ is continuous on } [0, 1],$$
$$U(t) \text{ is unitary circulant for all } t \in [0, 1].$$

Indeed, we can see that this coupling is an interpolation between the δ coupling described by a unitary matrix

$$U(0) = -\mathbb{I} + \frac{2}{n + i\alpha}\mathbb{J}, \quad \alpha \in \mathbb{R}.$$

where I is unit matrix and J denotes the matrix with all elements equal to one, and between coupling which we have studied earlier, namely

$$U(1) = R := \begin{pmatrix} 0 & 1 & 0 & \dots & 0 & 0 \\ 0 & 0 & 1 & & 0 & 0 \\ \vdots & & & \ddots & & \\ 0 & 0 & 0 & & 1 & 0 \\ 0 & 0 & 0 & & 0 & 1 \\ 1 & 0 & 0 & \dots & 0 & 0 \end{pmatrix}.$$

If we use (4.7) it is not hard to find (see [4]) that eigenvalues of $U(t)$ have the form

$$\lambda_k(t) = e^{-i(1-t)\gamma} \quad \text{for } k = 0,$$
$$\lambda_k(t) = -e^{i\pi t(\frac{2k}{n} - 1)} \quad \text{for } k \geq 1,$$

where $\gamma := \arg\frac{n+i\alpha}{n-i\alpha} \in (-\pi, \pi)$, i.e. $\frac{n+i\alpha}{n-i\alpha} = e^{-i\gamma}$. Moreover, by using identities (4.8) we can easily compute matrices $U(t)$ for all $t \in [0, 1]$.

4.4 Spectral condition

We find the spectral condition of a rectangular lattice quantum graph (Figure 1.4) in the same way as we did in Chapter 2 but this time we use the vertex coupling described by $U(t)$ from the previous section. In other words we have vertex condition in the following form

$$(U(t)-I)\begin{pmatrix}\psi_1(0_+)\\ \psi_2(0_+)\\ \psi_3(0_+)\\ \psi_4(0_+)\end{pmatrix}+i(U(t)+I)\begin{pmatrix}\psi_1'(0_+)\\ \psi_2'(0_+)\\ -\psi_3'(0_+)\\ -\psi_4'(0_+)\end{pmatrix}=0$$

where ψ_i, $i=1,2,3,4$ are functions in Ansatz (2.16). Substituting (2.17) into this condition we get system of linear equations for coefficients a_1, a_2, b_1, b_2 in the matrix from

$$[(U(t)-I)M-k(U(t)+I)N]\begin{pmatrix}a_1\\ b_1\\ a_2\\ b_2\end{pmatrix}=0,$$

where matrices M, N are given by

$$M=\begin{pmatrix}1 & 1 & 0 & 0\\ 0 & 0 & 1 & 1\\ e^{i(\theta_1+kl_1)} & e^{i(\theta_1-kl_1)} & 0 & 0\\ 0 & 0 & e^{i(\theta_2+kl_2)} & e^{i(\theta_2-kl_2)}\end{pmatrix},$$

$$N=\begin{pmatrix}1 & -1 & 0 & 0\\ 0 & 0 & 1 & -1\\ -e^{i(\theta_1+kl_1)} & e^{i(\theta_1-kl_1)} & 0 & 0\\ 0 & 0 & -e^{i(\theta_2+kl_2)} & e^{i(\theta_2-kl_2)}\end{pmatrix}.$$

Using the second identity in (4.8) and putting determinant equal to zero we get

$$\det[(D-I)F^*M-k(D+I)F^*N]=0,$$

where

$$D=\begin{pmatrix}e^{-i(1-t)\alpha} & 0 & 0 & 0\\ 0 & -e^{-\frac{i}{2}t\pi} & 0 & 0\\ 0 & 0 & -1 & 0\\ 0 & 0 & & -e^{\frac{i}{2}t\pi}\end{pmatrix}, \tag{4.9}$$

$$F^*=\begin{pmatrix}1 & 1 & 1 & 1\\ 1 & -1 & -1 & i\\ 1 & -1 & 1 & -1\\ 1 & -i & -1 & i\end{pmatrix}. \tag{4.10}$$

This determinant is equal to

$$D=512e^{i(\theta_1+\theta_2)}e^{-i\frac{(1-\gamma)t}{2}}[V_3k^3+V_2k^2+V_1k+V_0] \tag{4.11}$$

where

$$
\begin{aligned}
V_3 &= -\cos\frac{(1-t)\gamma}{2}\sin^2\frac{\pi t}{4}\Big[\sin(kl_1)\big(\cos(\theta_2)+\cos(kl_2)\big)+\sin(kl_2)\big(\cos(\theta_1)+\cos(kl_1)\big)\Big],\\
V_2 &= 2\sin\frac{(1-t)\gamma}{2}\sin^2\frac{\pi t}{4}\Big[\big(\cos(\theta_1)+\cos(kl_1)\big)\big(\cos(\theta_2)+\cos(kl_2)\big)\Big],\\
V_1 &= \cos\frac{(1-t)\gamma}{2}\cos^2\frac{\pi t}{4}\Big[\sin(kl_1)\big(\cos(\theta_2)-\cos(kl_2)\big)+\sin(kl_2)\big(\cos(\theta_1)-\cos(kl_1)\big)\Big],\\
V_0 &= -2\sin\frac{(1-t)\gamma}{2}\cos^2\frac{\pi t}{4}\Big[\sin(kl_1)\sin(kl_2)\Big].
\end{aligned}
$$

We can check the correctness of this spectral condition by comparison with the previous results. First, if we put $l := l_1 = l_2$ then we obtain the spectral condition in the same form as it is in [4].

Moreover, if we put $t = 1$ then the terms V_2 and V_0 disappear thus by using simple mathematical operations on V_3 and V_1 we get the spectral condition in the form (2.20).

On the other hand if we put $t = 0$ then we get the spectral condition has the form

$$\sin kl_1\big(\cos\theta_2-\cos kl_2\big)+\sin kl_2\big(\cos\theta_1-\cos kl_1\big)-\frac{2}{k}\tan(\frac{\gamma}{2})\sin kl_1\sin kl_2=0.$$

If we use the fact that for $n = 4$ is $\tan(\frac{\gamma}{2}) = \frac{\alpha}{4}$ then we obtain the spectral condition exactly in the form (3.4).

We do not have to forgot the negative spectrum which we obtain by substituting $\kappa = ik$:

$$\kappa^3\hat{V}_3+\hat{V}_2\kappa^2+\kappa\hat{V}_1-\hat{V}_0=0 \tag{4.12}$$

where

$$
\begin{aligned}
\hat{V}_3 &= -\cos\frac{(1-t)\gamma}{2}\sinh^2\frac{\pi t}{4}\Big[\sinh(\kappa l_1)\big(\cos(\theta_2)+\cosh(\kappa l_2)\big)+\sinh(\kappa l_2)\big(\cos(\theta_1)+\cosh(\kappa l_1)\big)\Big],\\
\hat{V}_2 &= 2\sin\frac{(1-t)\gamma}{2}\sin^2\frac{\pi t}{4}\Big[\big(\cos(\theta_1)+\cosh(\kappa l_1)\big)\big(\cos(\theta_2)+\cosh(\kappa l_2)\big)\Big],\\
\hat{V}_1 &= \cos\frac{(1-t)\gamma}{2}\cos^2\frac{\pi t}{4}\Big[\sinh(\kappa l_1)\big(\cos(\theta_2)-\cosh(\kappa l_2)\big)+\sinh(\kappa l_2)\big(\cos(\theta_1)-\cosh(\kappa l_1)\big)\Big],\\
\hat{V}_0 &= -2\sin\frac{(1-t)\gamma}{2}\cos^2\frac{\pi t}{4}\Big[\sinh(\kappa l_1)\sinh(\kappa l_2)\Big].
\end{aligned}
$$

4.5 Quadratic form

Before we star to analyze the spectral condition we find out the quadratic form of the Hamiltonian $\mathcal{H}$. In order to do that we use Remark 1.3 and Theorem 1.2. First we have to find out matrices $\mathbb{A}(t) = U(t) - \mathbb{I}$ and $\mathbb{B}(t) = i(U(t) + \mathbb{I})$. We know that

$$
\begin{aligned}
\mathbb{A}(t) = U(t)-\mathbb{I} &= \frac{1}{4}F(D-\mathbb{I})F^\star,\\
\mathbb{B}(t) = i(U(t)+\mathbb{I}) &= \frac{i}{4}F(D+\mathbb{I})F^\star,
\end{aligned}
$$

where D, resp. F are defined in (4.9), resp. (4.10). Computing those expressions we obtain

$$\mathbb{A}(t) = \begin{pmatrix} e^{-i(1-t)\gamma}-5-2\cos(\frac{\pi t}{2}) & e^{-i(1-t)\gamma}+1+2\sin(\frac{\pi t}{2}) & e^{-i(1-t)\gamma}-1+2\cos(\frac{\pi t}{2}) & e^{-i(1-t)\gamma}+1-2\sin(\frac{\pi t}{2}) \\ e^{-i(1-t)\gamma}+1-2\sin(\frac{\pi t}{2}) & e^{-i(1-t)\gamma}-5-2\cos(\frac{\pi t}{2}) & e^{-i(1-t)\gamma}+1+2\sin(\frac{\pi t}{2}) & e^{-i(1-t)\gamma}-1+2\cos(\frac{\pi t}{2}) \\ e^{-i(1-t)\gamma}-1+2\cos(\frac{\pi t}{2}) & e^{-i(1-t)\gamma}+1-2\sin(\frac{\pi t}{2}) & e^{-i(1-t)\gamma}-5-2\cos(\frac{\pi t}{2}) & e^{-i(1-t)\gamma}+1+2\sin(\frac{\pi t}{2}) \\ e^{-i(1-t)\gamma}+1+2\sin(\frac{\pi t}{2}) & e^{-i(1-t)\gamma}-1+2\cos(\frac{\pi t}{2}) & e^{-i(1-t)\gamma}+1-2\sin(\frac{\pi t}{2}) & e^{-i(1-t)\gamma}-5-2\cos(\frac{\pi t}{2}) \end{pmatrix},$$

$$\mathbb{B}(t) = \begin{pmatrix} e^{-i(1-t)\gamma}+3-2\cos(\frac{\pi t}{2}) & e^{-i(1-t)\gamma}+1+2\sin(\frac{\pi t}{2}) & e^{-i(1-t)\gamma}-1+2\cos(\frac{\pi t}{2}) & e^{-i(1-t)\gamma}+1-2\sin(\frac{\pi t}{2}) \\ e^{-i(1-t)\gamma}+1-2\sin(\frac{\pi t}{2}) & e^{-i(1-t)\gamma}+3-2\cos(\frac{\pi t}{2}) & e^{-i(1-t)\gamma}+1+2\sin(\frac{\pi t}{2}) & e^{-i(1-t)\gamma}-1+2\cos(\frac{\pi t}{2}) \\ e^{-i(1-t)\gamma}-1+2\cos(\frac{\pi t}{2}) & e^{-i(1-t)\gamma}+1-2\sin(\frac{\pi t}{2}) & e^{-i(1-t)\gamma}+3-2\cos(\frac{\pi t}{2}) & e^{-i(1-t)\gamma}+1+2\sin(\frac{\pi t}{2}) \\ e^{-i(1-t)\gamma}+1+2\sin(\frac{\pi t}{2}) & e^{-i(1-t)\gamma}-1+2\cos(\frac{\pi t}{2}) & e^{-i(1-t)\gamma}+1-2\sin(\frac{\pi t}{2}) & e^{-i(1-t)\gamma}+3-2\cos(\frac{\pi t}{2}) \end{pmatrix}.$$

Using Remark 1.3 we find out that

$$\begin{aligned} \mathrm{Ran}P_D &= \mathrm{Ker}\mathbb{B} = \mathrm{Span}\{(-1,1,-1,1)^T\} \\ \mathrm{Ran}P_N &= \mathrm{Ker}\mathbb{A} = \emptyset, \\ P_R &= \mathbb{I} - P_N - P_D. \end{aligned}$$

Now we can compute $\Lambda = \mathbb{B}^{-1}\mathbb{A}P_R$ and we get

$$\Lambda = \begin{pmatrix} \frac{(\cos\frac{\pi t}{2}+\sin\frac{\pi t}{2}-1)e^{-i(1-t)\gamma}-\cos\frac{\pi t}{2}+\sin\frac{\pi t}{2}+1}{2(e^{-i(1-t)\gamma}+1)(\cos(\frac{\pi t}{2})-1)} & -\frac{\sin(\frac{\pi t}{2})}{\cos(\frac{\pi t}{2})-1} & \frac{(\cos\frac{\pi t}{2}+\sin\frac{\pi t}{2}-1)e^{-i(1-t)\gamma}-\cos\frac{\pi t}{2}+\sin\frac{\pi t}{2}+1}{2(e^{-i(1-t)\gamma}+1)(\cos(\frac{\pi t}{2})-1)} \\ \frac{(\cos\frac{\pi t}{2}+\sin\frac{\pi t}{2}-1)e^{-i(1-t)\gamma}-\cos\frac{\pi t}{2}+\sin\frac{\pi t}{2}+1}{2(e^{-i(1-t)\gamma}+1)(\cos(\frac{\pi t}{2})-1)} & 0 & \frac{(\cos\frac{\pi t}{2}-\sin\frac{\pi t}{2}-1)e^{-i(1-t)\gamma}-\cos\frac{\pi t}{2}-\sin\frac{\pi t}{2}+1}{2(e^{-i(1-t)\gamma}+1)(\cos(\frac{\pi t}{2})-1)} \\ \frac{(\cos\frac{\pi t}{2}-\sin\frac{\pi t}{2}-1)e^{-i(1-t)\gamma}-\cos\frac{\pi t}{2}-\sin\frac{\pi t}{2}+1}{2(e^{-i(1-t)\gamma}+1)(\cos(\frac{\pi t}{2})-1)} & -\frac{\sin(\frac{\pi t}{2})}{\cos(\frac{\pi t}{2})-1} & \frac{(\cos\frac{\pi t}{2}-\sin\frac{\pi t}{2}-1)e^{-i(1-t)\gamma}-\cos\frac{\pi t}{2}-\sin\frac{\pi t}{2}+1}{2(e^{-i(1-t)\gamma}+1)(\cos(\frac{\pi t}{2})-1)} \end{pmatrix}$$

Finally, the Theorem 1.2 claims that

$$h[f,f] = \sum_{e\in\mathcal{E}} \int_e \left|\frac{df}{dx}\right|^2 + \sum_{v\in\mathcal{V}} \langle \Lambda_v P_{R,v}F, P_{R,v}F\rangle,$$

If we maintain notation which we use in this chapter the quadratic form takes the following form for $t \in (0,1]$:

$$\begin{aligned} h[\psi,\psi] = \sum_{i=1}^{4}\int_{e_i}\left|\frac{d\psi}{dx}\right|^2 + \frac{1}{2(e^{-i(1-t)\gamma}+1)(\cos(\frac{\pi t}{2})-1)} \times \\ \times\Big[\big((\psi_3+\psi_1)(\psi_1+\psi_2+\psi_3)\cos(\frac{\pi t}{2}) + (\psi_1-\psi_3)(\psi_3-\psi_2+\psi_1)\sin(\frac{\pi t}{2}) - (\psi_3-\psi_1)(\psi_1+\psi_2+\psi_3)\big)e^{-i(1-t)\gamma} - \\ (\psi_3+\psi_1)(\psi_1+\psi_2+\psi_3)\cos(\frac{\pi t}{2}) + (\psi_1-\psi_3)(\psi_3-\psi_2+\psi_1)\sin(\frac{\pi t}{2}) - (\psi_3-\psi_1)(\psi_1+\psi_2+\psi_3)\Big], \end{aligned}$$

where we for sake of simplicity used the following notation

$$\begin{pmatrix}\psi_1\\ \psi_2\\ \psi_3\\ \psi_4\end{pmatrix} \equiv \begin{pmatrix}\psi_1(0_+)\\ \psi_2(0_+)\\ \psi_3(0_+)\\ \psi_4(0_+)\end{pmatrix}$$

In case $t = 0$ the quadratic form takes a simpler form

$$h[\psi,\psi] = \sum_{i=1}^{4}\int_{e_i}\left|\frac{d\psi}{dx}\right|^2 + \alpha|\psi(0_+)|^2$$

where $\psi(0_+) := \psi_1(0_+) = \psi_2(0_+) = \psi_3(0_+) = \psi_4(0_+)$ since coupling is continuous at the vertex.

4.6 Spectrum of a rectangular lattice: case $\alpha = 0$

Let us put $\alpha = 0$. This imply that γ is also equal to zero and the δ-coupling becomes the Kirchhoff coupling introduced above. Since $\gamma = 0$ we can see that terms V_0 and V_2 in (4.11) disappear. Taking only V_1 and V_3 into account we can simplify the positive, resp. negative spectral conditions into the following form

$$\begin{aligned} &\sin kl_1\Big(\frac{k^2\sin^2\frac{\pi}{4}t-\cos^2\frac{\pi}{4}t}{k^2\sin^2\frac{\pi}{4}t+\cos^2\frac{\pi}{4}t}\cos\theta_2+\cos kl_2\Big)+ \\ &\sin kl_2\Big(\frac{k^2\sin^2\frac{\pi}{4}t-\cos^2\frac{\pi}{4}t}{k^2\sin^2\frac{\pi}{4}t+\cos^2\frac{\pi}{4}t}\cos\theta_1+\cos kl_1\Big)=0, \end{aligned} \tag{4.13}$$

resp.

$$\begin{aligned} &\sinh\kappa l_1\Big(\frac{\kappa^2\sin^2\frac{\pi}{4}t+\cos^2\frac{\pi}{4}t}{\kappa^2\sin^2\frac{\pi}{4}t-\cos^2\frac{\pi}{4}t}\cos\theta_2+\cosh\kappa l_2\Big)+ \\ &\sinh\kappa l_2\Big(\frac{\kappa^2\sin^2\frac{\pi}{4}t+\cos^2\frac{\pi}{4}t}{\kappa^2\sin^2\frac{\pi}{4}t-\cos^2\frac{\pi}{4}t}\cos\theta_1+\cosh\kappa l_1\Big)=0, \end{aligned}$$

We can see that those conditions are much similar to those in Chapter 2, namely (2.20) and (2.21). On the other hand this time there is a family of functions

$$f_t^{(p)}(k) := \frac{k^2\sin^2\frac{\pi}{4}t-\cos^2\frac{\pi}{4}t}{k^2\sin^2\frac{\pi}{4}t+\cos^2\frac{\pi}{4}t}\quad t\in[0,1],$$

resp.

$$f_t^{(n)}(k) := \frac{\kappa^2\sin^2\frac{\pi}{4}t+\cos^2\frac{\pi}{4}t}{\kappa^2\sin^2\frac{\pi}{4}t-\cos^2\frac{\pi}{4}t}\quad t\in[0,1]$$

which interpolate between

$$f_0^{(p)}(k) = -1 \quad \text{and} \quad f_1^{(p)}(k) = \frac{(k^2-1)}{(k^2+1)},$$

resp.

$$f_0^{(n)}(\kappa) = -1 \quad \text{and} \quad f_1^{(n)}(\kappa) = \frac{(\kappa^2+1)}{(\kappa^2-1)}.$$

Let us first study the case $t = 0$. The spectral conditions take the form

$$\sin kl_1\Big(-\cos\theta_2+\cos kl_2\Big)+\sin kl_2\Big(-\cos\theta_1+\cos kl_1\Big)=0,$$

$$\sinh\kappa l_1\Big(-\cos\theta_2+\cosh\kappa l_2\Big)+\sinh\kappa l_2\Big(-\cos\theta_1+\cosh\kappa l_1\Big)=0.$$

We can immediately see that the first condition can be satisfied everywhere and the second one nowhere. Thus the positive spectrum consists of whole positive half-line and the negative spectrum is empty.

The case $t = 1$ was studied in Chapter 2. Now the cases where $t \in (0,1)$ are similar to the case $t = 1$ because all the functions $f_t^{(p)}(k)$, resp. $f_t^{(n)}(\kappa)$ have similar form for $t \in (0,1]$ (see Figure 4.1). This observation allows us to use similar generalized methods to establish the spectral properties as we used in Chapter 2.

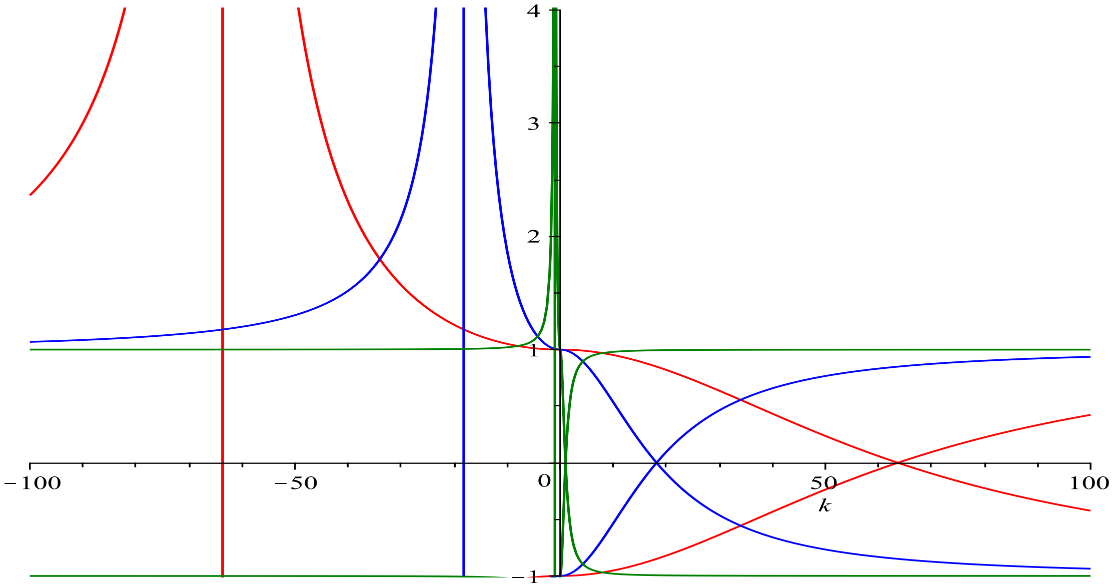

Figure 4.1: Interpolation of functions $\pm f_t^{(p)}(k)$ and $f_t^{(n)}(\kappa)$, $t \in [0,1]$. Note that $\pm f_0^{(p)}(k) = \pm 1$ and $f_0^{(n)}(\kappa) = \pm 1$. Red: $t = 0.02$. Blue: $t = 0.07$. Green: $t = 1$.

Proposition 4.2. *Let $\frac{l_1}{l_2}$ be rational number, i.e. $\frac{l_1}{l_2} = \frac{m}{n}$ for some $m, n \in \mathbb{N}$. Then $k = \frac{m\pi}{l_1} \equiv \frac{n\pi}{l_2}$ is an infinitely degenerate eigenvalue.*

Proof. The expression (4.13) claims that k belongs to the spectrum if

$$\sin(kl_1) = 0 \wedge \sin(kl_2) = 0 \Leftrightarrow (\exists m, n \in \mathbb{N})\Big(k = \frac{m\pi}{l_1} \wedge k = \frac{n\pi}{l_2}\Big) \Leftrightarrow$$
$$\Leftrightarrow (\exists m, n \in \mathbb{N})\Big(\frac{l_1}{l_2} = \frac{m}{n}\Big). \tag{4.14}$$

Thus $k = \frac{m\pi}{l_1} = \frac{n\pi}{l_2}$ belongs to the spectrum.

We will see later that in the vicinity of this point there are spectral gaps (see Theorem 4.1 below). This fact together with Theorem 1.4 imply that k belongs to the point spectrum. Moreover, the fact that this solution does not depend on θ_1, θ_2 imply that this point is infinitely degenerate eigenvalue. □

Corollary 4.1. *If $\frac{l_1}{l_2}$ is a rational number then the number of infinitely degenerate eigenvalues is infinite.*

Proof. It is clear that if $\frac{l_1}{l_2}$ is a rational number then there is an infinite number of points such that (4.14) is fulfilled. All those points are infinitely degenerate eigenvalues by Proposition 4.2. □

Lemma 4.1. *Suppose that $t \in (0,1]$ is fixed and $(\cos(kl_1) \neq \pm 1 \wedge \cos(kl_2) \neq \pm 1)$. Then a number k satisfying*

$$|\cos(kl_1)| > \left|\frac{k^2 \sin^2 \frac{\pi}{4}t - \cos^2 \frac{\pi}{4}t}{k^2 \sin^2 \frac{\pi}{4}t + \cos^2 \frac{\pi}{4}t}\right| \wedge |\cos(kl_2)| > \left|\frac{k^2 \sin^2 \frac{\pi}{4}t - \cos^2 \frac{\pi}{4}t}{k^2 \sin^2 \frac{\pi}{4}t + \cos^2 \frac{\pi}{4}t}\right| \tag{4.15}$$

and

$$\operatorname{sgn}\big[\sin(kl_2)\cos(kl_1)\big] = \operatorname{sgn}\big[\sin(kl_1)\cos(kl_2)\big] \tag{4.16}$$

does not belong to the spectrum.

Proof. The first condition (4.15) ensures that the both expressions in the square brackets in the (4.13) are not equal to zero. The second condition (4.16) ensures that the both summands in the (4.13) have the same sign. Consequently, left-hand side of the condition (4.13) can not vanish. □

Theorem 4.1. *For every $t \in (0, 1]$ and every $l_1, l_2 > 0$ there exists a spectral gap in the vicinity of each point of a set $\{\frac{m\pi}{l_1}, \frac{n\pi}{l_2}\}$, $m, n \in \mathbb{N}$.*

Remark 4.2. In particular, the points of the set $\{\frac{m\pi}{l_1}, \frac{n\pi}{l_2}\}_{m,n\in\mathbf{N}}$ may or may not belong to the spectrum in dependence if $\frac{l_1}{l_2}$ is rational or not.

Proof. Let $t \in (0, 1]$ be fixed. We show this statement for an arbitrary point of the set $\{\frac{n\pi}{l_1}\}$, $n \in \mathbb{N}$. For the points of the set $\{\frac{m\pi}{l_2}\}$, $m \in \mathbb{N}$, the proof would be analogous.

Let k' be an arbitrary fixed point of the set $\{\frac{n\pi}{l_1}\}_{n\in\mathbb{N}}$. This, in particular, means that $\cos(k'l_1) = \pm 1$. Now we divide the proof into two cases. The first case refers to $\cos(k'l_2) \neq \pm 1$ and the second one to $\cos(k'l_2) = \pm 1$.

1. Let's start with the first case. We have $k' \in \{\frac{n\pi}{l_1}\}_{n\in\mathbb{N}}$ such that

$$\cos(k'l_1) = \pm 1 \Leftrightarrow \sin(k'l_1) = 0 \quad \wedge \quad \cos(k'l_2) \neq \pm 1 \Leftrightarrow \sin(k'l_2) \neq 0.$$

It can be immediately seen from (2.20) that k' does not belong to the spectrum since the second summand is equal to zero and the first one is not.

Now let us consider a neighborhood of this point. Since $\sin(k'l_2) \neq 0$ and function $x \mapsto \sin(x)$ is a continuous then there exists a $\delta_1 > 0$ and a constant $C_1 > 0$ such that

$$|\sin(kl_2)| > C_1 \quad \text{for all } k \text{ such that} \quad |k' - k| < \delta_1. \tag{4.17}$$

Hence for all k from the δ_1-neighborhood we can divide the condition (2.20) by $\sin(kl_2)$ and we get

$$\begin{aligned}\Phi_1\big(k, \theta_1, \theta_2\big) := \Big[\Big(&\frac{k^2\sin^2\frac{\pi}{4}t - \cos^2\frac{\pi}{4}t}{k^2\sin^2\frac{\pi}{4}t + \cos^2\frac{\pi}{4}t}\cos\theta_1 + \cos kl_1\Big)\Big] + \\ &\frac{\sin(kl_1)}{\sin(kl_2)}\Big[\Big(\frac{k^2\sin^2\frac{\pi}{4}t - \cos^2\frac{\pi}{4}t}{k^2\sin^2\frac{\pi}{4}t + \cos^2\frac{\pi}{4}t}\cos\theta_2 + \cos kl_2\Big)\Big].\end{aligned} \tag{4.18}$$

Moreover, using assumption we know that $\sin(k'l_1) = 0$. Thus for every $\varepsilon > 0$ there exists $0 < \delta_2 < \delta_1$ such that

$$\left|\frac{\sin(kl_1)}{\sin(kl_2)}\Big[\frac{k^2\sin^2\frac{\pi}{4}t - \cos^2\frac{\pi}{4}t}{k^2\sin^2\frac{\pi}{4}t + \cos^2\frac{\pi}{4}t}\cos(\theta_2) + \cos(kl_2)\Big]\right| < \left|\frac{\sin(kl_1)}{C_1}\cdot 2\right| < \varepsilon, \tag{4.19}$$

for all k in δ_2-neighborhood $H^{(1)}_{k'}$ of k', i.e. $H^{(1)}_{k'} := \{\ k \in \mathbb{R} \mid |k' - k| < \delta_2\}$. There we considered (4.17) and the fact that

$$\left|\frac{k^2 \sin^2 \frac{\pi}{4}t - \cos^2 \frac{\pi}{4}t}{k^2 \sin^2 \frac{\pi}{4}t + \cos^2 \frac{\pi}{4}t} \cos(\theta_2) + \cos(kl_2)\right| \leq 2.$$

On the other hand $\cos(k'l_2) = \pm 1$. Hence there exist $\delta_3 > 0$ and a constant $C_2 > 0$ such that

$$\left|\frac{k^2 \sin^2 \frac{\pi}{4}t - \cos^2 \frac{\pi}{4}t}{k^2 \sin^2 \frac{\pi}{4}t + \cos^2 \frac{\pi}{4}t} \cos(\theta_1) + \cos(kl_1)\right| > C_2$$

for all k in the δ_3-neighborhood $H^{(2)}_{k'} := \{\ k \in \mathbb{R} \mid |k' - k| < \delta_3\}$ of k'.

Now if we choose ε in (4.19) as $\varepsilon := C_2$ then we get

$$\left|\frac{k^2 \sin^2 \frac{\pi}{4}t - \cos^2 \frac{\pi}{4}t}{k^2 \sin^2 \frac{\pi}{4}t + \cos^2 \frac{\pi}{4}t} \cos(\theta_1) + \cos(kl_1)\right| > C_2 \quad \wedge \tag{4.20}$$
$$\left|\frac{\sin(kl_1)}{\sin(kl_2)}\left[\frac{k^2 \sin^2 \frac{\pi}{4}t - \cos^2 \frac{\pi}{4}t}{k^2 \sin^2 \frac{\pi}{4}t + \cos^2 \frac{\pi}{4}t} \cos(\theta_2) + \cos(kl_2)\right]\right| < C_2$$

for all $k \in H_{k'} := H^{(1)}_{k'} \cap H^{(2)}_{k'}$. This implies that for every $k \in H_{k'}$ the expression (4.18) can not be equal to zero and thus $H_{k'}$ can not belong to the spectrum.

2. The second part of the proof takes into account the case when

$$\cos(k'l_1) = \pm 1 \Leftrightarrow \sin(k'l_1) = 0 \quad \wedge \quad \cos(k'l_2) = \pm 1 \Leftrightarrow \sin(k'l_2) = 0$$

for some $k' \in \{\frac{n\pi}{l_1}\}_{n \in \mathbb{N}}$.

Using Proposition 4.2 we find that k' is an infinitely degenerate eigenvalue.

On the other hand in the vicinity of this point the Lemma 4.1 the assumptions are fulfilled.

Indeed, since $\cos(k'l_1) = \cos(k'l_2) = \pm 1$ we can find $\delta > 0$ such that the first condition (4.15) is fulfilled on the interval $(k' - \delta, k' + \delta)$:

If $\cos(k'l_1) = \cos(k'l_2) = 1$ then functions $\cos(kl_1)$, $\cos(kl_2)$ are positive for all $k \in (k' - \delta, k' + \delta)$. In addition to that, the functions $\sin(kl_1)$, $\sin(kl_2)$ have the same sign on $(k' - \delta, k')$, resp. on $(k', k' + \delta)$. This implies that the condition (4.16) is satisfied on $(k' - \delta, k')$, resp. on $(k', k' + \delta)$.

On the other hand if $\cos(k'l_1) = 1$ and $\cos(k'l_2) = -1$ then functions $\cos(kl_1), \cos(kl_2)$ have opposite signs on $(k' - \delta, k' + \delta)$. The same statement is valid for functions $\sin(kl_1)$, $\sin(kl_2)$ on $(k' - \delta, k')$, resp. on $(k', k' + \delta)$. Thus the condition (4.16) is also satisfied on $(k' - \delta, k')$, resp. on $(k', k' + \delta)$.

The other cases are similar to the previous ones.

Finally, Lemma 4.1 implies that the intervals $(k' - \delta, k')$ and $(k', k' + \delta)$ do not belong to the spectrum. □

Proposition 4.3. *The gap width tends asymptotically to zero at the momentum scale for every $t \in (0,1]$.*

Proof. It can be seen from the condition (4.13) that gaps can only appear somewhere where k satisfy

$$|\cos(kl_1)| > \left|\frac{k^2 \sin^2 \frac{\pi}{4}t - \cos^2 \frac{\pi}{4}t}{k^2 \sin^2 \frac{\pi}{4}t + \cos^2 \frac{\pi}{4}t}\right| \vee |\cos(kl_2)| > \left|\frac{k^2 \sin^2 \frac{\pi}{4}t - \cos^2 \frac{\pi}{4}t}{k^2 \sin^2 \frac{\pi}{4}t + \cos^2 \frac{\pi}{4}t}\right|.$$

If we formally send k to infinity then we get

$$|\cos(kl_1)| > 1 \vee |\cos(kl_2)| > 1.$$

Function $k \mapsto \frac{k^2 \sin^2 \frac{\pi}{4}t - \cos^2 \frac{\pi}{4}t}{k^2 \sin^2 \frac{\pi}{4}t + \cos^2 \frac{\pi}{4}t}$ is strictly monotonous thus the gap width monotonically decreases to zero when momentum goes to infinity. □

Theorem 4.2. *Let us have the periodic rectangular lattice quantum graph (Figure 1.4) with the Hamiltonian $\mathcal{H} := -\frac{d^2}{dx^2}$ and with the vertex conditions determined by the matrix $U(t)$, $t \in (0,1]$. Then its spectrum has the following properties:*

Positive spectrum

- *For every $l_1, l_2 > 0$ there are infinitely many gaps. The gaps are located in the vicinity of the points $\{\frac{m\pi}{l_1}, \frac{n\pi}{l_2}\}$, $m, n \in \mathbb{N}$ in the momentum scale.*
- *If $\frac{l_1}{l_2}$ is a rational number then there are infinitely many infinitely degenerate eigenvalues.*
- *The gap width goes asymptotically to zero in the momentum scale.*

Negative spectrum

- *Point $-\cot(\frac{\pi}{4}t)$ always belongs to the spectrum. There exist spectral band in the vicinity of this point. Thus inf $\sigma(H) < -\cot(\frac{\pi}{4}t)$.*

4.7 Analytic solution $\alpha = 0$ - illustrated by plots

This section is a generalization of Section 2.2. Namely, $t \in [0,1]$ instead of $t = 1$ and correspondingly $k \mapsto \pm\frac{k^2 \sin^2 \frac{\pi}{4}t - \cos^2 \frac{\pi}{4}t}{k^2 \sin^2 \frac{\pi}{4}t + \cos^2 \frac{\pi}{4}t}$, $\kappa \mapsto \frac{\kappa^2 \sin^2 \frac{\pi}{4}t + \cos^2 \frac{\pi}{4}t}{\kappa^2 \sin^2 \frac{\pi}{4}t - \cos^2 \frac{\pi}{4}t}$ instead of $k \mapsto \pm\frac{k^2-1}{k^2+1}$, $\kappa \mapsto \frac{\kappa^2+1}{\kappa^2-1}$, respectively. We refer reader to this section where the detailed description can be found.

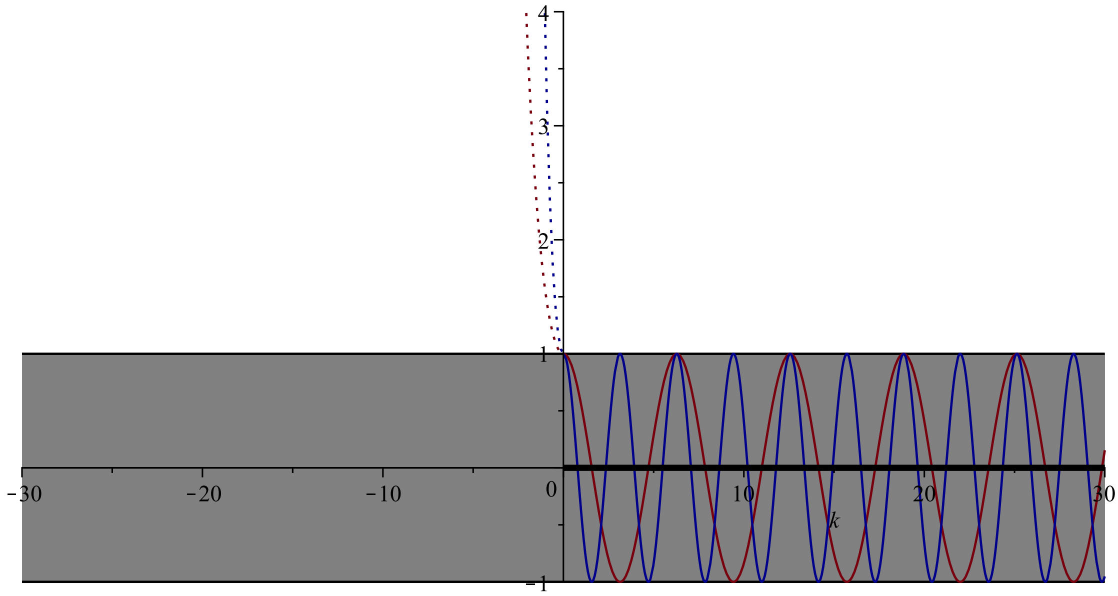

Figure 4.2: The situation for edge lengths $l_1 = 1$, $l_2 = 2$ and $t = 0$.

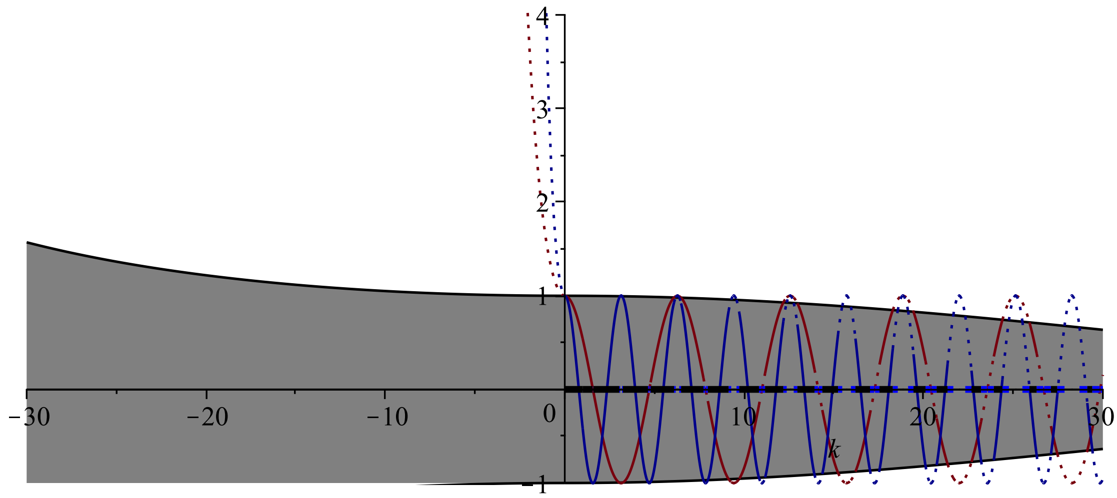

Figure 4.3: The situation for edge lengths $l_1 = 1$, $l_2 = 2$ and $t = 0.02$.

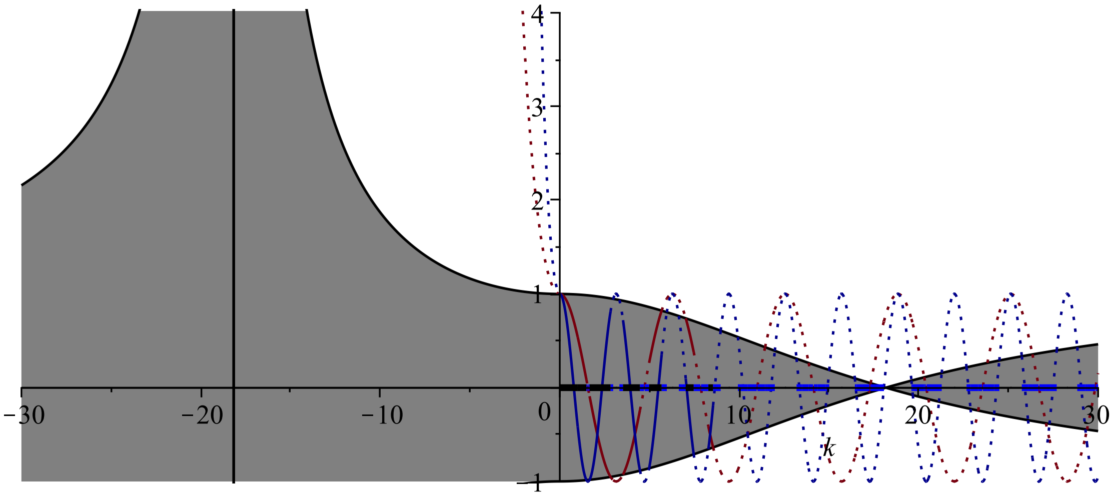

Figure 4.4: The situation for edge lengths $l_1 = 1$, $l_2 = 2$ and $t = 0.07$.

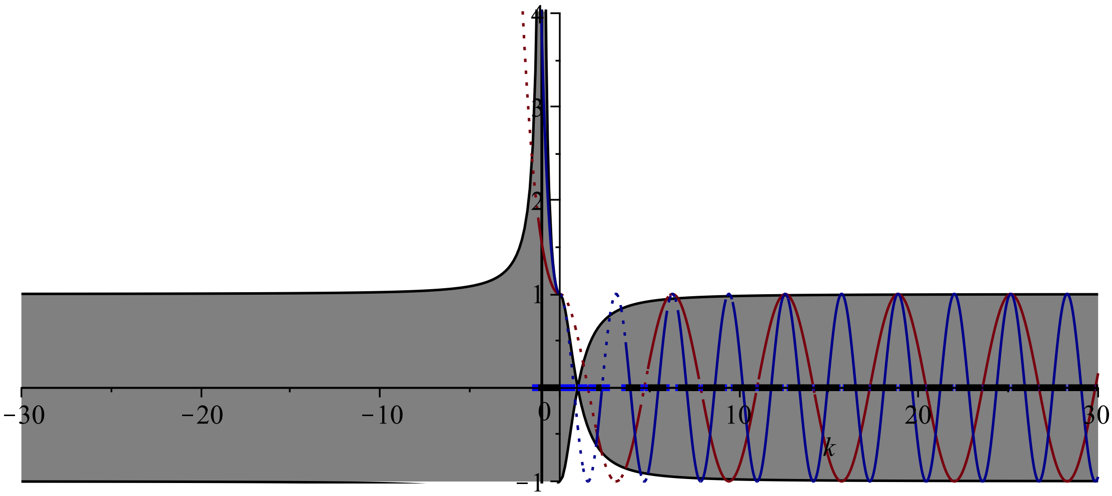

Figure 4.5: The situation for edge lengths $l_1 = 1$, $l_2 = 2$ and $t = 1$.

4.8 Numerical solutions $\alpha = 0$

The numerical solution shows that there are the gaps around the points $\{\frac{m\pi}{2}, \frac{n\pi}{2}\}$, $m, n \in \mathbb{N}$ for every $t \in (0, 1]$. It can be seen how the gaps are closing around those points if we send $t \to 0$. On the other hand at the bottom part of the figure we can see how the negative spectrum nicely follows the cotangent curve.

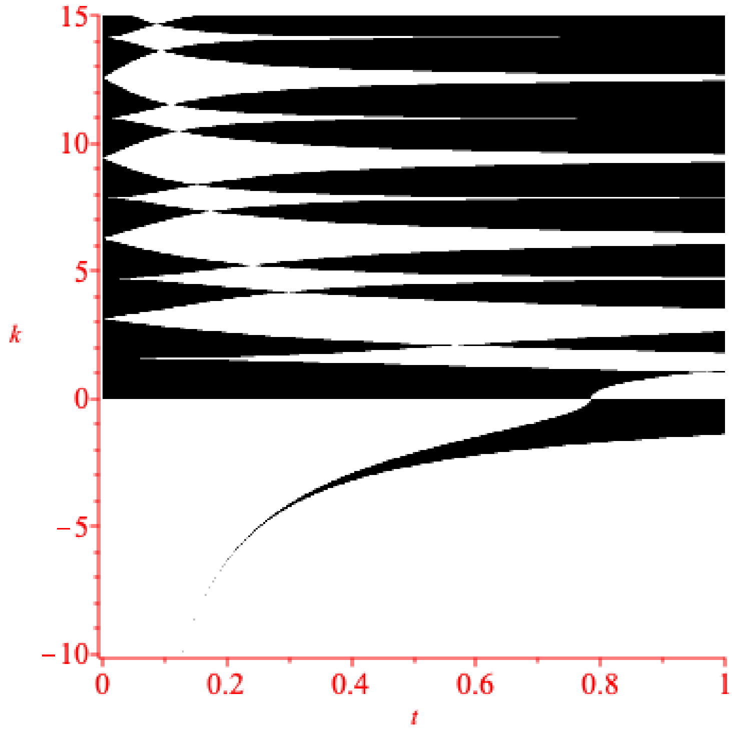

Figure 4.6: Numerical solution for $l_1 = 1$ and $l_2 = 2$.

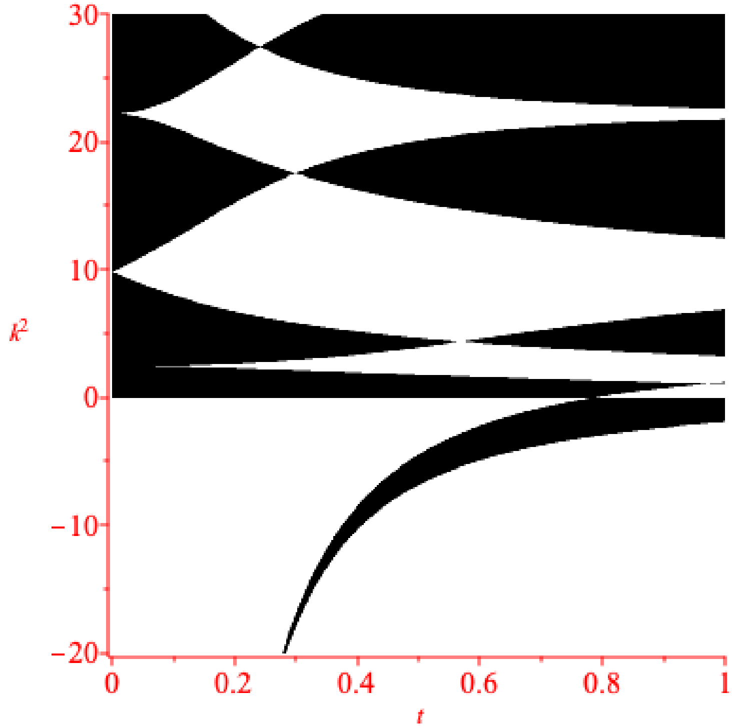

Figure 4.7: Numerical solution for $l_1 = 1$ and $l_2 = 2$.

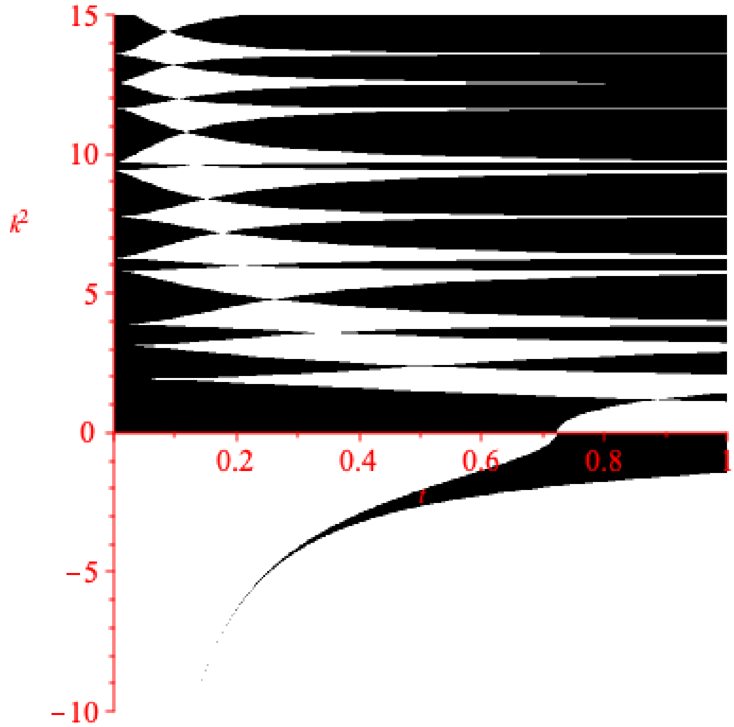

Figure 4.8: Numerical solution for $l_1 = 1$ and $l_2 = \frac{1+\sqrt{5}}{2}$.

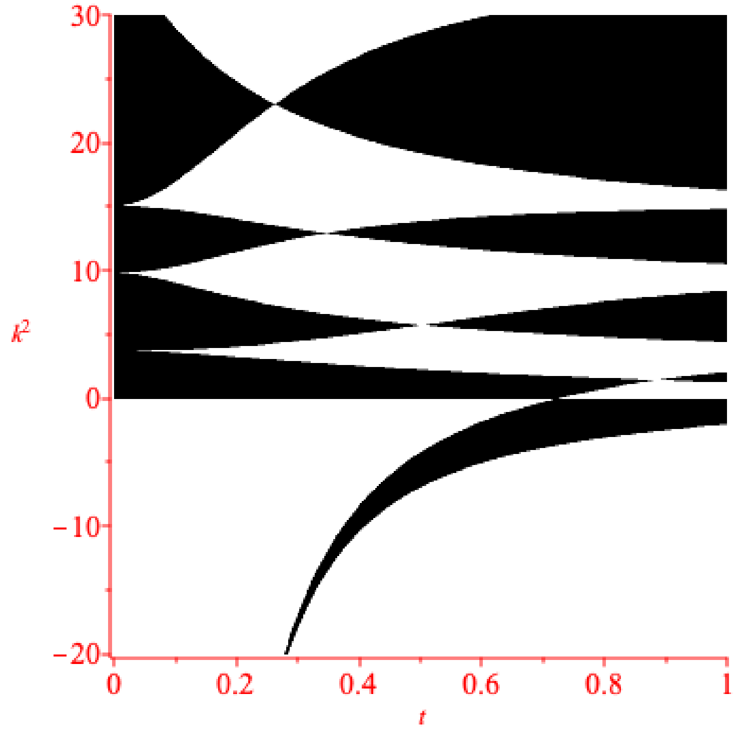

Figure 4.9: Numerical solution for $l_1 = 1$ and $l_2 = \frac{1+\sqrt{5}}{2}$.

4.9 Momentum and energy as function of θ_1, θ_2

In this section is shown low momentum resp. energy as function of $\theta_1, \theta_2 \in (-\pi, \pi]$. The case for $t = 0$ can be compared with computations which are made in [8, Section V.]

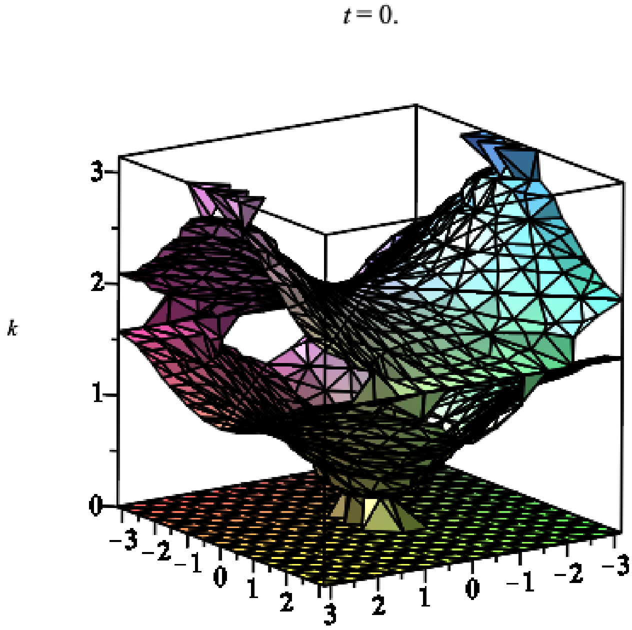

Figure 4.10: The momentum k as function of θ_1, θ_2. $l_1 = 1, l_2 = 2, t = 0$.

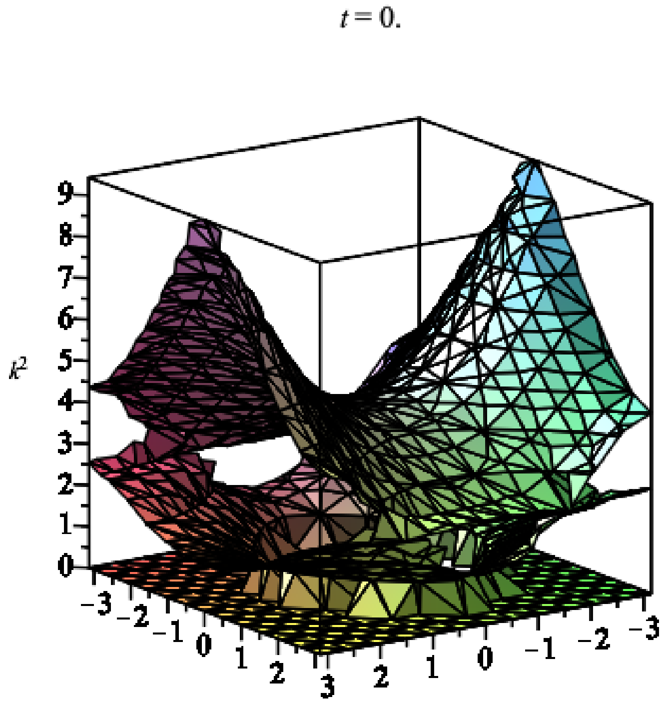

Figure 4.11: The energy k^2 as function of θ_1, θ_2. $l_1 = 1, l_2 = 2, t = 0$.

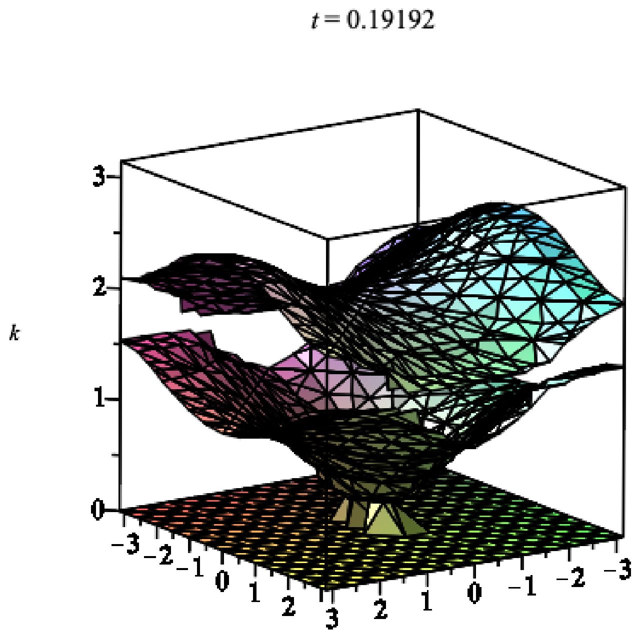

Figure 4.12: The momentum k as function of θ_1, θ_2. $l_1 = 1, l_2 = 2, t = 0.191$.

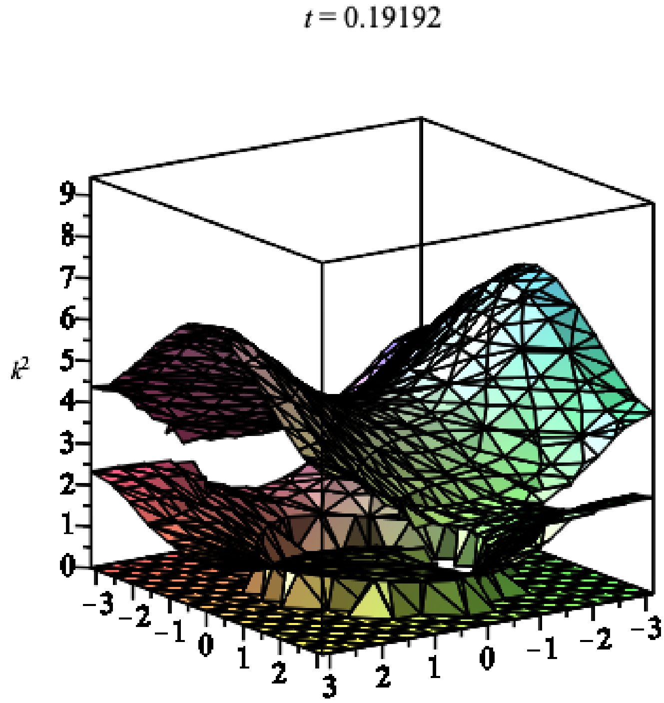

Figure 4.13: The energy k^2 as function of θ_1, θ_2. $l_1 = 1, l_2 = 2, t = 0.191$.

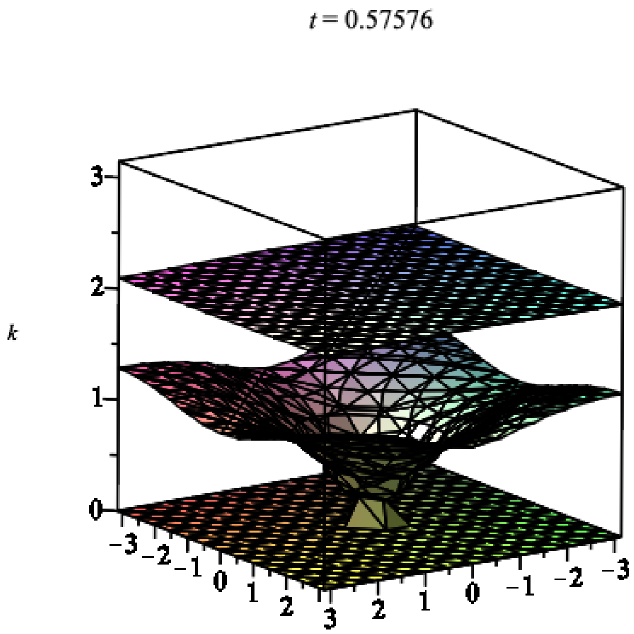

Figure 4.14: The momentum k as function of θ_1, θ_2. $l_1 = 1, l_2 = 2, t = 0.575$.

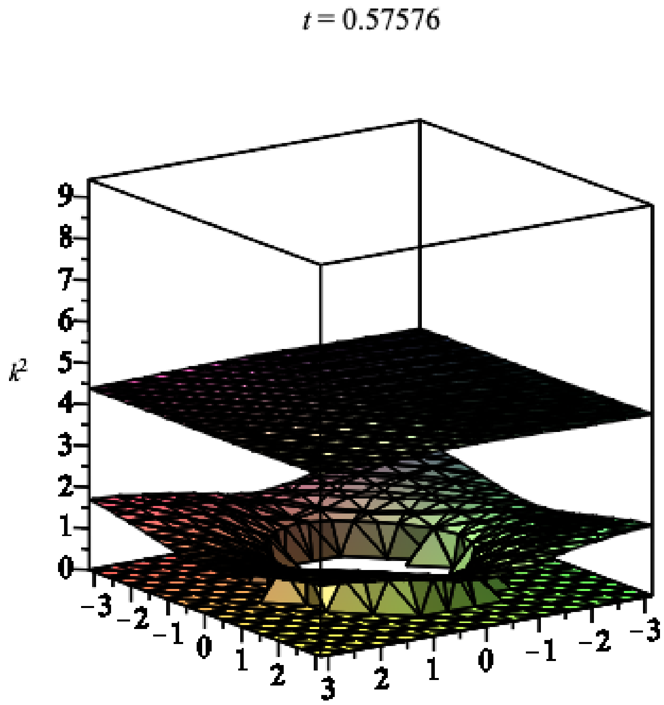

Figure 4.15: The energy k^2 as function of θ_1, θ_2. $l_1 = 1, l_2 = 2, t = 0.575$.

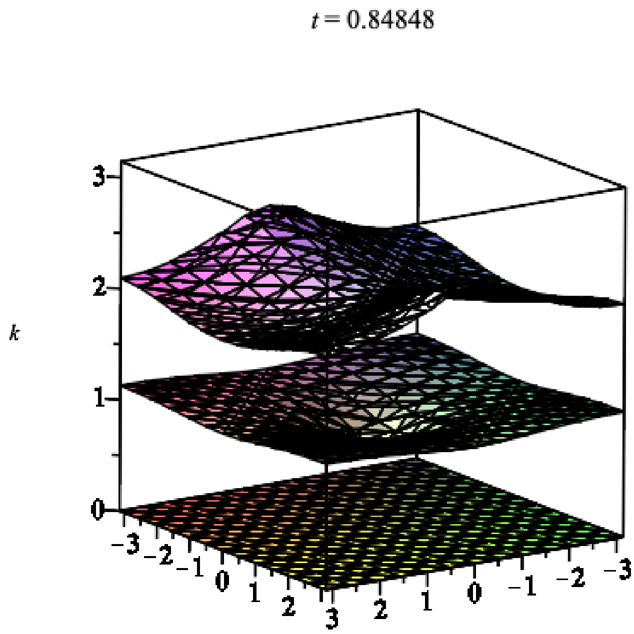

Figure 4.16: The momentum k as function of θ_1, θ_2. $l_1 = 1, l_2 = 2, t = 0.848$.

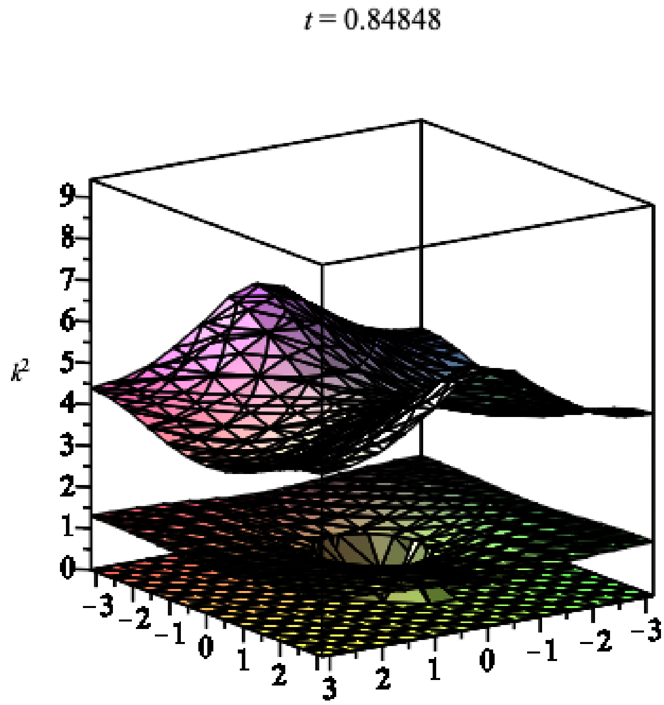

Figure 4.17: The energy k^2 as function of θ_1, θ_2. $l_1 = 1, l_2 = 2, t = 0.848$.

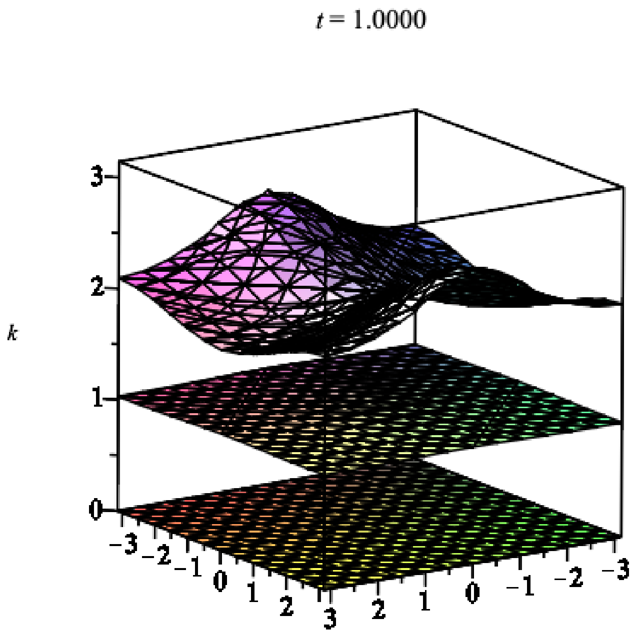

Figure 4.18: The momentum k as function of θ_1, θ_2. $l_1 = 1, l_2 = 2, t = 1$.

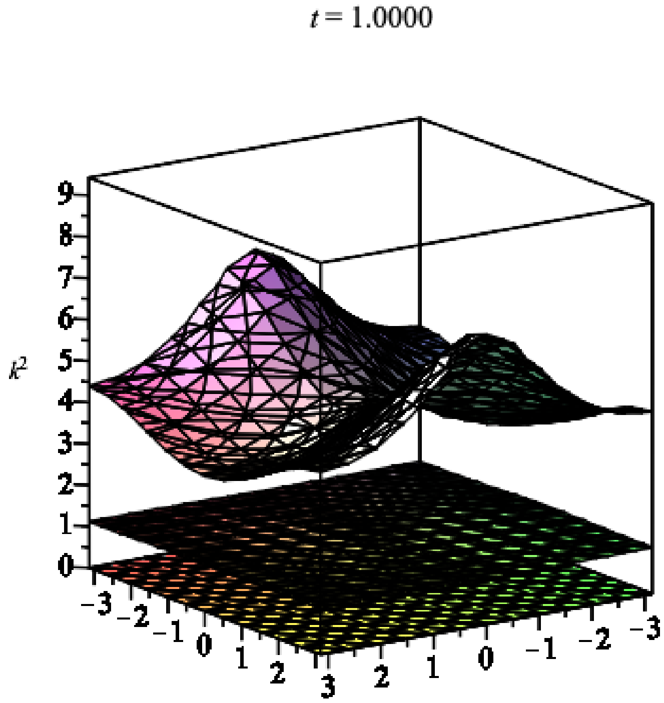

Figure 4.19: The energy k^2 as function of θ_1, θ_2. $l_1 = 1, l_2 = 2, t = 0.314$.

4.10 Spectrum of a rectangular lattice: case $\alpha \neq 0$

4.10.1 Positive spectrum

Spectral condition:

$$\begin{aligned}
&\sin(kl_1)\Big(\cos(kl_2) + \frac{k^2\sin^2(\frac{\pi t}{4}) - \cos^2(\frac{\pi t}{4})}{k^2\sin^2(\frac{\pi t}{4}) + \cos^2(\frac{\pi t}{4})}\cos(\theta_2)\Big) \\
&+ \sin(kl_2)\Big(\cos(kl_1) + \frac{k^2\sin^2(\frac{\pi t}{4}) - \cos^2(\frac{\pi t}{4})}{k^2\sin^2(\frac{\pi t}{4}) + \cos^2(\frac{\pi t}{4})}\cos(\theta_1)\Big) \\
&- \frac{2}{k}\tan(\frac{1-t}{2}\gamma)\frac{k^2\sin^2\frac{\pi t}{4}}{k^2\sin^2\frac{\pi t}{4} + \cos^2\frac{\pi t}{4}}(\cos\theta_1 + \cos kl_1)(\cos\theta_2 + \cos kl_2) \\
&+ \frac{2}{k}\tan(\frac{1-t}{2}\gamma)\frac{\cos^2\frac{\pi t}{4}}{k^2\sin^2\frac{\pi t}{4} + \cos^2\frac{\pi t}{4}}\sin(kl_1)\sin(kl_2) = 0
\end{aligned} \tag{4.21}$$

Theorem 4.3. *Let $\alpha \neq 0$ and $\frac{l_1}{l_2} \in \mathbb{Q}$ then for every $t \in (0,1)$ there is an infinitely many gaps in the spectrum.*

Proof. Suppose we have point k' such that $\cos(k'l_1) = \cos(k'l_2) = 1$. We have already proved that there exist a vicinity $(k'-\delta, k')$, resp. $(k', k'+\delta)$ of this point where the first two expressions in the (4.21) are both negative, resp. both positive. Indeed, we can use the second part of Theorem 4.1 and Lemma 4.1 and the following inequalities

$$\begin{aligned}
0 < \cos(kl_2) - \left|\frac{k^2\sin^2(\frac{\pi t}{4}) - \cos^2(\frac{\pi t}{4})}{k^2\sin^2(\frac{\pi t}{4}) + \cos^2(\frac{\pi t}{4})}\right| < \cos(kl_2) + \frac{k^2\sin^2(\frac{\pi t}{4}) - \cos^2(\frac{\pi t}{4})}{k^2\sin^2(\frac{\pi t}{4}) + \cos^2(\frac{\pi t}{4})}\cos(\theta_2), \\
0 < \cos(kl_1) - \left|\frac{k^2\sin^2(\frac{\pi t}{4}) - \cos^2(\frac{\pi t}{4})}{k^2\sin^2(\frac{\pi t}{4}) + \cos^2(\frac{\pi t}{4})}\right| < \cos(kl_1) + \frac{k^2\sin^2(\frac{\pi t}{4}) - \cos^2(\frac{\pi t}{4})}{k^2\sin^2(\frac{\pi t}{4}) + \cos^2(\frac{\pi t}{4})}\cos(\theta_1).
\end{aligned} \tag{4.22}$$

Now for arbitrary fixed k we see that function $\phi(\theta_1, \theta_2) = (\cos\theta_1 + \cos kl_1)(\cos\theta_2 + \cos kl_2)$ has its minimum and maximum as follows

$$\begin{aligned}
\min_{\theta_1,\theta_2\in(-\pi,\pi]} \phi(\theta_1,\theta_2) &= \min\{(\cos kl_1 - 1)(\cos kl_2 + 1), (\cos kl_1 + 1)(\cos kl_2 - 1)\}, \\
\max_{\theta_1,\theta_2\in(-\pi,\pi]} \phi(\theta_1,\theta_2) &= (\cos kl_1 + 1)(\cos kl_2 + 1).
\end{aligned} \tag{4.23}$$

Without loss of generality we can assume that the minimum corresponds to the first case. Moreover, let $\tan(\frac{1-t}{2}\gamma) > 0$. Under these assumptions we have the following inequalities

$$\begin{aligned}
-2\frac{1}{k}\tan(\frac{1-t}{2}\gamma)\frac{k^2\sin^2\frac{\pi t}{4}}{k^2\sin^2\frac{\pi t}{4} + \cos^2\frac{\pi t}{4}}(\cos\theta_1 + \cos kl_1)(\cos\theta_2 + \cos kl_2) > \\
-2\frac{1}{k}\tan(\frac{1-t}{2}\gamma)\frac{k^2\sin^2\frac{\pi t}{4}}{k^2\sin^2\frac{\pi t}{4} + \cos^2\frac{\pi t}{4}}(\cos kl_1 - 1)(\cos kl_2 + 1) > -C_1(\cos kl_1 - 1),
\end{aligned} \tag{4.24}$$

where we used (4.23) in the first inequality and the fact that there exist $C_1 < 0$ such that

$$-2\frac{1}{k}\tan(\frac{1-t}{2}\gamma)\frac{k^2\sin^2\frac{\pi t}{4}}{k^2\sin^2\frac{\pi t}{4}+\cos^2\frac{\pi t}{4}}(\cos kl_2+1) > -C_1, \quad \forall k>0$$

in the second inequality. Next we use the following limit

$$\lim_{k\to k'}\frac{1-\cos(kl_1)}{\sin(kl_1)}=0$$

which by the definition of a limit means that

$$(\forall\varepsilon_1>0)(\exists H_{k'}^{(1)})(\forall k\in H_{k'}^{(1)})(|1-\cos(kl_1)|<\varepsilon_1|\sin(kl_1)|). \tag{4.25}$$

Let us choose $\varepsilon_1 > 0$ as follows

$$\varepsilon_1 = \frac{1}{2|C_1|}\left(\cos(kl_1) - \left|\frac{k^2\sin^2(\frac{\pi t}{4})-\cos^2(\frac{\pi t}{4})}{k^2\sin^2(\frac{\pi t}{4})+\cos^2(\frac{\pi t}{4})}\right|\right) \tag{4.26}$$

Note that for some $\delta > 0$ this number is positive at least on $(k'-\delta, k')$ and $(k', k'+\delta)$ by (4.22). Substituting ε_2 into (4.25) we obtain

$$\begin{aligned}
&2\frac{1}{k}\tan(\frac{1-t}{2}\gamma)\frac{k^2\sin^2\frac{\pi t}{4}}{k^2\sin^2\frac{\pi t}{4}+\cos^2\frac{\pi t}{4}}(\cos\theta_1+\cos kl_1)(\cos\theta_2+\cos kl_2) < \\
&< C_1(\cos kl_1 - 1) < |C_1(\cos kl_1 - 1)| < \\
&\frac{1}{2}\left(\cos(kl_2) - \left|\frac{k^2\sin^2(\frac{\pi t}{4})-\cos^2(\frac{\pi t}{4})}{k^2\sin^2(\frac{\pi t}{4})+\cos^2(\frac{\pi t}{4})}\right|\right)|\sin(kl_1)| < \\
&\frac{1}{2}\sin(kl_1)\Big(\cos(kl_2) + \frac{k^2\sin^2(\frac{\pi t}{4})-\cos^2(\frac{\pi t}{4})}{k^2\sin^2(\frac{\pi t}{4})+\cos^2(\frac{\pi t}{4})}\cos(\theta_2)\Big)
\end{aligned} \tag{4.27}$$

In the first inequality we used (4.24), the second inequality is the property of absolute value, the third one is obtained by substitution of (4.26) into (4.25) and in the last one we used (4.22). Note that the last inequality is valid only on $H_{k'}^{(1)}$ since function $\sin(kl_1)$ is positive on this interval thus we can omit the absolute value, i.e. $\sin(kl_1) = |\sin(kl_1)|$. The foregoing inequalities thus hold on the interval $(k', k'+\delta)\cap H_{k'}^{(1)}$.

Similarly, we use the limit

$$\lim_{k\to k'}\frac{\sin(kl_1)\sin(kl_2)}{\sin(kl_1)}=0$$

and we find out that there exists a $H_{k'}^{(2)}$ such that on $(k', k'+\delta)\cap H_{k'}^{(2)}$ the following inequality hold

$$\begin{aligned}
&-2\frac{1}{k}\tan(\frac{1-t}{2}\gamma)\frac{\cos^2\frac{\pi t}{4}}{k^2\sin^2\frac{\pi t}{4}+\cos^2\frac{\pi t}{4}}\sin(kl_1)\sin(kl_2) < \\
&\frac{1}{2}\sin(kl_2)\Big(\cos(kl_1) + \frac{k^2\sin^2(\frac{\pi t}{4})-\cos^2(\frac{\pi t}{4})}{k^2\sin^2(\frac{\pi t}{4})+\cos^2(\frac{\pi t}{4})}\cos(\theta_1)\Big)
\end{aligned} \tag{4.28}$$

Finally inequalities (4.27) and (4.28) prove that the sum of last three terms in the spectral condition (4.21) is positive for all $k \in (k', k' + \delta) \cap H_{k'}^{(1)} \cap H_{k'}^{(2)}$ and we know that the first term is positive on $k \in (k', k' + \delta)$. In other words the spectral condition can not be zero on $k \in (k', k' + \delta) \cap H_{k'}^{(1)} \cap H_{k'}^{(2)}$ thus this interval can not belong to the spectrum.

It is not hard to see that if we would assume that $\tan(\frac{1-t}{2}\gamma) < 0$ we would get similar result on $k \in (k' - \delta, k') \cap H_{k'}^{(1)} \cap H_{k'}^{(2)}$. Moreover, in the same way we would have proved that there are the gaps in the left, resp. right vicinity of all points k' where $\cos(k'l_1) = \pm 1 \wedge \cos(k'l_2) = \pm 1$. Since we know that there is an infinite number of those points we proved that there are infinitely many gaps in the spectrum.

□

Theorem 4.4. *Let $\alpha \neq 0$, $\frac{l_1}{l_2} \in \mathbb{R} \setminus \mathbb{Q}$ and $t \in (0, 1)$ then for every $l_1, l_2 > 0$ hold:*

1. *If $\frac{l_1}{l_2}$ is Last admissible then there are infinitely many gaps in the spectrum.*

2. *For an arbitrary $\frac{l_1}{l_2}$ there exists an $\varepsilon_1 > 0$ such that for all $t > 1 - \varepsilon_1$ there are infinitely many gaps in the spectrum.*

3. *For an arbitrary $\frac{l_1}{l_2}$ there exists an $\varepsilon_2 > 0$ such that for all $t < \varepsilon_2$ there are infinitely many gaps in the spectrum.*

4. *For an arbitrary $\frac{l_1}{l_2}$ there exists an $\varepsilon_3 > 0$ such that for all $|\alpha| < \varepsilon_3$ there are infinitely many gaps in the spectrum.*

Proof. Without of loss of generality we may suppose that $l_1 \geq l_2$. First consider the following sequences

$$a_n = \frac{2\pi}{l_1}(n + \frac{a}{n}) = \frac{2\pi n}{l_1} + \frac{a2\pi}{l_1 n}, \quad n \in \mathbb{N}_0, \tag{4.29}$$

resp.

$$a'_n = \frac{2\pi}{l_1}(-\frac{a}{n} + n) = -\frac{a2\pi}{l_1 n} + \frac{2\pi n}{l_1}, \quad n \in \mathbb{N}_0. \tag{4.30}$$

where a is a so far unspecified real parameter.

Now let us consider three limit indicated below. We compute those limits only for the sequence $\{a_n\}_{n=1}^{\infty}$. It can be easily done for the sequence $\{a'_n\}_{n=1}^{\infty}$ and we will find that the limits have the same values.

$$\lim_{n\to\infty}\frac{1-\cos(a_n l_1)}{\cos(a_n l_1)-\frac{a_n^2\sin^2(\frac{\pi t}{4})-\cos^2(\frac{\pi t}{4})}{a_n^2\sin^2(\frac{\pi t}{4})+\cos^2(\frac{\pi t}{4})}}= \tag{4.31}$$

$$=\lim_{n\to\infty}\frac{1-\cos\frac{a2\pi}{n}\cos 2\pi n+\sin\frac{a2\pi}{n}\sin 2\pi n}{\cos\frac{a2\pi}{n}\cos 2\pi n+\sin\frac{a2\pi}{n}\sin 2\pi n-\frac{a_n^2\sin^2(\frac{\pi t}{4})-\cos^2(\frac{\pi t}{4})}{a_n^2\sin^2(\frac{\pi t}{4})+\cos^2(\frac{\pi t}{4})}}$$

$$=\lim_{n\to\infty}\frac{\Big(-\sum_{k=1}^{\infty}\frac{(-1)^k\left(\frac{2\pi a}{n}\right)^{2k}}{2k!}\Big)\Big(\sin^2\frac{\pi t}{4}(\frac{4\pi^2}{l_1^2}(n^2+2a+\frac{a^2}{n^2}))+\cos^2\frac{\pi t}{4}\Big)}{\Big(\sum_{k=1}^{\infty}\frac{(-1)^k\left(\frac{2\pi a}{n}\right)^{2k}}{2k!}\Big)\Big(\sin^2\frac{\pi t}{4}(\frac{4\pi^2}{l_1^2}(n^2+2a+\frac{a^2}{n^2}))+\cos^2\frac{\pi t}{4}\Big)+2\cos^2\frac{\pi t}{4}}$$

$$=\frac{\sin^2(\frac{\pi t}{4})4\pi^4a^2}{-\sin^2(\frac{\pi t}{4})\pi^4a^2+l_1^2\cos^2\frac{\pi t}{4}}$$

$$\lim_{n\to\infty}\frac{\sin(a_n l_1)}{\frac{1}{a_n}}=\lim_{n\to\infty}\Big(\sin\frac{a2\pi}{n}\cos 2\pi n+\cos\frac{a2\pi}{n}\sin 2\pi n\Big)\Big(\frac{2\pi n}{l_1}+\frac{a2\pi}{l_1 n}\Big)= \tag{4.32}$$

$$=\frac{2\pi}{l_1}\lim_{n\to\infty}\frac{\sin\frac{a2\pi}{n}}{\frac{1}{n}}=\frac{4\pi^2 a}{l_1}$$

$$\lim_{n\to\infty}\frac{1}{a_n}\frac{\frac{\cos^2\frac{\pi t}{4}}{a_n^2\sin^2\frac{\pi t}{4}+\cos^2\frac{\pi t}{4}}}{\cos(a_n l_1)-\frac{a_n^2\sin^2(\frac{\pi t}{4})-\cos^2(\frac{\pi t}{4})}{a_n^2\sin^2(\frac{\pi t}{4})+\cos^2(\frac{\pi t}{4})}}= \tag{4.33}$$

$$\lim_{n\to\infty}\frac{\cos^2\frac{\pi t}{4}}{\Big[\frac{2\pi}{l_1}(n+\frac{a}{n})\Big]\Big[\Big(\sum_{k=1}^{\infty}\frac{(-1)^k\left(\frac{2\pi a}{n}\right)^{2k}}{2k!}\Big)\Big(\sin^2\frac{\pi t}{4}(\frac{4\pi^2}{l_1^2}(n^2+2a+\frac{a^2}{n^2}))+\cos^2\frac{\pi t}{4}\Big)+2\cos^2\frac{\pi t}{4}\Big]}=0$$

Now let us introduce a new parameter $a'\in(0,a)$. This way we can get intervals $A_n:=(\frac{2\pi n}{l_1},\frac{2\pi n}{l_1}+\frac{2\pi a}{l_1 n})$ and $A_n':=(\frac{2\pi n}{l_1}-\frac{2\pi a}{l_1 n},\frac{2\pi n}{l_1})$ if we use the parameter a' instead of the parameter a in (4.29) and (4.30), respectively. This allows us to rewrite the foregoing sequences of numbers as sequences of functions and immediately write their limits.

$$\lim_{n\to\infty}\frac{1-\cos(kl_1)}{\cos(kl_1)-\frac{k^2\sin^2(\frac{\pi t}{4})-\cos^2(\frac{\pi t}{4})}{k^2\sin^2(\frac{\pi t}{4})+\cos^2(\frac{\pi t}{4})}}=\frac{\sin^2(\frac{\pi t}{4})4\pi^4a'^2}{-\sin^2(\frac{\pi t}{4})\pi^4a'^2+l_1^2\cos^2\frac{\pi t}{4}}, \tag{4.34}$$

$$\lim_{n\to\infty}\frac{\frac{1}{k}}{\sin(kl_1)}=\frac{l_1}{4\pi^2a'}, \tag{4.35}$$

$$\lim_{n\to\infty}\frac{1}{k}\frac{\frac{\cos^2\frac{\pi t}{4}}{k^2\sin^2\frac{\pi t}{4}+\cos^2\frac{\pi t}{4}}}{\cos(kl_1)-\frac{k^2\sin^2(\frac{\pi t}{4})-\cos^2(\frac{\pi t}{4})}{k^2\sin^2(\frac{\pi t}{4})+\cos^2(\frac{\pi t}{4})}}=0, \tag{4.36}$$

where $k=\frac{2\pi n}{l_1}+\frac{2\pi a'}{l_1 n}$, resp. $k=\frac{2\pi n}{l_1}-\frac{2\pi a'}{l_1 n}$ on $k\in A_n$, resp. $k\in A_n'$.

Moreover, we can repeat this procedure for l_2 and for the sequences

$$b_n = 2\pi(\frac{n}{l_2} + \frac{a}{nl_2}) = \frac{2\pi n}{l_2} + \frac{2\pi a}{l_2 n}, \quad n \in \mathbb{N}_0,$$

resp.

$$b'_n = 2\pi(-\frac{a}{nl_2} + \frac{n}{l_2}) = -\frac{2\pi a}{l_2 n} + \frac{2\pi n}{l_2}, \quad n \in \mathbb{N}_0,$$

and we get similar results. Namely,

$$\lim_{n\to\infty} \frac{1-\cos(kl_2)}{\cos(kl_2) - \frac{k^2\sin^2(\frac{\pi t}{4}) - \cos^2(\frac{\pi t}{4})}{k^2\sin^2(\frac{\pi t}{4}) + \cos^2(\frac{\pi t}{4})}} = \frac{\sin^2(\frac{\pi t}{4})4\pi^4 a'^2}{-\sin^2(\frac{\pi t}{4})\pi^4 a'^2 + l_2^2\cos^2\frac{\pi t}{4}} \tag{4.37}$$

$$\lim_{n\to\infty} \frac{\frac{1}{k}}{\sin(kl_2)} = \frac{l_2}{4\pi^2 a'} \tag{4.38}$$

$$\lim_{n\to\infty} \frac{1}{k} \frac{\frac{\cos^2\frac{\pi t}{4}}{k^2\sin^2\frac{\pi t}{4} + \cos^2\frac{\pi t}{4}}\sin(kl_i)}{\cos(kl_i) - \frac{k^2\sin^2(\frac{\pi t}{4}) - \cos^2(\frac{\pi t}{4})}{k^2\sin^2(\frac{\pi t}{4}) + \cos^2(\frac{\pi t}{4})}} = 0 \tag{4.39}$$

where $k = \frac{2\pi n}{l_2} + \frac{2\pi a'}{l_2 n}$, resp. $k = \frac{2\pi n}{l_2} - \frac{2\pi a'}{l_2 n}$ on $B_n := (\frac{2\pi n}{l_2}, \frac{2\pi n}{l_2} + \frac{2\pi a}{l_2 n})$, resp. $B'_n := (\frac{2\pi n}{l_2} - \frac{2\pi a}{l_2 n}, \frac{2\pi n}{l_2})$.

Now let us use the Dirichlet approximation theorem which implies that for every irrational number $\frac{l_1}{l_2}$ there are infinitely many fractions $\frac{p}{q}$ such that

$$\left|\frac{l_1}{l_2} - \frac{p}{q}\right| < \frac{1}{q^2}. \tag{4.40}$$

Since $l_1 < l_2$ by assumption, it is not hard to see that we can find an infinite sequence of fractions in the form $\frac{p_n}{q_n}$, $n \in \mathbb{N}$ with the following properties

1. $\{q_n\}_{n=1}^{\infty}$ is strictly growing: $\quad q_n < q_{n+1}, \quad \forall n \in \mathbb{N}$.
2. $\{p_n\}_{n=1}^{\infty}$ is strictly growing: $\quad p_n < p_{n+1} \quad \forall n \in \mathbb{N}$.
3. $p_n < q_n, \quad \forall n \in \mathbb{N}$.

Using this we can rewrite the (4.40) as follows

$$\left|\frac{2\pi q_n}{l_1} - \frac{2\pi p_n}{l_2}\right| < \frac{a2\pi}{l_1 q_n}. \tag{4.41}$$

and by using the third property we also get

$$\left|\frac{2\pi q_n}{l_1} - \frac{2\pi p_n}{l_2}\right| < \frac{a2\pi}{l_1 p_n}. \tag{4.42}$$

Let us for all $n \in \mathbb{N}$ define an interval

$$\delta_n = \begin{cases} (\frac{2\pi q_n}{l_1}, \frac{2\pi p_n}{l_2}), & \text{if } \frac{2\pi q_n}{l_1} < \frac{2\pi p_n}{l_2}, \\ (\frac{2\pi p_n}{l_2}, \frac{2\pi q_n}{l_1}), & \text{if } \frac{2\pi q_n}{l_1} > \frac{2\pi p_n}{l_2}. \end{cases}$$

We see that one of the following possibilities hold for every $n \in \mathbb{N}$:

$$\delta_n \subset A_{p_n} \quad \wedge \quad \delta_n \subset B'_{q_n}$$

or

$$\delta_n \subset A'_{p_n} \quad \wedge \quad \delta_n \subset B_{q_n}.$$

Finally, since $\{q_n\}_{n=1}^{\infty}$ and $\{q_n\}_{n=1}^{\infty}$ are strictly growing sub-sequences of $\{n\}_{n=1}^{\infty}$ we see that all the limits (4.34)-(4.36) and (4.37)-(4.39) hold for $\{\delta_n\}_{n=1}^{\infty}$. In other words, the Dirichlet approximation theorem implies the existence of the sequence of intervals $\{\delta_n\}_{n=1}^{\infty}$ such that the following limits hold for all $i \in \{1, 2\}$:

$$\lim_{n\to\infty} \frac{1-\cos(kl_i)}{\cos(kl_i) - \frac{k^2\sin^2(\frac{\pi t}{4})-\cos^2(\frac{\pi t}{4})}{k^2\sin^2(\frac{\pi t}{4})+\cos^2(\frac{\pi t}{4})}} = \frac{\sin^2(\frac{\pi t}{4})4\pi^4 a'^2}{-\sin^2(\frac{\pi t}{4})\pi^4 a'^2 + l_i^2\cos^2\frac{\pi t}{4}}, \tag{4.43}$$

$$\lim_{n\to\infty} \frac{\frac{1}{k}}{\sin(kl_i)} = \frac{l_i}{4\pi^2 a'}, \tag{4.44}$$

$$\lim_{n\to\infty} \frac{1}{k} \frac{\frac{\cos^2\frac{\pi t}{4}}{k^2\sin^2\frac{\pi t}{4}+\cos^2\frac{\pi t}{4}}\sin(kl_i)}{\cos(kl_i) - \frac{a_n^2\sin^2(\frac{\pi t}{4})-\cos^2(\frac{\pi t}{4})}{a_n^2\sin^2(\frac{\pi t}{4})+\cos^2(\frac{\pi t}{4})}} = 0, \tag{4.45}$$

when $k \in \delta_n$.

Now we combine the first two limits and we obtain for all $i, j \in \{1, 2\}, i \neq j$ the following limit

$$\lim_{n\to\infty} \frac{\frac{1}{k}2\tan\left(\frac{1-t}{2}\gamma\right)}{\sin(kl_j)} \frac{1-\cos(kl_i)}{\cos(kl_i) - \frac{k^2\sin^2(\frac{\pi t}{4})-\cos^2(\frac{\pi t}{4})}{k^2\sin^2(\frac{\pi t}{4})+\cos^2(\frac{\pi t}{4})}} = 2\tan\left(\frac{1-t}{2}\gamma\right)\frac{l_j l_i^2}{\pi^2} \frac{\sin^2(\frac{\pi t}{4})}{-a'\sin^2(\frac{\pi t}{4}) + \frac{l_i^2}{\pi^2 a'}\cos^2\frac{\pi t}{4}} \tag{4.46}$$

Let us make an assumption that this limit is equal to zero. We will discus the conditions required to this assumption to be fulfilled later. Now, if the limit is equal to zero we find out that for all $i, j \in \{1, 2\}, i \neq j$:

$$(\forall \varepsilon_2 > 0)(\exists n_2 \in \mathbb{N})(\forall n > n_2)(\forall k \in \delta_n)$$

$$\Big|\frac{1}{k}2\tan\left(\frac{1-t}{2}\gamma\right)\frac{k^2\sin^2\frac{\pi t}{4}}{k^2\sin^2\frac{\pi t}{4}+\cos^2\frac{\pi t}{4}}(1+\cos kl_i)(1-\cos kl_j)\Big| < \tag{4.47}$$

$$< 2\Big|\frac{1}{k}2\tan\left(\frac{1-t}{2}\gamma\right)(1-\cos kl_j)\Big| < 2\varepsilon_2\Big|\sin(kl_i)\Big(\cos(kl_j) - \frac{k^2\sin^2(\frac{\pi t}{4})-\cos^2(\frac{\pi t}{4})}{k^2\sin^2(\frac{\pi t}{4})+\cos^2(\frac{\pi t}{4})}\Big)\Big|$$

$$< 2\varepsilon_2\Big|\sin(kl_i)\Big(\cos(kl_j) + \frac{k^2\sin^2(\frac{\pi t}{4})-\cos^2(\frac{\pi t}{4})}{k^2\sin^2(\frac{\pi t}{4})+\cos^2(\frac{\pi t}{4})}\cos\theta_j\Big)\Big|,$$

where we used that

$$\Big|\frac{k^2\sin^2\frac{\pi t}{4}}{k^2\sin^2\frac{\pi t}{4}+\cos^2\frac{\pi t}{4}}(1+\cos kl_i)\Big| < 2, \quad \forall k \in \mathbb{R}.$$

Now we use the first expression in (4.23) and we divide inequality (4.47) into two cases:

1. $\tan\left(\frac{1-t}{2}\gamma\right) > 0$:

$$-\frac{1}{k}2\tan\big(\frac{1-t}{2}\gamma\big)\frac{k^2\sin^2\frac{\pi t}{4}}{k^2\sin^2\frac{\pi t}{4}+\cos^2\frac{\pi t}{4}}(\cos\theta_i-\cos kl_i)(\cos\theta_j-\cos kl_j) < \tag{4.48}$$
$$< 2\varepsilon_2\Big|\sin(kl_i)\Big(\cos(kl_j)+\frac{k^2\sin^2(\frac{\pi t}{4})-\cos^2(\frac{\pi t}{4})}{k^2\sin^2(\frac{\pi t}{4})+\cos^2(\frac{\pi t}{4})}\cos\theta_j\Big)\Big|$$

2. $\tan\left(\frac{1-t}{2}\gamma\right) < 0$:

$$\frac{1}{k}2\tan\big(\frac{1-t}{2}\gamma\big)\frac{k^2\sin^2\frac{\pi t}{4}}{k^2\sin^2\frac{\pi t}{4}+\cos^2\frac{\pi t}{4}}(\cos\theta_i-\cos kl_i)(\cos\theta_j-\cos kl_j) < \tag{4.49}$$
$$< \varepsilon_2\Big|\sin(kl_i)\Big(\cos(kl_j)+\frac{k^2\sin^2(\frac{\pi t}{4})-\cos^2(\frac{\pi t}{4})}{k^2\sin^2(\frac{\pi t}{4})+\cos^2(\frac{\pi t}{4})}\cos\theta_j\Big)\Big|$$

Similarly, by using the limit (4.45) we get

$$(\forall\varepsilon_3>0)(\exists n_3\in\mathbb{N})(\forall n>n_3)(\forall k\in\delta_n)$$
$$|\frac{1}{k}\frac{\cos^2\frac{\pi t}{4}}{k^2\sin^2\frac{\pi t}{4}+\cos^2\frac{\pi t}{4}}\sin kl_i\sin kl_j| < \varepsilon_3\Big|\sin(kl_i)\Big(\cos(kl_j)-\frac{k^2\sin^2(\frac{\pi t}{4})-\cos^2(\frac{\pi t}{4})}{k^2\sin^2(\frac{\pi t}{4})+\cos^2(\frac{\pi t}{4})}\Big)\Big| \tag{4.50}$$
$$< \varepsilon_3\Big|\sin(kl_i)\Big(\cos(kl_j)+\frac{k^2\sin^2(\frac{\pi t}{4})-\cos^2(\frac{\pi t}{4})}{k^2\sin^2(\frac{\pi t}{4})+\cos^2(\frac{\pi t}{4})}\cos\theta_j\Big)\Big|.$$

Finally, we refer reader to Theorem 4.1, namely to the expression (4.19), where if we re-scale the ε sufficiently we get, for arbitrary $n\in\mathbb{N}$, existence of the neighborhood $H_j^{(n)}$ of point $\frac{2\pi n}{l_j}$ such that for all $\varepsilon_1>0$ the following inequalities hold

$$\left|\sin(kl_j)\Big(\frac{k^2\sin^2\frac{\pi}{4}t-\cos^2\frac{\pi}{4}t}{k^2\sin^2\frac{\pi}{4}t+\cos^2\frac{\pi}{4}t}\cos(\theta_i)+\cos(kl_i)\Big)\right| < \tag{4.51}$$
$$< \varepsilon_1\left|\sin(kl_i)\Big(\frac{k^2\sin^2\frac{\pi}{4}t-\cos^2\frac{\pi}{4}t}{k^2\sin^2\frac{\pi}{4}t+\cos^2\frac{\pi}{4}t}\cos(\theta_j)+\cos(kl_j)\Big)\right|.$$

and

$$\left|\sin(kl_j)\Big(\frac{k^2\sin^2\frac{\pi}{4}t-\cos^2\frac{\pi}{4}t}{k^2\sin^2\frac{\pi}{4}t+\cos^2\frac{\pi}{4}t}\cos(\theta_i)+\cos(kl_i)\Big)\right| > 0. \tag{4.52}$$

Note that the two expressions in (4.52) have different sign on δ_n for all $n\in\mathbb{N}$.

Now if we choose $\varepsilon_1=\varepsilon_2=\varepsilon_3=\frac{1}{6}$ then if we use all those inequalities on the spectral condition 4.21) we get existence of n_0 such that for all $n>n_0$ this condition is neither strictly positive or strictly negative on $\delta_n\cap H_j^{(n)}$. In other words, the infinite sequence of intervals $\delta_n\cap H_j^{(n)}$ does not belong to the spectrum.

The last thing to do is to discuss cases when the limit (4.46) is equal to zero:

1. $a \to 0$:
   Indeed, since $a' \in (0, a)$ also goes to zero it is not hard to see that this limit is equal to zero.

   This condition can be satisfied only for Last admissible numbers (3.6). We know that for those numbers there for every $a > 0$ exist infinitely many pairs $(p,q) \in \mathbb{Z}^2$ such that $|\frac{l_1}{l_2} - \frac{p}{q}| < \frac{a}{q^2}$ thus the existence of sequence δ_n is ensured.

2. $t \to 0$, $t \to 1$:
   Again we see that the limit is equal to zero. In contrast with the first case now the condition is satisfied for all rational numbers.

3. $\gamma \to 0$:
   Similarly to the second case the condition is satisfied for all rational numbers.

Let us take a closer look on the previous cases. We consider only the second case. We would have proved the other cases by following the same arguments. Now let be parameters l_1, l_2, α in the limit (4.46) chosen arbitrary. For every $\varepsilon > 0$ we can choose sufficiently t such that the limit is equal to ε, i.e.

$$\lim_{n\to\infty} \frac{\frac{1}{k}2\tan\left(\frac{1-t}{2}\gamma\right)}{\sin(kl_j)} \frac{1-\cos(kl_i)}{\cos(kl_i) - \frac{k^2\sin^2(\frac{\pi t}{4}) - \cos^2(\frac{\pi t}{4})}{k^2\sin^2(\frac{\pi t}{4}) + \cos^2(\frac{\pi t}{4})}} = \varepsilon. \tag{4.53}$$

Using the definition of the limit we obtain

$$(\forall \tilde{\varepsilon} > 0)(\exists n_0 \in \mathbb{N})(\forall n > n_0)(\forall k \in \delta_n), \tag{4.54}$$

$$\left| \frac{\frac{1}{k}2\tan\left(\frac{1-t}{2}\gamma\right)}{\sin(kl_j)} \frac{1-\cos(kl_i)}{\cos(kl_i) - \frac{k^2\sin^2(\frac{\pi t}{4}) - \cos^2(\frac{\pi t}{4})}{k^2\sin^2(\frac{\pi t}{4}) + \cos^2(\frac{\pi t}{4})}} - \varepsilon \right| < \tilde{\varepsilon}, \tag{4.55}$$

which is equivalent to

$$\left| \frac{\frac{1}{k}2\tan\left(\frac{1-t}{2}\gamma\right)}{\sin(kl_j)} \frac{1-\cos(kl_i)}{\cos(kl_i) - \frac{k^2\sin^2(\frac{\pi t}{4}) - \cos^2(\frac{\pi t}{4})}{k^2\sin^2(\frac{\pi t}{4}) + \cos^2(\frac{\pi t}{4})}} \right| < \tilde{\varepsilon} + \varepsilon =: \varepsilon_2. \tag{4.56}$$

There we used well known inequality $|a| - |b| < |a - b|$. Since $\varepsilon_2 > 0$ can be chosen arbitrary we see that inequality (4.10.1) is used correctly.

□

4.10.2 Negative spectrum

We get the spectral condition by substituting $\kappa = ik$ into (4.21):

$$\begin{aligned}
&\sinh(\kappa l_1)\left(\left(\kappa^2 \sin^2\frac{\pi t}{4} - \cos^2\frac{\pi t}{4}\right)\cosh(\kappa l_2) + \left(\kappa^2 \sin^2(\frac{\pi t}{4}) + \cos^2(\frac{\pi t}{4})\right)\cos(\theta_2)\right)\\
&+\sinh(\kappa l_2)\left(\left(\kappa^2 \sin^2\frac{\pi t}{4} - \cos^2\frac{\pi t}{4}\right)\cosh(\kappa l_1) + \left(\kappa^2 \sin^2(\frac{\pi t}{4}) + \cos^2(\frac{\pi t}{4})\right)\cos(\theta_1)\right)\\
&+\frac{2}{\kappa}\tan(\frac{1-t}{2}\gamma)\kappa^2\sin^2\frac{\pi t}{4}(\cos\theta_1 + \cosh\kappa l_1)(\cos\theta_2 + \cosh\kappa l_2)\\
&-\frac{2}{\kappa}\tan(\frac{1-t}{2}\gamma)\cos^2\frac{\pi t}{4}\sinh(\kappa l_1)\sinh(\kappa l_2) = 0
\end{aligned} \tag{4.57}$$

4.11 Numerical solution $\alpha \neq 0$

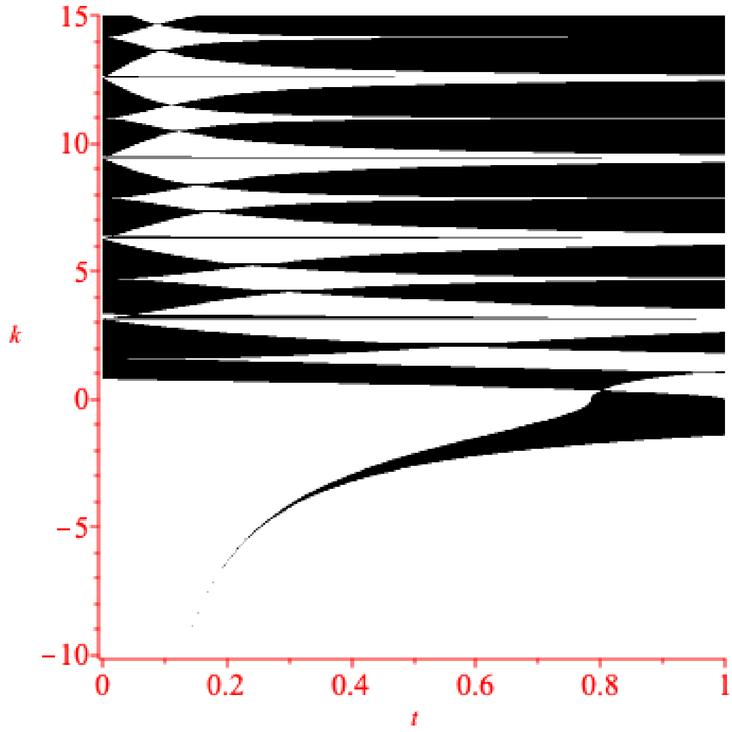

Figure 4.20: Numerical solution for $l_1 = 1$, $l_2 = 2$ and $\alpha = 1$

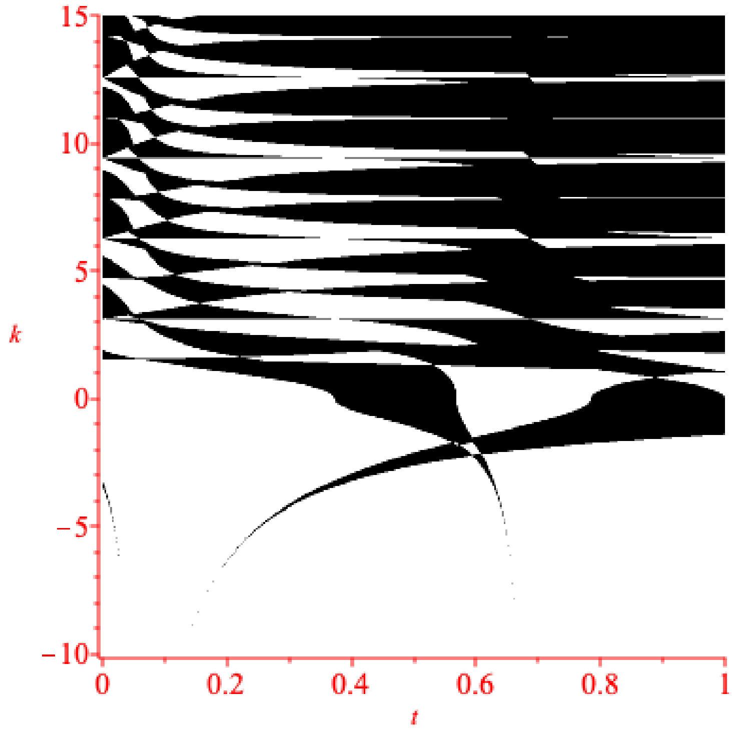

Figure 4.21: Numerical solution for $l_1 = 1$, $l_2 = 2$ and $\alpha = 10$

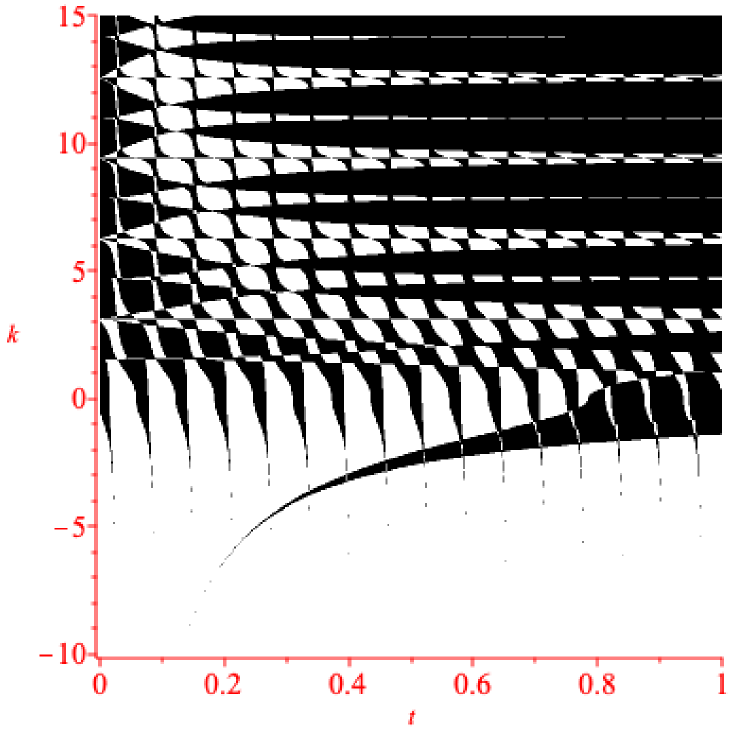

Figure 4.22: Numerical solution for $l_1 = 1$, $l_2 = 2$ and $\alpha = 100$

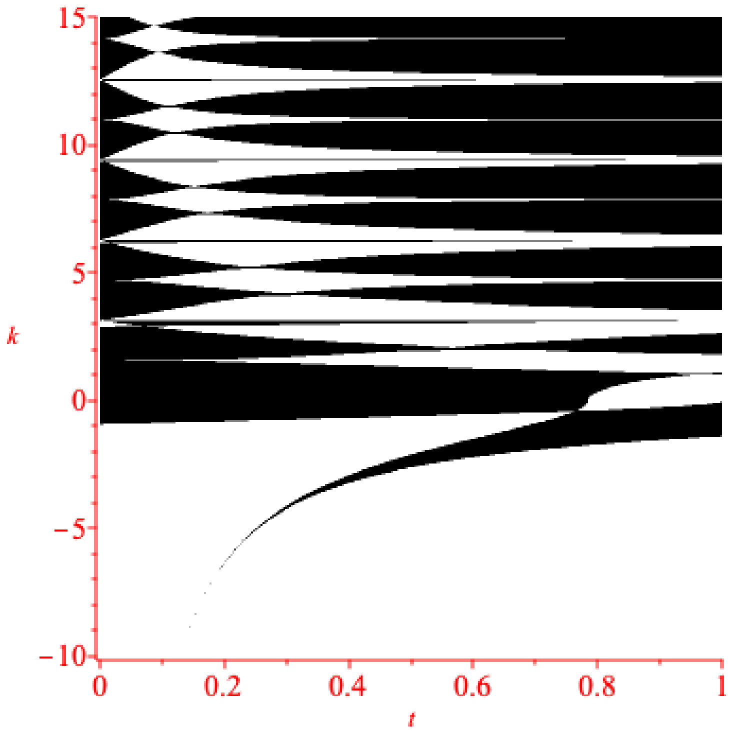

Figure 4.23: Numerical solution for $l_1 = 1$, $l_2 = 2$ and $\alpha = -1$

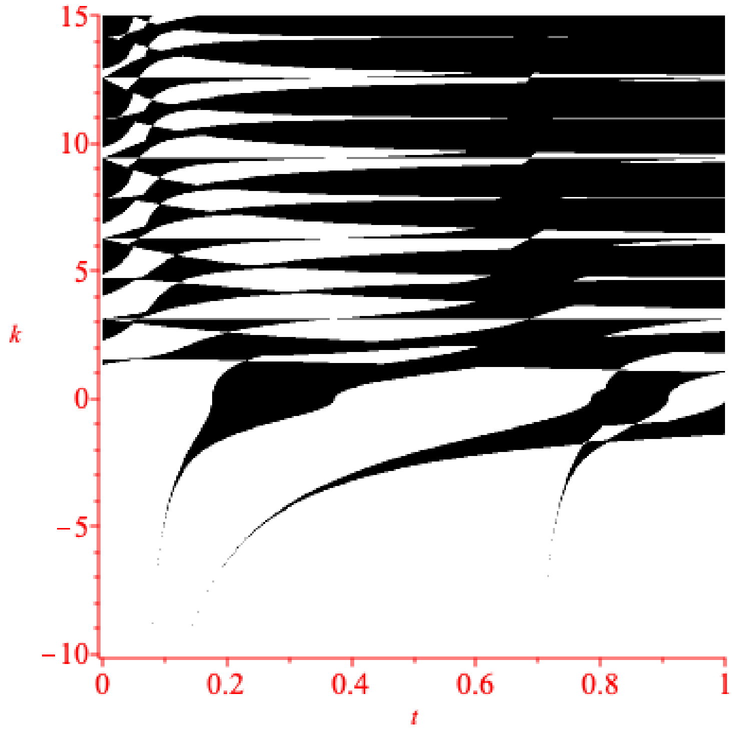

Figure 4.24: Numerical solution for $l_1 = 1$, $l_2 = 2$ and $\alpha = -10$

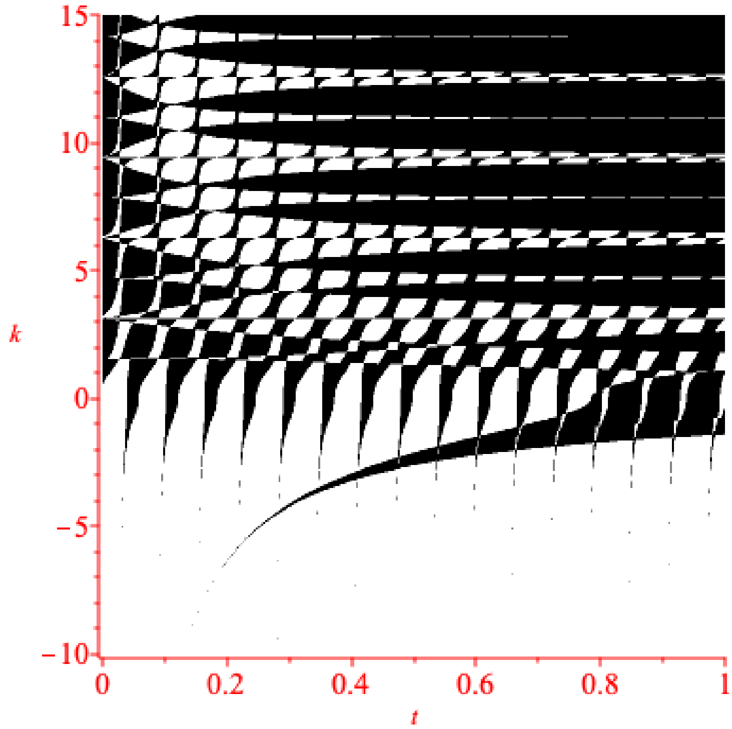

Figure 4.25: Numerical solution for $l_1 = 1$, $l_2 = 2$ and $\alpha = -100$

Conclusion

We have studied the rectangular lattice quantum graph with class of interpolating couplings which is given by family of unitary matrices $U(t) : t \in [0,1], \alpha \in \mathbb{R}$ such that

$$\begin{gathered} U(0) = -I + \frac{2}{n + i\alpha} J \quad \text{and} \quad U(1) = R, \\ \text{the map } t \mapsto U(t) \text{ is continuous on } [0,1], \\ U(t) \text{ is unitary circulant for all } t \in [0,1]. \end{gathered} \tag{4.58}$$

where I is unit matrix, J denotes the matrix with all elements equal to one and $U(1)$ is defined as

$$U(1) = R := \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \end{pmatrix}.$$

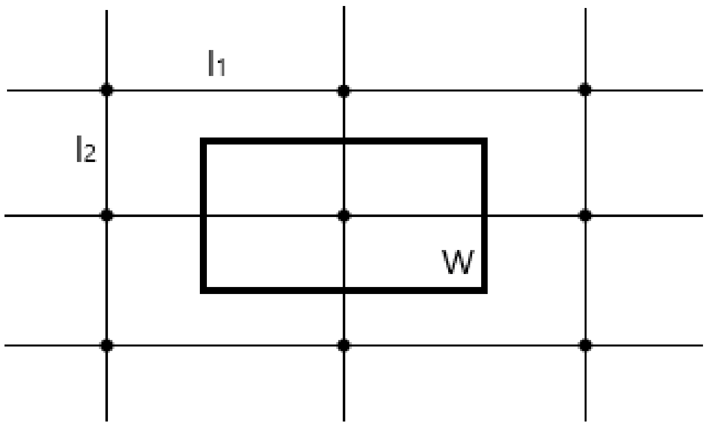

Figure 4.26: The rectangular lattice quantum graph.

We established the spectral condition which determines the spectrum:

Positive spectrum

$$\begin{aligned}
&\sin(kl_1)\Big(\cos(kl_2)+\frac{k^2\sin^2(\frac{\pi t}{4})-\cos^2(\frac{\pi t}{4})}{k^2\sin^2(\frac{\pi t}{4})+\cos^2(\frac{\pi t}{4})}\cos(\theta_2)\Big)\\
&+\sin(kl_2)\Big(\cos(kl_1)+\frac{k^2\sin^2(\frac{\pi t}{4})-\cos^2(\frac{\pi t}{4})}{k^2\sin^2(\frac{\pi t}{4})+\cos^2(\frac{\pi t}{4})}\cos(\theta_1)\Big)\\
&-2\frac{1}{k}\tan(\frac{1-t}{2}\gamma)\frac{k^2\sin^2\frac{\pi t}{4}}{k^2\sin^2\frac{\pi t}{4}+\cos^2\frac{\pi t}{4}}(\cos\theta_1+\cos kl_1)(\cos\theta_2+\cos kl_2)\\
&+2\frac{1}{k}\tan(\frac{1-t}{2}\gamma)\frac{\cos^2\frac{\pi t}{4}}{k^2\sin^2\frac{\pi t}{4}+\cos^2\frac{\pi t}{4}}\sin(kl_1)\sin(kl_2)=0
\end{aligned} \tag{4.59}$$

Negative spectrum

$$\begin{aligned}
&\sinh(\kappa l_1)\Bigg(\Big(\kappa^2\sin^2\frac{\pi t}{4}-\cos^2\frac{\pi t}{4}\Big)\cosh(\kappa l_2)+\Big(\kappa^2\sin^2(\frac{\pi t}{4})+\cos^2(\frac{\pi t}{4})\Big)\cos(\theta_2)\Bigg)\\
&+\sinh(\kappa l_2)\Bigg(\Big(\kappa^2\sin^2\frac{\pi t}{4}-\cos^2\frac{\pi t}{4}\Big)\cosh(\kappa l_1)+\Big(\kappa^2\sin^2(\frac{\pi t}{4})+\cos^2(\frac{\pi t}{4})\Big)\cos(\theta_1)\Bigg)\\
&+\frac{2}{\kappa}\tan(\frac{1-t}{2}\gamma)\kappa^2\sin^2\frac{\pi t}{4}(\cos\theta_1+\cosh\kappa l_1)(\cos\theta_2+\cosh\kappa l_2)\\
&-\frac{2}{\kappa}\tan(\frac{1-t}{2}\gamma)\cos^2\frac{\pi t}{4}\sinh(\kappa l_1)\sinh(\kappa l_2)=0
\end{aligned} \tag{4.60}$$

Theorem 4.5. *Let us have the periodic rectangle lattice quantum graph (Figure 4.26) with the Hamiltonian $\mathcal{H} := -\frac{d^2}{dx^2}$ and with the vertex conditions determined by (4.58). Then its spectrum has following properties:*

1. $t = 0$:
   (a) $\alpha = 0$:
      i. ***Positive spectrum:***
         - *The spectrum is the positive half-line, i.e.* $\sigma(\mathcal{H}) = [0, \infty]$.
      ii. ***Negative spectrum:***
         - *The negative spectrum is empty.*
   (b) $\alpha \neq 0$:
      i. ***Positive spectrum:***
         - *If θ is rational or Last admissible number then the spectrum has infinitely many gaps for $\alpha \neq 0$.*
         - *For badly approximable θ there exist $\gamma > 0$ such that $\gamma < \alpha < \pi^2 \cdot \min\Big\{\frac{\nu(\theta)}{l_2}, \frac{\nu(\theta)^{-1}}{l_1}\Big\}$ for $\alpha > 0$, resp. $\gamma < |\alpha| < \pi^2 \cdot \min\Big\{\frac{\nu(\theta)}{l_1}, \frac{\nu(\theta)^{-1}}{l_2}\Big\}$ for $\alpha < 0$ the spectrum has no gaps above the threshold.*

- *For all $\theta \in \mathbb{R}$ the spectrum has infinitely many gaps if $\alpha > \pi^2 \cdot \min\left\{\frac{\nu(\theta)}{l_2}, \frac{\nu(\theta)^{-1}}{l_1}\right\}$ for $\alpha > 0$, resp. $|\alpha| > \pi^2 \cdot \min\left\{\frac{\nu(\theta)}{l_1}, \frac{\nu(\theta)^{-1}}{l_2}\right\}$ for $\alpha < 0$.*

ii. ***Negative spectrum:***

- *The negative spectrum is non-empty if and only if $\alpha > 0$.*

2. $t = 1$:

(a) $\alpha \in \mathbb{R}$ *(the spectral condition does not depend on α):*

i. ***Positive spectrum:***

- *For every $\theta \in \mathbb{R}$ there is an infinitely many gaps. The gaps are located in the vicinity of the points $\{\frac{m\pi}{l_1}, \frac{n\pi}{l_2}\}$, $m, n \in \mathbb{N}$.*
- *If θ is rational number then there is an infinitely many infinitely degenerate eigenvalues.*
- *The gap width goes asymptotically to zero in the momentum scale.*

ii. ***Negative spectrum:***

- *Momentum -1 always belongs to the spectra. There exist a spectral band in the vicinity of this point. Thus inf $\sigma(H) < -1$.*

3. $t \in (0, 1)$:

(a) $\alpha = 0$:

i. ***Positive spectrum:***

- *For every $\theta \in \mathbb{R}$ there is an infinitely many gaps. The gaps are located in the vicinity of the points $\{\frac{m\pi}{l_1}, \frac{n\pi}{l_2}\}$, $m, n \in \mathbb{N}$.*
- *If θ is rational number then there is an infinitely many infinitely degenerate eigenvalues.*
- *The gap width goes asymptotically to zero in the momentum scale.*

ii. ***Negative spectrum:***

- *Momentum $-\cot(\frac{\pi}{4}t)$ always belongs to the spectra. There exist a spectral band in the vicinity of this point. Thus inf $\sigma(H) < -\cot(\frac{\pi}{4}t)$.*

(b) $\alpha \neq 0$:

i. ***Positive spectrum:***

- *If θ is rational or Last admissible number then there is infinitely many gaps in the spectrum.*
- *For arbitrary θ there exist $\varepsilon_1 > 0$ such that for all $t > 1 - \varepsilon_1$ there is infinitely many gaps in the spectrum.*
- *For arbitrary θ there exist $\varepsilon_2 > 0$ such that for all $\alpha < \varepsilon_2$ there is infinitely many gaps in the spectrum.*
- *For an arbitrary $\frac{l_1}{l_2}$ there exists an $\varepsilon_3 > 0$ such that for all $|\alpha| < \varepsilon_3$ there are infinitely many gaps in the spectrum.*

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