Gaps in the spectrum of a periodic quantum graph with periodically distributed $\delta'$-type interactions

Diana Barseghyan$^{1,2}$ and Andrii Khrabustovskyi$^{3,4}$

$^1$Department of Mathematics, University of Ostrava, 70103 Ostrava, Czech Republic
$^2$Nuclear Physics Institute ASCR, 25068 Řež near Prague, Czech Republic
$^3$Institute of Analysis, Karlsruhe Institute of Technology, D-76133 Karlsruhe, Germany

E-mail: diana.barseghyan@osu.cz and andrii.khrabustovskyi@kit.edu

Received 17 February 2015, revised 27 April 2015
Accepted for publication 30 April 2015
Published 2 June 2015

Abstract

We consider a family of quantum graphs $\{ (\Gamma, A_\epsilon) \}_{\epsilon > 0}$, where $\Gamma$ is a $\mathbb{Z}^n$-periodic metric graph and the periodic Hamiltonian $A_\epsilon$ is defined by the operation $-\epsilon^{-1} \frac{\partial^2}{\partial s^2}$ on the edges of $\Gamma$ and either $\delta'$-type conditions or the Kirchhoff conditions at its vertices. Here $\epsilon > 0$ is a small parameter. We show that the spectrum of $A_\epsilon$ has at least $m$ gaps as $\epsilon \to 0$ ($m \in \mathbb{N}$ is a predefined number), moreover the location of these gaps can be nicely controlled via a suitable choice of the geometry of $\Gamma$ and of coupling constants involved in $\delta'$-type conditions.

Keywords: periodic quantum graphs, $\delta'$-type interactions, spectral gaps

1. Introduction

The name ‘quantum graph’ is usually used for a pair $(\Gamma, A)$, where $\Gamma$ is a network-shaped structure of vertices connected by edges (‘metric graph’) and $A$ is a second order self-adjoint differential operator (‘Hamiltonian’), which is determined by differential operations on the edges and certain interface conditions at the vertices. Quantum graphs arise naturally in mathematics, physics, chemistry and engineering as models of wave propagation in quasi-one-dimensional systems looking like a narrow neighbourhood of a graph. One can mention, in particular, quantum wires, photonic crystals, dynamical systems, scattering theory and many other applications. For a broad overview and comprehensive bibliography on this topic we refer to the recent monograph [3].
In many applications (for instance, to graphen and carbon nano-structures—see [15, 17]) periodic infinite graphs are studied. The metric graph $\Gamma$ is called periodic ($\mathbb{Z}^n$-periodic) if there is a group $G \cong \mathbb{Z}^n$ acting isometrically, properly discontinuously and co-compactly on $\Gamma$ (see [3, definition 4.1.1.]). Roughly speaking $\Gamma$ is glued from countably many copies of a certain compact graph $Y$ (‘period cell’) and each $g \in G$ maps $Y$ to one of these copies.

In what follows in order to simplify the presentation (but without any loss of generality) we will assume that $\Gamma$ is embedded into $\mathbb{R}^d$ with $d = 3$ as $n = 1, 2$ and $d = n$ as $n \geq 3$ and is invariant under translations through linearly independent vectors $e_1, ..., e_n$, i.e.,

$$\Gamma = \Gamma + e_j, \ j = 1, ..., n.$$ (1)

These vectors produce an action of $\mathbb{Z}^n$ on $\Gamma$. Such an embedding can be always realized.

An example of $\mathbb{Z}^2$-periodic graph is presented on figure 1, its period cell is highlighted in bold lines.

The Hamiltonian $A$ on a periodic metric graph $\Gamma$ is said to be periodic if it commutes with the action of $\mathbb{Z}^n$ on $\Gamma$. It is well-known (see, e.g., [3, chapter 4]) that the spectrum of such operators has a band structure, i.e. it is a locally finite union of compact intervals called bands. In general the neighbouring bands may overlap. The bounded open interval $(\alpha, \beta) \subset \mathbb{R}$ is called a gap if it has an empty intersection with the spectrum, but its ends belong to it. In general the presence of gaps in the spectrum is not guaranteed. For example if $\Gamma$ is a rectangular lattice and $A$ is defined by the operation $-\delta^2/\delta x^2$ on its edges and the Kirchhoff conditions at the vertices, then the spectrum $\sigma(A)$ of the operator $A$ has no gaps, namely $\sigma(A) = [0, \infty)$. Existence of spectral gaps is important because of various applications, for example in physics of photonic crystals.

There are several ways how to create quantum waveguides with spectral gaps. One of them is to use decorating graphs. Namely, given a fixed graph $I_0$ we ‘decorate’ it attaching to each vertex of $I_0$ a copy of certain fixed graph $I_1$, the obtained graph we denote by $\Gamma$. Spectral properties of such graphs were studied in [21], where operators defined on functions on vertices were considered (‘discrete graphs’). The case of quantum graphs was studied in [16] and it was proved that gaps open up in the spectrum of the operator defined by the operation $-\delta^2/\delta x^2$ on the edges of $\Gamma$ and the Kirchhoff conditions at the vertices (other conditions are also allowed). These gaps are located around eigenvalues of a certain Hamiltonian on $I_1$.

Also one can use a ‘spider decoration’ procedure: in each vertex we disconnect the edges emerging from it and then connect their loose endpoints by a certain additional graph (‘spider’). Such a decorating procedure was probably used for the first time in [2, 6], more results on gap opening one can find in [19].

Another way to create gaps is to substitute the Kirchhoff conditions at the vertices by more ‘advanced’ ones instead of to perturb a graph geometry. For example, let $\Gamma$ be a rectangular lattice and $A$ be defined by the operation $-\delta^2/\delta x^2$ on its edges and $\delta$ conditions at the vertices, i.e. the functions from dom($A$) are continuous at all vertices and the sum of their derivatives is proportional to the value of a function at the vertex with a coupling constant $\alpha \in \mathbb{R}$ (the case $\alpha = 0$ corresponds to the Kirchhoff conditions). Then (see [6, 7]) the spectrum $\sigma(A)$ has infinitely many gaps provided $\alpha \neq 0$ and the lattice-spacing ratio satisfies some additional mild assumptions.

The goal of the current paper is to study spectral properties of some specific class of periodic quantum graphs. The main peculiarity of these graphs is that their spectral gaps can be nicely controlled via a suitable choice of the graph geometry and of coupling constants involved in interface conditions at its vertices.

In particular, for a given $m \in \mathbb{N}$ we construct a family $\{ (\Gamma, A_\epsilon) \}_{\epsilon > 0}$ of periodic quantum graphs having at least $m$ gaps as $\epsilon$ is small enough and moreover the first $m$ gaps converge to predefined intervals as $\epsilon \to 0$. The graph $\Gamma$ is constructed as follows. We take an arbitrary $\mathbb{Z}^n$
periodic graph $\Gamma$ with vectors $e_1, \ldots, e_n$ producing an action of $\mathbb{Z}^n$ on it and attach to $\Gamma_0$ a family of compact graphs $Y_{ij}, i = (i_1, \ldots, i_m) \in \mathbb{Z}^n$, $j = 1, \ldots, m$ satisfying $Y_0 + \sum_{k=1}^m i_k e_k = Y_j$.

We denote by $\Gamma$ the obtained graph (an example is presented on figure 2) and consider on it the Hamiltonian $A_\varepsilon$ defined by the operation

$$-\varepsilon^{-1} \frac{d^2}{dx^2}$$

on its edges and the Kirchhoff conditions in all its vertices except the points of attachment of $Y_j$ to $\Gamma_0$—in these points we pose $\delta'$-type conditions (in the case of vertex with two outgoing edges they coincide with the usual $\delta'$ conditions at a point on the line—see [1, section I.4]). The required structure for the spectrum of $A_\varepsilon$ is achieved via a suitable choice of coupling constants involved in $\delta'$-type conditions and of ‘sizes’ of attached graphs. The geometry of the attached graphs is inessential: one can control the location of spectral gaps just by attaching the graphs $Y_j$ consisting of only one edge with a suitably chosen length.

2. Setting of the problem and main result

2.1. Graph $\Gamma$

Let 

$$\Gamma = (\mathcal{V}, \mathcal{E}, \mathcal{Y}, \mathcal{I})$$

be a connected $\mathbb{Z}^n$-periodic metric graph. Here

- by $\mathcal{V}$ we denote the set of its vertices,
- by $\mathcal{E}$ we denote the set of its edges,
- by $\mathcal{Y}$ we denote the set of its vertices.

Figure 1. An example of $\mathbb{Z}^2$-periodic graph.

Figure 2. The example of the graph $\Gamma$. Here $m = 2$. 

- periodic graph $\Gamma_0$ with vectors $e_1, \ldots, e_n$ producing an action of $\mathbb{Z}^n$ on it and attach to $\Gamma_0$ a family of compact graphs $Y_{ij}, i = (i_1, \ldots, i_m) \in \mathbb{Z}^n$, $j = 1, \ldots, m$ satisfying $Y_0 + \sum_{k=1}^m i_k e_k = Y_j$.
the map \( \gamma : \mathcal{E} \to \mathcal{V} \times \mathcal{V} \) assigns to each edge \( e \) its initial and terminal points (we denote them \( \gamma^{-}(e) \) and \( \gamma^{+}(e) \), correspondingly),
- the function \( l : \mathcal{E} \to (0, \infty) \) assigns to the edge \( e \) its length \( l(e) \).

We suppose that the degree of each vertex (i.e., the number of edges emanating from it) is finite. In order to simplify the presentation we assume that \( \Gamma \) is embedded into \( \mathbb{R}^d \), where \( d = 3 \) as \( n = 1, 2 \) and \( d = n \) as \( n \geq 3 \).

On each edge \( e \in \mathcal{E} \) we introduce the local coordinate \( x_e \in [0, l(e)] \) in such a way that \( x_e = 0 \) corresponds to \( \gamma^{-}(e) \) and \( x_e = l(e) \) corresponds to \( \gamma^{+}(e) \). One can assume that \( \Gamma \) has no loops (i.e. there is no edge \( e \) with \( e \in \gamma^{-}(e) \)), otherwise one can break them into pieces by introducing a new intermediate vertex. For \( v \in \mathcal{V} \) we denote

\[
\{ \gamma^{-}(e), \gamma^{+}(e) \}.
\]

In a natural way the function \( l \) gives rise to a metric on \( \Gamma \). In what follows by \( \partial Y \) (or \( \text{int} Y \)), \( \partial \mathcal{Z} \) we denote, correspondingly, the interior, the closure, the boundary of a subset \( Z \subset \Gamma \) with respect to this metric. In particular, \( \partial \Gamma \) consists of the vertices of \( \Gamma \) of degree 1.

The \( \mathbb{Z}^n \)-periodicity of \( \Gamma \) means that there are linearly independent vectors \( e_1, ..., e_n \) satisfying (1). By \( Y \) we denote a period cell of \( \Gamma \), that is a compact subset of \( \Gamma \) satisfying

\[
Y \cap \left( Y + \sum_{k=1}^{n} i_k e_k \right) = \emptyset \text{ for an arbitrary } i = (i_1, ..., i_n) \in \mathbb{Z}^n \setminus \{0\},
\]

\[
\Gamma = \bigcup_{i \in \mathbb{Z}^n} \left( Y + \sum_{k=1}^{n} i_k e_k \right).
\]

We notice that period cell is not uniquely defined.

The period cell \( Y \) can be always chosen in such a way that \( \partial Y \) does not contain any vertex \( v \in \mathcal{V} \setminus \partial \Gamma \) (see figure 1). Under such a choice of the period cell the boundary \( \partial Y \) of \( Y \) consists of two disjoint parts \( \partial_{\text{int}} Y \) and \( \partial_{\text{ext}} Y \), where

- \( \partial_{\text{int}} Y \) consists of vertices of \( \Gamma \) of degree 1 belonging to \( Y \),
- \( \partial_{\text{ext}} Y \) consists of vertices of \( Y \) of degree 1 lying in the interiors of certain edges of \( \Gamma \).

An example of \( \mathbb{Z}^2 \)-periodic graph is presented on figure 1. Its period cell \( Y \) is presented in more details on figure 3 and one has

\[
\partial_{\text{int}} Y = \{ v_{13}, v_{14}, v_{15}, v_{16} \}, \quad \partial_{\text{ext}} Y = \{ v_1, v_5, v_6, v_{11} \}.
\]

Additionally, we suppose that \( Y \) can be expressed as a union of \( m + 1 \) compact subsets,

\[
Y = \bigcup_{j=0}^{m} Y_j, \quad m \in \mathbb{N}, \tag{2}
\]

satisfying the following conditions:

(i) \( \partial Y_j \neq \emptyset \),
(ii) \( Y_j \) are connected,
(iii) \( \text{int} \{ Y_j \cap Y_k \} = \emptyset \) provided \( j \neq k \),
\[ \text{i.e. } Y_j \text{ and } Y_k \text{ may have only common vertices, not edges}, \]
(iv) \( \partial_{\text{ext}} Y \subset \partial Y_0 \),
(v) the sets \( V_j := \partial Y_0 \cap \partial Y_j \), \( j = 1, \ldots, m \) are nonempty,

(vi) if \( j, k \neq 0 \) and \( j \neq k \) then either \( \partial Y_j \cap \partial Y_k = \emptyset \) or \( \partial Y_j \cap \partial Y_k \subset \partial Y_0 \).

(3)

Remark 2.1. In fact, decomposition (2) satisfying (3) is always possible for an arbitrary graph \( \Gamma \neq \mathbb{R} \) under a suitable choice of a period cell. Let us formulate this statement more accurately. At first we notice that for an arbitrary \( s \in \mathbb{N} \) condition (1) holds with \( e^*_j := se_j \) instead of \( e_j \), \( j = 1, \ldots, n \) (i.e., \( \Gamma \) is periodic with respect to the period cell \( Y^x := sY \)). It is easy to see that if \( \Gamma \neq \mathbb{R} \) then \( Y^x \) contains \( m \) edges \( \tilde{e}_1, \ldots, \tilde{e}_m \) satisfying

\[
\tilde{e}_i \cap \tilde{e}_j = \emptyset \quad \text{as} \quad i \neq j, \quad Y_0 := Y^x \setminus \bigcup_{j=1}^m \tilde{e}_j \quad \text{is a connected set}, \quad Y_0 \neq \emptyset, \quad \partial_{\text{ext}} Y^x \subset \partial Y_0
\]

provided \( s \) is large enough. We set \( Y_j := \tilde{e}_j, \ j = 1, \ldots, m \). Obviously, \( Y^x = \bigcup_{j=0}^m Y_j \) and conditions (3) hold true.

It is easy to see that \( \bigcup_{j=1}^m V_j \subset Y \). One can assume that the set \( \bigcup_{j=1}^m V_j \) belongs to \( \mathcal{V} \), otherwise if some of its points belongs to the interior of an edge then we can add it to \( \mathcal{V} \) (as a vertex with two outgoing edges). Finally, for \( i = (i_1, \ldots, i_n) \in \mathbb{Z}^n, \ j \in \{1, \ldots, m\} \) we set

\[
V_{ij} = V_j + \sum_{k=1}^n i_k e_k.
\]

The points belonging to \( V_{ij} \) will support our \( \delta^* \)-type conditions.
Also we will use the notation
\[ Y_j := Y_j + \sum_{k=1}^{n} i_k e_k, \quad i = (i_1, ..., i_n) \in \mathbb{Z}^n, j \in \{0, ..., m\}. \]

Let us come back to the example depicted on figure 3. There are several possibilities to decompose the period cell in a way described above. For example, one has \( Y = Y_0 \cup Y_1 \), where
\[ Y_0 \text{ consists of the edges } e_1, e_2, e_3, e_4, e_5, e_6, e_7, e_8, e_9, e_{10}, e_{12}, e_{13}, e_{14}, e_{16}, \] (solid lines),
\[ Y_1 \text{ consists of the edges } e_3, e_7, e_{11}, e_{15}, e_{17}, e_{18}, e_{19}, e_{20}, \] (dashed–dotted lines).

The set \( Y \) consists of the vertices \( v_3, v_6, v_9, v_{12} \).

One can also decompose \( Y \) in a more “advanced” way, for example as a union of six sets:
\[ Y_0 \text{ consists of the edges } e_1, e_2, e_3, e_4, e_5, e_6, e_7, e_8, e_9, e_{10}, e_{12}, e_{13}, e_{14}, e_{16}, \]
\[ Y_1 \text{ consists of the edges } e_7, e_{11}, e_{15}, e_{17}, e_{18}, e_{19}, e_{20}, \]
\[ Y_2 \text{ consists of the edge } e_3, \]
\[ Y_3 \text{ consists of the edge } e_7, \]
\[ Y_4 \text{ consists of the edge } e_{11}, \]
\[ Y_5 \text{ consists of the edge } e_{15}. \]

Then \( \mathcal{V}_1 = \{v_3, v_6, v_9, v_{12}\}, \mathcal{V}_2 = \{v_3\}, \mathcal{V}_3 = \{v_6\}, \mathcal{V}_4 = \{v_9\}, \mathcal{V}_5 = \{v_{12}\}. \)

2.2. Hamiltonian \( \mathcal{A}_\varepsilon \)

In what follows if \( u : \Gamma \to \mathbb{C} \) and \( e \in \mathcal{E} \) then by \( u_e \) we denote the restriction of \( u \) onto \( e \). Via a local coordinate \( x_e \) we identify \( u_e \) with a function on \( (0, l(e)) \).

We introduce several functional spaces on \( \Gamma \). The space \( L^2(\Gamma) \) consists of functions that are measurable and square integrable on each edge \( e \) and such that
\[ \|u\|_{L^2(\Gamma)} := \sum_{e \in \mathcal{E}} \|u_e\|_{L^2(0,l(e))}^2 = \sum_{e \in \mathcal{E}} \int_{0}^{l(e)} |u_e(x_e)|^2 dx_e < \infty. \]

The space \( \widetilde{H}^k(\Gamma), k \in \mathbb{N} \) consists of functions on \( \Gamma \) belonging to the Sobolev space \( H^k(\Gamma) \) on each edge and satisfying
\[ \|u\|_{\widetilde{H}^k(\Gamma)} := \sum_{e \in \mathcal{E}} \|u_e\|_{H^k(0,l(e))}^2 = \sum_{e \in \mathcal{E}} \int_{0}^{l(e)} \left| \frac{d^k u_e(x_e)}{dx_e^k} \right|^2 dx_e < \infty. \]

Finally, the set \( \mathcal{H}(\Gamma) \) consists of functions \( u \in \widetilde{H}^1(\Gamma) \) satisfying the following conditions at vertices of \( \Gamma \):

- if \( v \in \mathcal{V} \setminus \bigcup_{i \in \mathbb{Z}^n} \bigcup_{j=1}^{m} \mathcal{V}_j \) then \( u \) is continuous at \( v \), i.e. the limiting value of \( u(x) \) when \( x \) approaches \( v \) is independent of \( e \). We denote this value by \( u(v) \);
- if \( v \in \mathcal{V}_j \) for some \( i = (i_1, ..., i_n) \in \mathbb{Z}^n, j \in \{1, ..., m\} \) then
  - the limiting value of \( u(x) \) when \( x \) approaches \( v \) along \( e \in \mathcal{E}(v) \cap \mathcal{V}_j \) is independent of \( e \).
  - the limiting value of \( u(x) \) when \( x \) approaches \( v \) along \( e \in \mathcal{E}(v) \cap \mathcal{V}_j \) is independent of \( e \).
    - We denote this value by \( u_0(v) \);
    - We denote this value by \( u_j(v) \).

Now, we describe the family of operators \( \mathcal{A}_\varepsilon \), which will be the main object of our interest in this paper. In \( L^2(\Gamma) \) we introduce the sesquilinear form \( a_\varepsilon \),
\[ \text{dom}(a_e) = H(\Gamma), \]
\[ a_e[u, w] = \varepsilon^{-1} \sum_{e \in \mathcal{E}} \int_{\mathbb{R}} \frac{du_x}{dx} \frac{dw_x}{dx} + \sum_{i \in \mathbb{Z}^+} \sum_{j=1}^{m} \sum_{v_j} q_j \left( u_0(v) - u_j(v) \right) \left( w_0(v) - w_j(v) \right), \]

where \( q_j \) are positive constants. The definition of \( a_e[u, w] \) makes sense: the second term in the right-hand side of (4) (we denote it \( \delta[u, w] \)) is finite, namely one has the estimate
\[ |\delta[u, w]|^2 \leq C ||u||^2_{H^1(\Gamma)} ||w||^2_{H^1(\Gamma)} \]

following from the standard trace inequality
\[ ||u(l)||^2 \leq 2 \left( \|u\|_{L^2(0, l)}^2 + l \|u\|_{L^2(0, l)}^2 \right), \quad \forall u \in H^1(0, l). \]

Furthermore, it is straightforward to check that the form \( a_e[u, v] \) is symmetric, densely defined, closed and positive. Then (see, e.g., [20, theorem VIII.15]) there exists the unique self-adjoint and positive operator \( \tilde{\mathcal{A}}_e \) associated with the form \( a_e \), i.e.
\[ (\mathcal{A}_e u, v)_{L^2(\Gamma)} = a_e[u, v], \quad \forall u \in \text{dom}(\mathcal{A}_e), \forall v \in \text{dom}(a_e). \]

The definitional domain of the operator \( \mathcal{A}_e \) consists of functions \( u \in H(\Gamma) \) belonging to \( H^2(\Gamma) \) and satisfying the following conditions at the vertices (additionally to the conditions needed to be in \( H(\Gamma) \)):

- if \( v \in \mathcal{V} \setminus \bigcup_{j=1}^{m} \{v_j\} \) then
  \[ \sum_{e \in \mathcal{E}(v)} \frac{du_x}{dx} \bigg|_{x = 0} = 0 \]
  (Kirchhoff conditions),

  where
  \[ x_v = \begin{cases} x_e, & \text{if } v = \gamma^-(e), \\ x_v = l(e) - x_e, & \text{if } v = \gamma^+(e), \end{cases} \]

  (i.e. \( x_v \) is a natural coordinate on \( e \in \mathcal{E}(v) \) such that \( x_v = 0 \) at \( v \));

- if \( v \in \mathcal{V}_0, \ i \in \mathbb{Z}^n, \ j \in \{1, \ldots, m\} \) one has the following conditions at \( v \):
  \[ -\varepsilon^{-1} \sum_{e \in \mathcal{E}(v) \setminus \mathcal{V}_0} \frac{du_x}{dx} \bigg|_{x = 0} + q_j \left( u_0(v) - u_j(v) \right) = 0, \]
  \[ -\varepsilon^{-1} \sum_{e \in \mathcal{E}(v) \cap \mathcal{V}_0} \frac{du_x}{dx} \bigg|_{x = 0} + q_j \left( u_j(v) - u_0(v) \right) = 0. \]

The operator \( \mathcal{A}_e \) acts as follows:
\[ (\mathcal{A}_e u)_e = -\varepsilon^{-1} \frac{d^2u_e}{dx^2}, \quad e \in \mathcal{E}. \]

\textbf{Remark 2.2.} Suppose that \( v \in \mathcal{V}_0 \) (for some \( i \in \mathbb{Z}^n, j \in \{1, \ldots, m\} \)) has two outgoing edges, \( e \in \mathcal{E}(v) \cap \mathcal{V}_0 \) and \( \tilde{e} \in \mathcal{E}(v) \cap \mathcal{V}_0 \). Then, evidently, conditions (5) are equivalent to
\[
\frac{d u_e}{dx_e} \bigg|_{x_e=0} + \frac{d u_{\tilde{e}}}{dx_{\tilde{e}}} = 0, \qquad \kappa \frac{du_e}{dx_e} \bigg|_{x_e=0} = \left( u_e \bigg|_{x_e=0} - u_{\tilde{e}} \bigg|_{x_{\tilde{e}}=0} \right), \qquad \kappa = \left( q_j \epsilon \right)^{-1},
\]

(recall that \( x_e \in [0, l(e)] \) and \( x_{\tilde{e}} \in [0, l(\tilde{e})] \) are the natural coordinates on \( e \) and \( \tilde{e} \), correspondingly, such that \( x_e = x_{\tilde{e}} = 0 \) at \( v \)). Thus we obtain the usual \( \delta' \) conditions at a point on the line [1, section I.4] that explains why we use the term ‘\( \delta' \)-type conditions’ for (5). Various analogues of \( \delta' \) conditions for graphs are discussed in [7].

**Remark 2.3.** The name ‘\( \delta' \)-conditions’ is misleading because such Hamiltonians cannot be obtained using families of scaled zero-mean potentials (see [22]). However one can approximate them by a triple of \( \delta \) potentials and then by regular \( \delta \)-like ones following an idea put forward in [4] and then made mathematically rigorous in [9]. The problem of approximating all singular vertex couplings (in particular, \( \delta' \)-type ones) in a quantum graph is solved in [5].

### 2.3. The main result

Before to formulate the result let us introduce several notations. We denote

- \( l_j \), \( j = 0, ..., m \) the total length of all edges belonging to \( Y_j \),
- \( N_j \), \( j = 1, ..., m \) we denote the number of points belonging to the set \( Y_j \).

Then for \( j = 1, ..., m \) we set:

\[
a_j := \frac{N_j q_j}{l_j}.
\]  \( (6) \)

It is assumed that the numbers \( a_j \) are pairwise non-equivalent. We renumber them in the ascending order, that is

\[
a_j < a_{j+1}, \quad \forall j = 1, ..., m - 1.
\]  \( (7) \)

Finally, we consider the following equation (with unknown \( \lambda \in \mathbb{C} \)):

\[
F(\lambda) := 1 + \sum_{j=1}^{m} \frac{a_j l_j}{l_0 (a_j - \lambda)} = 0.
\]  \( (8) \)

It is straightforward to show that if (7) holds then equation (8) has exactly \( m \) roots, they are real and interlace with \( a_j \). We denote them by \( b_j \), \( j = 1, ..., m \) supposing that they are renumbered in the ascending order, i.e.

\[
a_j < b_j < a_{j+1}, \quad j = 1, ..., m - 1, \quad a_m < b_m < \infty.
\]  \( (9) \)

We are now in position to formulate the first main result of this work.

**Theorem 2.1.** Let \( L > 0 \) be an arbitrary number. Then the spectrum of the operator \( A_\epsilon \) in \([0, L]\) has the following structure for \( \epsilon \) small enough:

\[
\sigma(A_\epsilon) \cap [0, L] = [0, L] \setminus \bigcup_{j=1}^{m} (a_j(\epsilon), b_j(\epsilon)),
\]  \( (10) \)

where the endpoints of the intervals \( (a_j(\epsilon), b_j(\epsilon)) \) satisfy the relations

\[
\lim_{\epsilon \to 0} a_j(\epsilon) = a_j, \quad \lim_{\epsilon \to 0} b_j(\epsilon) = b_j, \quad j = 1, ..., m.
\]  \( (11) \)

In the last section we will present our second result (theorem 4.1): we will show that under a
suitable choice of the graph \( \Gamma \) and the coupling constants \( q_j \) the limit intervals \((a_j, b_j)\) coincide with predefined ones.

Theorem 2.1 will be proven in the next section. We postpone the outline of the proof to the end of subsection 3.1 because we need to introduce first some more notations.

3. Proof of theorem 2.1

3.1. Preliminaries

The Floquet–Bloch theory establishes a relationship between the spectrum of \( A_{\epsilon} \) and the spectra of appropriate operators on \( Y \). Namely, let

\[ \theta \in \mathbb{T}^n = \left\{ \theta = (\theta_1, \ldots, \theta_n) \in \mathbb{C}^n, \left| \theta_k \right| = 1 \text{ for all } k = 1, \ldots, n \right\}. \]

We denote by \( H^0(\Gamma) \) the set of functions \( u : \Gamma \to \mathbb{C} \) satisfying

- \( \forall e \in E : u_e \in H^1(e) \),
- \( u \) is continuous at all vertices belonging to \( \mathcal{V} \setminus \left( \bigcup_{v \in \mathcal{V}} V_v \right) \),
- at the vertices belonging to \( \bigcup_{v \in \mathcal{V}} V_v \) \( u \) satisfies the same conditions as functions from \( H(\Gamma) \),
- \( u \) is \( \theta \)-periodic, that is

\[ \forall x \in \Gamma : u(x + e_k) = \theta_k u(x), \quad k = 1, \ldots, n \]

(if \( \theta = (1, 1, \ldots, 1) \) (respectively, \( \theta = -(1, 1, \ldots, 1) \)) one has periodic (respectively, antiperiodic) conditions).

Then we introduce the sesquilinear form \( a_{\epsilon}^{\theta} \) defined as follows (below the notation \( E(Y) \) stays for the set of edges of \( Y \)):

\[
\text{dom}(a_{\epsilon}^{\theta}) = \left\{ u = v|_Y, \; v \in H^0(\Gamma) \right\},
\]

\[
a_{\epsilon}^{\theta}[u, w] = e^{-1} \sum_{e \in E(Y)} \int_{0}^{1(e)} \frac{du_e}{dx_e} \frac{dw_e}{dx_e} + \sum_{j=1}^{m} \sum_{v \in \mathcal{V}_j} q_{j} (u_0(v) - u_j(v))(w_0(v) - w_j(v)).
\]

We define \( A_{\epsilon}^{\theta} \) as the operator acting in \( L_2(Y) \) being associated with the form \( a_{\epsilon}^{\theta} \). Since \( Y \) is compact, \( A_{\epsilon}^{\theta} \) has a purely discrete spectrum. We denote by \( \{ \lambda_k^{\theta}(\epsilon) \}_{k \in \mathbb{N}} \) the sequence of eigenvalues of \( A_{\epsilon}^{\theta} \) arranged in the ascending order and repeated according to their multiplicity.

One has the following representation (see [3, chapter 4]):

\[ \sigma(A_{\epsilon}) = \bigcup_{\theta \in \mathbb{T}^n} \left\{ \lambda_k^{\theta}(\epsilon) \right\}, \quad k \in \mathbb{N}, \]

Moreover, for any fixed \( k \in \mathbb{N} \) the set

\[ L_k(\epsilon) := \bigcup_{\theta \in \mathbb{T}^n} \left\{ \lambda_k^{\theta}(\epsilon) \right\} \]

is a compact interval (\( k \)-th spectral band).

By \( H(Y) \) we denote the set of functions \( u : Y \to \mathbb{C} \) satisfying

- \( \forall e \in E(Y) : u_e \in H^1(e) \),
- \( u \) is continuous at all vertices of \( Y \) except those ones belonging to \( \bigcup_{j=1}^{m} V_j \).
at the vertices from $\bigcup_{j=1}^{m} Y_j$ $u$ satisfies the same conditions as functions from $H(Y)$. Then we introduce the operator $A^N_\epsilon$ (respectively, $A^D_\epsilon$) as the operator acting in $L_2(Y)$ and associated with the sesquilinear form $a^N_\epsilon$ (respectively, $a^D_\epsilon$) defined as follows:

$$\text{dom}(A^N_\epsilon) = H(Y), \ a^N_\epsilon[u, w] = a^\theta_\epsilon[u, w],$$

(respectively, $\text{dom}(A^D_\epsilon) = \{ u \in H(Y): u = 0 \text{ on } \partial_{\text{ext}} Y \}, \ a^D_\epsilon[u, w] = a^\theta_\epsilon[u, w]$.)

The subscript $N$ (respectively, $D$) indicates that functions from $\text{dom}(A^N_\epsilon)$ (respectively, $\text{dom}(A^D_\epsilon)$) satisfy the Neumann (respectively, Dirichlet) boundary conditions on $\partial Y$.

The spectra of the operators $A^N_\epsilon$ and $A^D_\epsilon$ are purely discrete. We denote by $\{ \lambda_k^N(\epsilon) \}_{k \in \mathbb{N}}$ (respectively, $\{ \lambda_k^D(\epsilon) \}_{k \in \mathbb{N}}$) the sequence of eigenvalues of $A^N_\epsilon$ (respectively, of $A^D_\epsilon$) arranged in the ascending order and repeated according to their multiplicity.

Using the min–max principle and the enclosures

$$\text{dom}(A^N_\epsilon) \supset \text{dom}(A^\theta_\epsilon) \supset \text{dom}(A^D_\epsilon),$$

we obtain that

$$\forall k \in \mathbb{N}, \forall \theta \in \mathbb{T}^n: \lambda_k^N(\epsilon) \leq \lambda_k^\theta(\epsilon) \leq \lambda_k^D(\epsilon). \ (14)$$

Finally, we present the result of Simon [23, theorem 4.1], which will be widely used during the proof. In order to simplify its presentation we introduce an auxiliary definition.

**Definition 3.1.** Let $a$ be a symmetric, closed and positive sesquilinear form in a Hilbert space $H$ with a domain $\text{dom}(a)$, which is not necessary dense in $H$. Let $A$ be a positive self-adjoint operator acting in the subspace $\text{dom}(a)$ of $H$ and associated with the form $a$. Then the operator $R$ defined by the formula

$$R = \begin{cases} (A + I)^{-1} & \text{on } \text{dom}(a), \ I \text{ is the identity operator}, \\ 0 & \text{on } H \ominus \text{dom}(a) \end{cases}$$

is said to be the generalized resolvent corresponding to the form $a$.

**Theorem 3.1.** (Simon [23]) let $\{a_\epsilon\}_{\epsilon > 0}$ be a family of closed positive symmetric sesquilinear forms in a Hilbert space $H$, by $\{R_\epsilon\}_{\epsilon > 0}$ we denote the corresponding family of generalized resolvents. Suppose that $a_\epsilon$ increases monotonically as $\epsilon$ decreases, i.e.

if $\epsilon_1 \geq \epsilon_2$ then $\text{dom}(a_{\epsilon_2}) \supset \text{dom}(a_{\epsilon_1})$ and $a_{\epsilon_2}[u, u] \leq a_{\epsilon_1}[u, u], \forall u \in \text{dom}(a_{\epsilon_1})$.

Then the positive symmetric sesquilinear form $a_0$ defined by

$$\text{dom}(a_0) := \left\{ u \in \bigcap_{\epsilon > 0} \text{dom}(a_{\epsilon}): \sup_{\epsilon > 0} a_{\epsilon}[u, u] < \infty \right\}, \ a_0[u, v] = \lim_{\epsilon \to 0} a_{\epsilon}[u, v]$$

is closed, and moreover

$$\forall u \in H: R_\epsilon u \to R_0 u \text{ as } \epsilon \to 0,$$

where $R_0$ is the generalized resolvent corresponding to the form $a_0$.

With these preliminaries we are able to give a short scheme of the proof of theorem 2.1. In view of (12)–(14) the left end (respectively, the right end) of the $k$th spectral band $L_k(\epsilon)$ is situated between the $k$th Neumann eigenvalue $\lambda_k^N(\epsilon)$ and the $k$th periodic eigenvalue $\lambda_k^\theta(\epsilon)$. 

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\[ \theta = (1, \ldots, 1) \] (respectively, between the \( k \)th antiperiodic eigenvalue \( \lambda_k^N(\varepsilon) \), \( \theta = -(1, \ldots, 1) \) and the \( k \)th Dirichlet eigenvalue \( \lambda_k^D(\varepsilon) \)). Our main task is to prove that they both converge to \( b_k^1 \) as \( k \rightarrow \infty \) and converge to infinity as \( k > m \). These results taken together constitute the claim of theorem 2.1. Our analysis will be based on Simon’s theorem formulated above.

We notice that the band ends need not in general coincide with the corresponding periodic/antiperiodic eigenvalues, even in case \( n = 1 \) (see [8, 10]). What matters is that we can enclose them between two values which converge to the same limit as \( \varepsilon \rightarrow 0 \).

3.2. Asymptotic behaviour of Neumann and periodic eigenvalues

In this subsection we study the behaviour as \( \varepsilon \rightarrow 0 \) of the eigenvalues of the operators \( A^N_\varepsilon \) and \( A^\theta_\varepsilon \), \( \theta = (1, 1, \ldots, 1) \).

Obviously, \( \lambda_1^N(\varepsilon) = 0 \). For the subsequent eigenvalues we will prove the following lemma.

Lemma 3.1. One has

\[
\lim_{\varepsilon \rightarrow 0} \lambda_k^N(\varepsilon) = b_{k-1}, \quad k = 2, \ldots, m + 1, \\
\lim_{\varepsilon \rightarrow 0} \lambda_k^N(\varepsilon) = \infty, \quad k \geq m + 2. 
\]

Proof. The family of forms \( \{ a_\varepsilon^N \} \) increases monotonically as \( \varepsilon \rightarrow 0 \) and we may apply theorem 3.1. Namely, let us introduce the limit form \( a_0^N \),

\[
\text{dom}(a_0^N) := \left\{ u \in H(Y) : \sup_{\varepsilon > 0} a_\varepsilon^N[u, u] < \infty \right\}, \quad a_0^N[u, v] = \lim_{\varepsilon \rightarrow 0} a_\varepsilon^N[u, v].
\]

Evidently \( \text{dom}(a_0^N) \) consists of piecewise constant functions, which are continuous in \( Y_j \) for each \( j = 0, \ldots, m \) (this last one follows from (2) to (3) and the definition of \( H(\Gamma) \)). Thus \( \text{dom}(a_0^N) \) is an \( (m + 1) \)-dimensional subspace of \( L_2(Y) \) consisting of functions \( u \) of the form \( u(x) = \sum_{j=0}^m u_j \chi_j(x) \), where \( u_j \) are constants, \( \chi_j \) are the indicator functions of \( Y_j \)

and, clearly,

\[
a_0^N[u, v] = \sum_{j=1}^m q_j N_j(\mathbf{u}_0 - \mathbf{u}_j)(\mathbf{v}_0 - \mathbf{v}_j).
\]

We denote by \( A_0^N \) a self-adjoint operator acting in \( \text{dom}(a_0^N) = \text{dom}(a_0^N) \) and associated with the form \( a_0^N \). It is straightforward to check that it acts as follows:

\[
A_0^N u = \left( \sum_{k=1}^m q_k N_k t_0^{-1}(\mathbf{u}_0 - \mathbf{u}_k) \right) \mathbf{z}_0(x) + \sum_{j=1}^m q_j N_j l_j^{-1}(\mathbf{u}_j - \mathbf{u}_0) \chi_j(x).
\]

The operator \( A_0^N \) can be regarded as a Hermitian operator in \( C^{m+1} \) equipped with the scalar product \( (x, y)_{C^{m+1}} = \sum_{j=0}^m l_j \mathbf{x}_j \mathbf{y}_j \). We denote by

\[
0 \leq \lambda_1^N(0) \leq \lambda_2^N(0) \leq \ldots \leq \lambda_{m+1}^N(0)
\]

its eigenvalues arranged in the ascending order and repeated according to their multiplicity. It is easy to see that.
Later we will prove
\[ \lambda_k^N(0) = b_{k-1}, \quad k = 2, \ldots, m + 1. \] (18)

We denote by \( R_0^N : L_2(Y) \to L_2(Y) \) the generalized resolvent corresponding to the form \( a_0^N \). Its spectrum is a union of eigenvalues
\[ \mu_k^N(0) = (\lambda_k^N(0) + 1)^{-1}, \quad k = 1, \ldots, m + 1 \] (19)
and the point \( \mu = 0 \), which is an eigenvalue of infinity multiplicity.

Now, applying theorem 3.1 we conclude that
\[ \forall u \in L_2(Y) : \left( A_{\varepsilon}^N + I \right)^{-1} u \to R_0^N u \text{ as } \varepsilon \to 0. \] (20)

Moreover, since the operators \( (A_{\varepsilon}^N + I)^{-1} \) and \( R_0^N \) are compact and \( (A_{\varepsilon}^N + I)^{-1} \geq (A_0^N + I)^{-1} \geq 0 \) as \( \varepsilon_1 \geq \varepsilon_2 \) then by virtue of the result of Kato [11, theorem VIII-3.5] (20) can be improved to the norm convergence
\[ \| \left( A_{\varepsilon}^N + I \right)^{-1} - R_0^N \| \to 0 \text{ as } \varepsilon \to 0, \]
whence, using the classical perturbation theory, we obtain the convergence of spectra, namely
\[ \lim_{\varepsilon \to 0} (\lambda_k^N(\varepsilon) + 1)^{-1} = \mu_k^N(0) \text{ as } k = 1, \ldots, m + 1, \]
\[ \lim_{\varepsilon \to 0} (\lambda_k^N(\varepsilon) + 1)^{-1} = 0 \text{ as } k \geq m + 2. \] (21)

Taking into account (19) we obtain from (21):
\[ \lim_{\varepsilon \to 0} \lambda_k^N(\varepsilon) = \lambda_k^N(0) \text{ as } k = 1, \ldots, m + 1, \quad \lim_{\varepsilon \to 0} \lambda_k^N(\varepsilon) = \infty \text{ as } k \geq m + 2. \]

Thus, to complete the proof of lemma 3.1 it remains to prove (18).

In view of (16) \( \lambda_k^N(0), \quad k = 1, \ldots, m + 1 \) are the eigenvalues of the \((m + 1) \times (m + 1)\) matrix
\[
A = \begin{pmatrix}
\sum_{j=1}^{m} q_j N_j l_0^{-1} - q_1 N_1 l_0^{-1} & -q_2 N_2 l_0^{-1} & \ldots & -q_m N_m l_0^{-1} \\
-q_1 N_1 l_1^{-1} & q_1 N_1 l_1^{-1} & 0 & \ldots & 0 \\
-q_2 N_2 l_2^{-1} & 0 & q_2 N_2 l_2^{-1} & \ldots & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
-q_m N_m l_m^{-1} & 0 & 0 & \ldots & q_m N_m l_m^{-1}
\end{pmatrix}
\]
They are the roots of the characteristic equation
\[ \det(A - \lambda I) = 0. \]

We denote by \( M(i_1, i_2, \ldots, i_k) \) the minor of the matrix \( A \) staying on the intersection of \( i_1 \)th, \( i_2 \)th, \ldots, \( i_k \)th rows and the columns with the same numbers. One has the following formula (see, e.g., [18, section 2.13.2]):
\[ \det(A - \lambda I) = \sum_{k=0}^{m+1} \lambda^m + (-1)^m + 1 - k \]  

(22)

where

\[ E_0 = 1, \quad E_k = \sum_{1 \leq i_1 < i_2 < \ldots < i_k \leq m + 1} M(i_1, i_2, \ldots, i_k) \] as \( k \geq 1 \).  

(23)

It is clear that \( E_{m+1} = \det(A) = 0 \) since the sum of all columns of \( A \) is zero. For \( 2 \leq k \leq m \) we represent \( E_k \) as a sum of two terms:

\[ E_k = \sum_{1 \leq i_1 < i_2 < \ldots < i_k \leq m} M(i_1 + 1, i_2 + 1, \ldots, i_k + 1) + \sum_{1 \leq i_1 < \ldots < i_k \leq m} M(1, i_2 + 1, \ldots, i_k + 1). \]  

(24)

One has (below \( 1 \leq i_1 < i_2 < \ldots < i_k \leq m \)):

\[ M(i_1 + 1, i_2 + 1, \ldots, i_k + 1) = \begin{vmatrix} q_{i_1 N_0 l_{i_1}} & 0 & \ldots & 0 \\ 0 & q_{i_2 N_0 l_{i_2}} & \ldots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \ldots & q_{i_k N_0 l_{i_k}} \end{vmatrix} = \prod_{a=1}^{k} q_{i_a N_0 l_{i_a}}. \]  

(25)

And (below \( 1 \leq i_2 < \ldots < i_k \leq m \))

\[ M(1, i_2 + 1, \ldots, i_k + 1) \]

\[ = \begin{vmatrix} \sum_{j=1}^{m} q_{j N_0 l_{j_0}} & -q_{i_2 N_0 l_{i_2}} & \ldots & -q_{i_k N_0 l_{i_k}} \\ -q_{i_2 N_0 l_{i_2}} & q_{i_2 N_0 l_{i_2}} & \ldots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ -q_{i_k N_0 l_{i_k}} & 0 & \ldots & q_{i_k N_0 l_{i_k}} \end{vmatrix} = \prod_{a=2}^{k} q_{i_a N_0 l_{i_a}}. \]  

(26)

The first determinant in the right-hand side of (26) is equal to zero since the sum all columns of the corresponding matrix is equal to zero. As a result we obtain:
Via a simple algebraic calculations it is not hard to get from (27) that

\[
\sum_{1 \leq i_1 < \ldots < i_k \leq m} M(1, i_2 + 1, \ldots, i_k + 1) = l_0^{-1} \sum_{1 \leq i_1 < i_2 < \ldots < i_k \leq m} \left( \prod_{a=1}^{k} q_i^a N_i l_i^{-1} \right) \left( \sum_{a=1}^{k} l_i \right).
\]

(28)

Combining (24), (25), (28) and taking into account the definition of \( a_j \) one arrives at

\[
E_k = \sum_{1 \leq i_1 < i_2 < \ldots < i_k \leq m} \left( \prod_{a=1}^{k} a_i \right) \left( 1 + l_0^{-1} \sum_{a=1}^{k} l_i \right).
\]

(29)

We have proved (29) for \( 2 \leq k \leq m \). For \( k = 1 \) it holds as well:

\[
E_1 \equiv \text{tr} A = \sum_{i=1}^{m} q_i N_i l_0^{-1} + \sum_{i=1}^{m} q_i N_i l_i^{-1} = \sum_{i=1}^{m} a_i \left( 1 + l_0^{-1} l_i \right).
\]

Now let us study the function \( F(\lambda) \) staying in the right-hand side of equation (8). One has

\[
F(\lambda) = \prod_{j=1}^{m} \frac{1}{a_j - \lambda} \left( \sum_{k=0}^{m} \binom{m}{k} (-1)^{m-k} \sum_{1 \leq i_1 < i_2 < \ldots < i_k \leq m} \left( \prod_{a=1}^{k} a_i \right) \left( 1 + l_0^{-1} \sum_{a=1}^{k} l_i \right) \right).
\]

(30)

Grouping the terms with the same exponents of \( \lambda \) one can easily obtain:

\[
F(\lambda) = \prod_{j=1}^{m} \frac{1}{a_j - \lambda} \sum_{k=0}^{m} \binom{m}{k} (-1)^{m-k} \left( \sum_{1 \leq i_1 < i_2 < \ldots < i_k \leq m} \left( \prod_{a=1}^{k} a_i \right) \left( 1 + l_0^{-1} \sum_{a=1}^{k} l_i \right) \right).
\]

(31)

or, using (22), (29) and taking into account that \( E_{m+1} = 0 \), we obtain:

\[
F(\lambda) = \prod_{j=1}^{m} \frac{1}{a_j - \lambda} \sum_{k=0}^{m} \lambda^{m-k} (-1)^{m-k} E_k
\]

\[
= \frac{1}{-\lambda \prod_{j=1}^{m} (a_j - \lambda)} \sum_{k=0}^{m} \lambda^m + 1-k (-1)^m + 1-k E_k
\]

\[
= \frac{1}{-\lambda \prod_{j=1}^{m} (a_j - \lambda)} \sum_{k=0}^{m} \lambda^m + 1-k (-1)^m + 1-k E_k
\]

\[
= \frac{1}{-\lambda \prod_{j=1}^{m} (a_j - \lambda)} \det(A - \lambda I),
\]

(32)

whence, taking into account (9) and (17), we easily obtain (18). The lemma is proved. \( \square \)
The same asymptotics are valid for the eigenvalues of the operator $A_0^\theta$ as $\theta = (1, 1, ..., 1)$.

**Lemma 3.2.** One has

\[
\lim_{\epsilon \to 0} \lambda_k^\theta(\epsilon) = b_{k-1}, \quad k = 2, ..., m + 1, \\
\lim_{\epsilon \to 0} \lambda_k^\theta(\epsilon) = \infty, \quad k \geq m + 2
\]

provided $\theta = (1, 1, ..., 1)$.

**Proof.** It is easy to see that functions $u$ of the form (15) belong to $\text{dom}(a_0^\theta)$ provided $\theta = (1, 1, ..., 1)$, whence, evidently, the limit form $a_0^\theta$ coincides with the form $a_0^0$. In the rest the proof repeats word-by-word the proof of lemma 3.1. □

3.3. Asymptotic behaviour of dirichlet and $\theta$-periodic eigenvalues ($\theta = (1, 1, ..., 1)$)

In this subsection we study the behaviour as $\epsilon \to 0$ of the eigenvalues of the operators $A_\epsilon^D$ and $A_\epsilon^\theta$, $\theta \neq (1, 1, ..., 1)$.

**Lemma 3.3.** One has

\[
\lim_{\epsilon \to 0} \lambda_k^D(\epsilon) = a_k, \quad k = 1, ..., m, \\
\lim_{\epsilon \to 0} \lambda_k^\theta(\epsilon) = \infty, \quad k \geq m + 1
\]

**Proof.** For the proof we employ the same method as in the proof of lemma 3.1. Namely, we again introduce the limit form $a_0^D[u, u]$ by

$$\text{dom}(a_0^D) = \left\{ u \in H(Y), \ u \big|_{Y_0} = 0: \ \sup_{\epsilon > 0} a_\epsilon^D[u, u] < \infty \right\}, \quad a_0^D[u, v] = \lim_{\epsilon \to 0} a_\epsilon^D[u, v].$$

It is clear that $\text{dom}(a_0^D)$ consists of piecewise constant functions, which are continuous in $Y_j^s$ for each $j = 1, ..., m$ and equal to zero in $Y_0$. Thus $\text{dom}(a_0^D)$ is an $m$-dimensional subspace of $L^2(Y)$ consisting of functions $u$ of the form

$$u(x) = \sum_{j=1}^m u_j \chi_j(x), \quad \text{where } u_j \text{ are constants, } \chi_j \text{ is an indicator function of } Y_j$$

and

$$a_0^D[u, v] = \sum_{j=1}^m q_j N_j u_j v_j.$$

We denote by $A_0^D$ a bounded and self-adjoint operator acting in $\text{dom}(a_0^D) = \text{dom}(a_0^D)$ and associated with the form $a_0^D$. It acts as follows:
Repeating word-by-word the arguments of the proof of lemma 3.1 we conclude that

\[
\lim_{\epsilon \to 0} \lambda_k^D(\epsilon) = \lambda_k^D(0), \quad k = 1, \ldots, m, \\
\lim_{\epsilon \to 0} \lambda_k^D(\epsilon) = \infty, \quad k \geq m + 1,
\]

where \( \lambda_k^D(0) \) is the \( k \)th eigenvalue of the operator \( \mathcal{A}_0^D \). It follows from (33) that

\[
\lambda_k^D(0) = q_j N_j l_j^{-1} = a_k.
\]

The lemma is proved. \( \square \)

The same asymptotics are valid for the eigenvalues of the operator \( \mathcal{A}_\theta^D \) as \( \theta \not\supset (1, 1, \ldots, 1) \).

**Lemma 3.4.** One has

\[
\lim_{\epsilon \to 0} \lambda_k^\theta(\epsilon) = a_k, \quad k = 1, \ldots, m, \\
\lim_{\epsilon \to 0} \lambda_k^\theta(\epsilon) = \infty, \quad k \geq m + 1.
\]

Provided \( \theta \not\supset (1, 1, \ldots, 1) \).

**Proof.** The definition domain of the form \( a_\theta^\theta \) consists of functions \( u \) having the form (15) and belonging to \( \text{dom}(a_\theta^\theta) \). It is easy to see that if \( \theta \not\supset (1, 1, \ldots, 1) \) then \( u_0 = 0 \) (otherwise \( u \not\in \text{dom}(a_\theta^\theta) \)). Thus the limit form \( a_0^\theta \) coincides with the form \( a_0^D \) provided \( \theta \not\supset (1, 1, \ldots, 1) \). In the rest the proof repeats word-by-word the proof of lemma 3.3. \( \square \)

The claim of theorem 2.1 follows directly from (12)–(14) and lemmata 3.1–3.4.

**4. Periodic quantum graphs with asymptotically predefined spectral gaps**

In this section we will show that under a suitable choice of the graph \( \Gamma \) and the coupling constants \( q_j \) the limit intervals \( (a_j, b_j) \) coincide with predefined ones.

Let \( \Gamma \) be a \( \mathbb{Z}^n \)-periodic graph with a periodic cell \( Y \) admitting decomposition (2) and (3). Recall that the notation \( l_j \) stays for the total length of all edges belonging to the set \( Y_j \) \((j = 0, \ldots, m)\), by \( N_j \) we denote the number of points belonging to the set \( Y_j \) \((j = 1, \ldots, m)\)—see section 2, where these notations are introduced. Also in the same way as before we introduce the numbers \( a_j \) and \( b_j \) \((j = 1, \ldots, m)\).

**Theorem 4.1.** Let \( L > 0 \) be an arbitrarily large number and let \( (a_j, b_j) \) \((j = 1, \ldots, m, m \in \mathbb{N})\) be arbitrary intervals satisfying

\[
0 < a_1, \quad a_j < b_j < a_{j+1}, \quad j = 1, m-1, \quad a_m < b_m < L.
\]
Suppose that the numbers $l_j$, $j = 0, ..., m$, satisfy
\begin{equation}
    l_j = l_0 \frac{\beta_j - \alpha_j}{\alpha_j} \prod_{i=\max\{0,j\} \neq j}^{m} \left( \frac{\beta_i - \alpha_i}{\alpha_i - \alpha_j} \right) \tag{35}
\end{equation}
Then one has
\begin{equation}
    a_j = \alpha_j, \quad b_j = \beta_j, \quad j = 1, ..., m \tag{36}
\end{equation}
provided
\begin{equation}
    q_j = \frac{\alpha_j l_j}{N_j}, \quad j = 1, ..., m. \tag{37}
\end{equation}

\textbf{Remark 4.1.} Since the intervals $(\alpha_j, \beta_j)$ satisfy (34) then
\[ \forall j: \beta_j > \alpha_j, \quad \forall i \neq j: \text{sign}(\beta_i - \alpha_j) = \text{sign}(\alpha_i - \alpha_j) \neq 0 \]
and therefore the quantity staying in the right-hand side of (35) is positive.

\textbf{Remark 4.2.} Results, similar to theorem 4.1 (i.e., construction of periodic operators with gaps that are close to given intervals), were obtained by one of the authors in [12] for Laplace–Beltrami operators on periodic Riemannian manifolds, in [13] for periodic elliptic divergence type operators in $\mathbb{R}^n$, and in [14] for Neumann Laplacians in periodic domains in $\mathbb{R}^n$.

\textbf{Proof.} Plugging (37) into (6) we obtain the first equality of (36).
Recall that the numbers $b_j$ are the roots of the equation (8) written in the ascending order. Therefore, in order to prove the second equality in (36) one has to show that
\begin{equation}
    \forall i = 1, ..., m: \quad 1 + \sum_{j=1}^{m} \frac{\alpha_j l_j}{l_0(\alpha_j - \beta_i)} = 0. \tag{38}
\end{equation}
Let us consider (38) as the linear algebraic system of $m$ equations with unknowns $l_j$, $j = 1, ..., m$. It was proved in [12, lemma 4.1] that this system has the unique solution defined by formula (35). This implies the second equality in (36). Theorem 4.1 is proved. \hfill \Box

It is easy to construct the graph $\Gamma \subset \mathbb{R}^d$ satisfying (2), (3) and (35). For example, one can proceed as follows. Let $I_0$ be an arbitrary $\mathbb{Z}^n$-periodic metric graph, $e_1, ..., e_n$ be vectors producing an action of $\mathbb{Z}^n$ on $I_0$ (i.e., (1) holds). We denote by $Y_0$ its period cell. Let $v_1, ..., v_m$ be arbitrary points belonging to $Y_0$. Let $Y_j, j = 1, ..., m$ be arbitrary compact graphs satisfying $Y_i \cap Y_j = \emptyset$ as $i \neq j$ and $Y_j \cap I_0 = \{v_j\}$. We denote
\[ Y_j = Y_j + \sum_{k=1}^{n} l_k e_k, \quad i = (i_1, ..., i_n) \in \mathbb{Z}^n \]
and, finally,
\[ \Gamma = I_0 \cup \bigcup_{i \in \mathbb{Z}^n} \bigcup_{j=1}^{m} Y_j. \]
The graph $\Gamma$ is presented on figure 2 (here the graph in $\mathbb{Z}$-periodic, $m = 2$). The set

$$Y := \bigcup_{j=0}^{m} Y_j$$

is a period cell of $\Gamma$. It is easy to see that the sets $Y_j$ satisfy conditions (3). Obviously, they can be chosen in such a way that (35) holds—the simplest way is to take

$$Y_j = \{ \text{single edge of the length } l_j \text{ defined by formula (35)} \}.$$

Acknowledgments

The authors express their gratitude to Professor Pavel Exner for fruitful discussion on the results. The work of DB is supported by the Czech Science Foundation (GACR), the project 14-02476S ‘Variations, geometry and physics’, by the project ‘Support of Research in the Moravian-Silesian Region 2013’ and by the University of Ostrava. AK is grateful for hospitality extended to him during several visits to the Department of Mathematics of University of Ostrava where a part of this work was done.

References

[1] Albeverio S, Gesztesy F, Høegh-Krohn R and Holden H 2005 *Solvable Models in Quantum Mechanics* 2nd edn (New York: Chelsea) with an appendix by P Exner
[2] Avron J E, Exner P and Last Y 1994 Periodic Schrödinger operators with large gaps and Wannier–Stark ladders *Phys. Rev. Lett.* 72 896–9
[3] Berkolaiko G and Kuchment P 2013 *Introduction to Quantum Graphs* (Providence, RI: American Mathematical Society)
[4] Cheon T and Shigezuka T 1998 Realizing discontinuous wave functions with renormalized short-range potentials *Phys. Lett. A* 243 111–6
[5] Cheon T, Exner P and Turek O 2010 Approximation of a general singular vertex coupling in quantum graphs *Ann. Phys., NY* 325 548–78
[6] Exner P 1995 Lattice Kronig–Penney models *Phys. Rev. Lett.* 74 3503–6
[7] Exner P 1996 Contact interactions on graph superlattices *J. Phys. A: Math. Gen.* 29 87–102
[8] Exner P, Kuchment P and Winn B 2010 On the location of spectral edges in $\mathbb{Z}$-periodic media *J. Phys. A: Math. Theor.* 43 474022
[9] Exner P, Neidhardt H and Zagrebnov V 2001 Potential approximations to $\delta'$: an inverse Klauder phenomenon with norm-resolvent convergence *Commun. Math. Phys.* 224 593–612
[10] Harrison J, Kuchment P, Sobolev A and Winn B 2007 On occurrence of spectral edges for periodic operators inside the Brillouin zone *J. Phys. A: Math. Gen.* 40 7597–618
[11] Kato T 1966 *Perturbation Theory for Linear Operators* (New York: Springer)
[12] Khrabustovskyi A 2012 Periodic Riemannian manifold with preassigned gaps in the spectrum of Laplace–Beltrami operator *J. Differ. Equ.* 252 2339–618
[13] Khrabustovskyi A 2013 Periodic elliptic operators with asymptotically preassigned spectrum *Asymptotic Anal.* 82 1–37
[14] Khrabustovskyi A 2014 Opening up and control of spectral gaps of the Laplacian in periodic domains *J. Math. Phys.* 55 121502
[15] Korotyaev E and Lobanov I 2007 Schrödinger operators on zigzag nanotubes *Ann. Henri Poincaré* 8 1151–76
[16] Kuchment P 2005 Quantum graphs: II. Some spectral properties of quantum and combinatorial graphs *J. Phys. A: Math. Gen.* 38 4887–900
[17] Kuchment P and Post O 2007 On the spectra of carbon nano-structures *Commun. Math. Phys.* 275 805–26
[18] Marcus M and Minc H 1964 *A Survey of Matrix Theory and Matrix Inequalities* (Boston: Allyn and Bacon)
[19] Ong B-S 2006 Spectral problems of optical waveguides and quantum graphs PhD Thesis Texas A&M University
[20] Reed M and Simon B 1972 Methods of Modern Mathematical Physics: I. Functional Analysis (New York: Academic)
[21] Schenker J H and Aizenman M 2000 The creation of spectral gaps by graph decoration Lett. Math. Phys. 53 253–62
[22] Šeba P 1986 Some remarks on the δ'-interaction in one-dimension Rep. Math. Phys. 24 111–20
[23] Simon B 1978 A canonical decomposition for quadratic forms with applications to monotone convergence theorems J. Funct. Anal. 28 377–85