

# ANALYSIS OF THE DISPERSION EQUATION FOR THE SCHRÖDINGER OPERATOR ON PERIODIC METRIC GRAPHS

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## Abstract

The spectral analysis of the Schrödinger operator on cubic lattice type graphs is developed. Similarly to the quantum mechanical tight-binding approximation, using the well known concept of the Dirichlet-to-Neumann map asymptotic formulae for localized negative spectral bands of the Schrödinger operator on a periodic metric graph are established. The results are illustrated by numerical calculations.

## 1 Introduction

The main goal of this paper is to develop the spectral analysis of the Schrödinger operator on cubic lattice type graphs [8]. Similarly to the quantum mechanical tight-binding approximation we will get asymptotic formulae for localized spectral bands of the Schrödinger operator on a periodic graph. It is known that the tight-binding method gives the natural approximation for well-localized energy bands of the solid [1]. On the other hand, the corresponding one-dimensional lattice may serve as an approximation for the solid body [11].

Our consideration consists of the following three steps. First, in Section 2 we deal with star-like connected graph  $\Gamma_\infty$  of  $N$  infinite rays and some compact part  $\Gamma_0$ . We suppose that our self-adjoint operator has a simple isolated eigenvalue  $E_0$ .

Then for an even  $N$  in Section 5 a periodical graph  $\tilde{\Gamma}_T$  (and an operator  $\tilde{\mathcal{L}}_T$  on it) will be constructed by the use of a cell-graph  $\Gamma_T$ , where  $\Gamma_T$  looks like  $\Gamma_\infty$  with finite intervals  $[0, T/2]$  instead of the rays. Due to the Floquet-Bloch theory the spectrum of the operator has a band structure in a regular case [11]. A natural parameter (quasi-momentum)  $\mathbf{p} \in \mathbf{R}^{N/2}$  appears as a result of reducing of the periodical problem on the fundamental subgraph  $\Gamma_T$ . We obtain a dispersion equation  $\Phi(E, \mathbf{p}) = 0$  from which

one may get the energy  $E = E(\mathbf{p})$  as a many-valued function of the quasi-momentum  $\mathbf{p}$ . Using the dispersion equation we will prove that in a fixed neighborhood of  $E_0$  for any rather big  $T$  there is precisely one isolated spectral band. For  $T \rightarrow +\infty$  the band shrinks to the point  $E_0$ . A similar result on the line was obtained earlier [19].

Finally an asymptotic formula for the energy band, as  $T$  goes to infinity, will be proven in Section 6. The main results are formulated using the well known concept of the Dirichlet-to-Neumann map (Sections 3 and 4). For completeness we discuss the case  $T = 0$  in the last section 7. Some numerical calculations one can find in Appendices B and C.

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## 2 Schrödinger operator on the non-periodic graph

Let us consider the one-dimensional Schrödinger operator  $\mathcal{L}$  on a star-like connected graph  $\Gamma_\infty$  constructed of a compact part  $\Gamma_0$  represented as a finite set of oriented edges and a finite number  $N$  of semi-infinite rays  $\mathbf{R}_+$ :  $0 \leq x < \infty$ , joined at nodes.<sup>1)</sup> Then any function  $u$  from the domain  $D(\mathcal{L})$  of the operator  $\mathcal{L}$

$$u \in D(\mathcal{L}) \subset L^2(\Gamma_\infty) = L^2(\Gamma_0) \oplus \bigoplus_{j=1}^N L^2(\mathbf{R}_+)$$

has the following representation  $u := \{u_j, j = 0, 1, \dots, N\}$  with  $u_0 \in W^{2,2}(\Gamma_0) \subset L^2(\Gamma_0)$  and  $u_j \in W^{2,2}(\mathbf{R}_+) \subset L^2(\mathbf{R}_+)$ ,  $j \geq 1$ . As usual, for any  $u$  and  $v$  from  $L^2(\Gamma_\infty)$  we define a scalar product by the following formula

$$\langle u, v \rangle = \langle u, v \rangle_{L^2(\Gamma_\infty)} := \langle u_0, v_0 \rangle_{L^2(\Gamma_0)} + \sum_{j=1}^N \langle u_j, v_j \rangle_{L^2(\mathbf{R}_+)}.$$

The operator  $\mathcal{L}$  acts on  $u \in D(\mathcal{L})$  as

$$\begin{aligned} \mathcal{L}u &= v, \quad v := \{v_j, j = 0, 1, \dots, N\} \in L^2(\Gamma_\infty), \\ v_0 &= l_0 u_0 := -u_0'' + q u_0, \quad \text{and} \quad v_j = -u_j'', \quad j \geq 1, \end{aligned}$$

where  $q$  is a real bounded measurable potential on  $\Gamma_0$ .

We suppose that some self-adjoint boundary conditions  $\gamma$  connect the boundary values of each wave function  $u \in D(\mathcal{L})$  at the incident edges and rays (see for instance [4, 7, 2]), i.e., at any node  $\nu \in \Gamma_\infty$  the vector of values  $\vec{\psi}_\nu$  of the wave function  $u$  and the vector of values  $\vec{\psi}'_\nu$  of its derivatives in the direction from  $\nu$  are subjected to a selfadjoint condition

$$\gamma : \quad A\vec{\psi}_\nu + B\vec{\psi}'_\nu = 0, \quad \nu \in \Gamma_\infty, \quad (1)$$

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<sup>1</sup>Some of the rays may have a common point at the origin.

where the square matrices  $A = A(\nu)$  and  $B = B(\nu)$  are such that  $AB^* = BA^*$  and  $AA^* + BB^* > 0$  (see [7], Lemma 2.2).

Note that the operator  $A - iB$  is invertible because of the equation  $(A - iB)(A^* + iB^*) = AA^* + BB^* > 0$  and one may rewrite the condition (1) in the following form

$$(I + U)\vec{\psi}_\nu + i(I - U)\vec{\psi}'_\nu = 0, \quad (2)$$

where  $I$  is the unit matrix and  $U = U(\nu) := (A - iB)^{-1}(A + iB)$  is a unitary matrix, i.e.,  $UU^* = I$ .

Thus, the operator  $\mathcal{L} = \mathcal{L}(\gamma)$  is selfadjoint, i.e.,  $\mathcal{L} = \mathcal{L}^*$ ,

$$\langle \mathcal{L}u, v \rangle = \langle u, \mathcal{L}v \rangle, \quad \text{with } \{u, v\} \subset D(\mathcal{L}), \quad (3)$$

and its continuous spectrum fills the positive half-axis (cf. [2], Theorem 2.4). Moreover, it follows from Krein's resolvent formula that the spectrum  $\sigma(\mathcal{L})$  of the operator  $\mathcal{L}$  contains at most a finite number of negative eigenvalues of a finite multiplicity. Therefore, the operator  $\mathcal{L}$  is bounded from below.

## 2.1 Example

Consider a "ring"  $0 \leq x \leq 4$  with the periodical boundary conditions  $u_0(0) = u_0(4)$  and  $u'_0(+0) = u'_0(4 - 0)$ . We assume that four semi-infinite rays  $[0, +\infty)$  are attached to the ring at vertices  $\{1, 2, 3, 4\} \subset [0, 4]$  with the same selfadjoint boundary condition at each node on wave functions (cf. [2]): for a given  $\beta \in \mathbf{C}$

$$\begin{cases} u_0(j - 0) = u_0(j + 0) = u_0(j), \\ u_j(0) = \beta u_0(j), \\ u'_0(j + 0) - u'_0(j - 0) + \bar{\beta}u'_j(+0) = 0, \end{cases} \quad (4)$$

with  $1 \leq j \leq 4$  and  $4 + 0 = +0$  convention. So,  $\Gamma_0 = \cup_{0 \leq j \leq 3} [j, j + 1]$ . If we represent the conditions (4) in the form (1)

$$\begin{pmatrix} 1 & -1 & 0 \\ 0 & \beta & -1 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} u_0(j - 0) \\ u_0(j + 0) \\ u_j(0) \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 1 & 1 & \bar{\beta} \end{pmatrix} \begin{pmatrix} -u'_0(j - 0) \\ u'_0(j + 0) \\ u'_j(0) \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \quad (5)$$

then the matrix  $AB^* = 0$  is hermitian and  $\text{rank}(A, B) = 3$  for any  $\beta \in \overline{\mathbf{C}}$ . The latter is equivalent to the condition  $AA^* + BB^* > 0$ . In this case the representation (2) is much more complicated than (5), because

$$U := \frac{-1}{2 + |\beta|^2} \begin{pmatrix} -|\beta|^2 & 2 & 2\bar{\beta} \\ 2 & -|\beta|^2 & 2\bar{\beta} \\ 2\beta & 2\beta & |\beta|^2 - 2 \end{pmatrix}. \quad (6)$$

Thus, the operator  $\mathcal{L} = \mathcal{L}(\beta)$  is a selfadjoint operator and due to selfadjointness of the matrix  $U$  in (6) we have

$$\langle \mathcal{L}(\beta)u, u \rangle \geq \int_{\Gamma_0} q|u_0|^2 dx, \quad u \in D(\mathcal{L}(\beta)). \quad (7)$$

Choosing  $\beta = 1$  we receive "zero-current" condition, but choosing  $\beta = 0$  or  $\beta = \infty$  we get that the ring is decoupled from the rays. That is the operator  $\mathcal{L}(0)$  is the orthogonal sum of four identical selfadjoint operators  $-d^2/dx^2$  on the rays with Dirichlet boundary conditions  $u_j(0) = 0$ ,  $j = 1, 2, 3, 4$ , and of the selfadjoint operator  $-d^2/dx^2 + q(x)$  with periodical boundary conditions on the ring  $[0, 4]$ ,  $0 = 4$ .

In the case  $\beta = \infty$  the operator  $\mathcal{L}(\infty)$  is the orthogonal sum of four identical selfadjoint operators  $-d^2/dx^2$  on the rays with Neumann boundary conditions  $u'_j(0) = 0$ ,  $j = 1, 2, 3, 4$ , and of four selfadjoint operators  $-d^2/dx^2 + q(j+x)$ ,  $j = 0, 1, 2, 3$ , on the interval  $x \in [0, 1]$  with Dirichlet boundary conditions  $f(0) = f(1) = 0$ .

For the sake of simplicity we set  $q(x) = -a^2$ ,  $0 < a = \text{const}$ , so that for any finite complex number  $\beta$  and any positive number  $a$  the operator  $\mathcal{L} = \mathcal{L}(\beta; a)$  has a negative eigenvalue (see below). For instance, the number  $-a^2$  is the eigenvalue of the operator  $\mathcal{L}(0; a)$  with the eigenfunction  $u = \{u_0 \equiv 1, u_j \equiv 0, j \geq 1\} \in L^2(\Gamma_\infty)$ .

### 3 Restrictions on the ring

In this section we will consider restrictions  $\mathcal{L}_0$  and  $\mathcal{L}_1$  of the operator  $\mathcal{L}$  on sets

$$D_0 = D(\mathcal{L}_0) := \{u \in D(\mathcal{L}) : u_j(0) = 0, j = 1, 2, \dots, N\}$$

and

$$D_1 = D(\mathcal{L}_1) := \{u \in D(\mathcal{L}) : u'_j(0) = 0, j = 1, 2, \dots, N\}.$$

We are going to prove that a part  $l_{\mathcal{D}}$  (or  $l_{\mathcal{N}}$ ) of the operator  $\mathcal{L}_0$  (or  $\mathcal{L}_1$ ) on the ring  $\Gamma_0$ ,  $\Gamma_0 \neq \emptyset$ , will be a selfadjoint operator in  $L^2(\Gamma_0)$  with the domain

$$D(l_{\mathcal{D}/\mathcal{N}}) := \{f \in W^{2,2}(\Gamma_0) : \text{there is } F \in D_{0/1} \text{ with } F_0 = f\}.$$

First, note that for any  $u$  and  $v$  from  $D(\mathcal{L})$  by partial integration we obtain

$$\begin{aligned} \langle \mathcal{L}u, v \rangle &= \langle l_0 u_0, v_0 \rangle_{L^2(\Gamma_0)} + \sum_{j=1}^N \int_0^\infty (-u''_j) \overline{v_j} dx \\ &= \langle l_0 u_0, v_0 \rangle_{L^2(\Gamma_0)} + \sum_{j=1}^N \left( u'_j(+0) \overline{v_j(0)} + \int_0^\infty u'_j \overline{v'_j} dx \right). \end{aligned}$$

On the other hand

$$\langle u, \mathcal{L}v \rangle = \langle u_0, l_0 v_0 \rangle_{L^2(\Gamma_0)} + \sum_{j=1}^N \int_0^\infty u_j (-\overline{v''_j}) dx$$

$$= \langle u_0, l_0 v_0 \rangle_{L^2(\Gamma_0)} + \sum_{j=1}^N \left( u_j(0) \overline{v'_j(+0)} + \int_0^\infty u'_j \overline{v'_j} dx \right).$$

So, by (3) we get

$$\langle l_0 u_0, v_0 \rangle_{L^2(\Gamma_0)} - \langle u_0, l_0 v_0 \rangle_{L^2(\Gamma_0)} = \sum_{j=1}^N (u_j(0) \overline{v'_j(+0)} - u'_j(+0) \overline{v_j(0)}), \quad \{u, v\} \subset D(\mathcal{L}). \quad (8)$$

Now, we note that if the conditions  $\gamma$  such that for any  $u$  and  $v$  from the domain of the operator  $\mathcal{L}$

$$\sum_{j=1}^N (u_j(0) \overline{v'_j(+0)} - u'_j(+0) \overline{v_j(0)}) = 0,$$

then the operator  $\mathcal{L}$  is an orthogonal sum of an internal selfadjoint part (on the ring  $\Gamma_0$ ) and some external selfadjoint one (on the union of the rays). Thus, in the case restrictions of the domain of the external operator do not change the domain of the internal selfadjoint part of the operator  $\mathcal{L}$ . So, without loss of generality we may assume that for any  $j \geq 1$  there are such  $u$  and  $v$  from  $D(\mathcal{L})$  that  $u_j(0) = 1$  and  $v'_j(+0) = 1$ .

By (8) we have that  $l_{\mathcal{D}}$  and  $l_{\mathcal{N}}$  are symmetric operators. To describe the domain  $D(l_{\mathcal{D}}^*)$  (or  $D(l_{\mathcal{N}}^*)$ ) of the adjoint operator  $l_{\mathcal{D}}^*$  ( $l_{\mathcal{N}}^*$ ) we need to find such functions  $g \in L^2(\Gamma_0)$  that the functional:  $f \rightarrow \langle l_0 f, g \rangle_{L^2(\Gamma_0)}$  is bounded on the set  $D(l_{\mathcal{D}})$  (or  $D(l_{\mathcal{N}})$ ). It is clear that  $g \in W^{2,2}(\Gamma_0)$  and that any function  $g$  inherits the conditions  $\gamma$  in the sense that there is an extension  $G \in D(\mathcal{L})$  with  $G_0 = g$  (see Appendix A for details). So, the domain  $D(l_{\mathcal{D}}^*)$  is a subset of the restriction of the set  $D(\mathcal{L})$  on the graph  $\Gamma_0$ .

Now, one may use the equation (8) to check the selfadjointness of the operators  $l_{\mathcal{D}}$  and  $l_{\mathcal{N}}$ . Let  $f, g \in D(l_{\mathcal{D}}^*)$  (or  $f, g \in D(l_{\mathcal{N}}^*)$ ), then

$$\langle l_{\mathcal{D}/\mathcal{N}}^* f, g \rangle_{L^2(\Gamma_0)} - \langle f, l_{\mathcal{D}/\mathcal{N}}^* g \rangle_{L^2(\Gamma_0)} = \sum_{j=1}^N (F_j(0) \overline{G'_j(+0)} - F'_j(+0) \overline{G_j(0)}),$$

where  $F, G \in D(\mathcal{L})$ ,  $F_0 = f$ , and  $G_0 = g$ . If in addition  $f \in D(l_{\mathcal{D}})$  (or  $f \in D(l_{\mathcal{N}})$ ) then we have

$$0 = \langle l_{\mathcal{D}} f, g \rangle_{L^2(\Gamma_0)} - \langle f, l_{\mathcal{D}}^* g \rangle_{L^2(\Gamma_0)} = - \sum_{j=1}^N F'_j(+0) \overline{G_j(0)}$$

(or  $\sum_{j=1}^N F_j(0) \overline{G'_j(+0)} = 0$ ). It is immediate from this identity that if the boundary conditions  $\gamma$  does not contain a condition which looks like  $u'_s(+0) = 0$  (or  $u_s(0) = 0$ ) for some index  $s$ ,  $1 \leq s \leq N$ , then for each  $g \in D(l_{\mathcal{D}}^*)$  ( $g \in D(l_{\mathcal{N}}^*)$ ) and any  $G \in D(\mathcal{L})$  with  $G_0 = g$  we have  $G_j(0) = 0$  (or  $G'_j(+0) = 0$ ) for every  $j$ ,  $1 \leq j \leq N$ . So,  $l_{\mathcal{D}} = l_{\mathcal{D}}^*$  and  $l_{\mathcal{N}} = l_{\mathcal{N}}^*$ .

### 3.1 Example

The cases  $\beta = 0, \infty$  have been considered in Section 2.1. Let  $\beta$  be a finite complex number,  $\beta \neq 0$ . According to the conditions (4) the additional condition  $u_j(0) = 0$  implies  $u_0(j) = 0$ . Therefore, the domain  $D(l_{\mathcal{D}})$  of the operator  $l_{\mathcal{D}} = l_{\mathcal{D}}(\beta)$  is a set of such functions  $f(x)$  on the interval  $[0, 4]$  that  $f(j) = 0, j = 0, 1, 2, 3, 4$ , and  $f(j+x) \in W^{2,2}([0, 1]), j = 0, 1, 2, 3, x \in [0, 1]$ . On the other hand if  $u'_j(+0) = 0$  then  $u'_0(j+0) = u'_0(j-0)$ . Thus, for the domain of the operator  $l_{\mathcal{N}} = l_{\mathcal{N}}(\beta)$  we have

$$D(l_{\mathcal{N}}) = \{f \in W^{2,2}([0, 4]), f(0) = f(4), f'(+0) = f'(4-0)\}. \quad (9)$$

Finally, we note that the operator  $l_{\mathcal{D}}$  is an orthogonal sum of four selfadjoint operators with Dirichlet boundary conditions, similar to the case  $\beta = \infty$ , and the operator  $l_{\mathcal{N}}$  is a selfadjoint operator with periodical boundary conditions, as in the case  $\beta = 0$ .

## 4 Dirichlet-to-Neumann map

Instead of explicit describing the compact part  $\Gamma_0 \subset \Gamma_\infty$  and the boundary conditions  $\gamma$  it is convenient to use an analytic matrix-valued function  $\Lambda(z), z \in \mathbf{C}$ , known as *Dirichlet-to-Neumann map* (see [21, 20]).

We suppose that for given graph  $\Gamma_\infty$  and boundary conditions  $\gamma$  and for a fixed complex number  $z$  the condition  $l_0 u_0 = z u_0$  implies  $u_0 \equiv 0$  for any  $u \in D(\mathcal{L})$  with  $u_j(0) = 0, j = 1, 2, \dots, N$ . Then for any  $u = \{u_j, j \geq 0\} \in D(\mathcal{L})$  with  $l_0 u_0 = z u_0$  we may define a linear transformation  $\Lambda(z): \mathbf{C}^N \rightarrow \mathbf{C}^N$  such that

$$\vec{u}' = \Lambda(z)\vec{u}, \quad (10)$$

where

$$\vec{u} := \begin{pmatrix} u_1(0) \\ u_2(0) \\ \vdots \\ u_N(0) \end{pmatrix} \quad \text{and} \quad \vec{u}' := \begin{pmatrix} u'_1(+0) \\ u'_2(+0) \\ \vdots \\ u'_N(+0) \end{pmatrix}.$$

It is natural to call the inverse transformation  $\Lambda^{-1}(z)$  as *Neumann-to-Dirichlet map*.

The matrix-valued function  $\Lambda(z)$  contains all information we need about the compact graph  $\Gamma_0$ , the boundary conditions, and the operator  $l_0$  on  $L^2(\Gamma_0)$ .

It is clear that  $\Lambda(z)$  is an analytic function on  $\mathbf{C} \setminus \mathbf{R}_+$  with a discrete set of singularities on the negative part of the real axis. For instance, in the case  $\Gamma_0 = \emptyset$  selfadjoint boundary conditions of the form (2) leads to the representation

$$\Lambda = i(I - U)^{-1}(I + U), \quad \det(I - U) \neq 0, \quad (11)$$

and  $\Lambda$  does not depend on  $z$ .

Now, let  $u \in D(\mathcal{L})$  with  $l_0 u_0 = z u_0$ ,  $\Gamma_0 \neq \emptyset$ . Then by (8) for any  $z \in \mathbf{C}$  we get

$$\begin{aligned} 2i\Im z \|u_0\|_{L^2(\Gamma_0)}^2 &= \langle l_0 u_0, u_0 \rangle_{L^2(\Gamma_0)} - \langle u_0, l_0 u_0 \rangle_{L^2(\Gamma_0)} = \sum_{j=1}^N (u_j(0) \overline{u'_j(+0)} - u'_j(+0) \overline{u_j(0)}) \\ &= \langle \vec{u}, \vec{u}' \rangle_{\mathbf{C}^N} - \langle \vec{u}', \vec{u} \rangle_{\mathbf{C}^N} = \langle \vec{u}, \Lambda(z) \vec{u} \rangle_{\mathbf{C}^N} - \langle \Lambda(z) \vec{u}, \vec{u} \rangle_{\mathbf{C}^N} = -2i\Im \langle \Lambda(z) \vec{u}, \vec{u} \rangle_{\mathbf{C}^N}. \end{aligned}$$

Hence, for any  $u \in D(\mathcal{L})$  with  $l_0 u_0 = z u_0$  we have

$$\Im \langle \Lambda \vec{u}, \vec{u} \rangle_{\mathbf{C}^N} = -\Im z \|u_0\|_{L^2(\Gamma_0)}^2. \quad (12)$$

It means that the matrix  $\Lambda(z) \not\equiv \text{const}$ ,  $\Lambda(z)$  is invertible if  $\Im z \neq 0$ , and  $\Lambda(\xi)$  is a hermitian matrix on the real axis,  $\xi \in \mathbf{R}$ . If  $\xi$  is such a real number that  $\Lambda(\xi)$  exists then  $\Lambda(\xi + z)$  is a regular function on some disk  $|z| < r$  with  $r > 0$  and by (12) we get  $0 > \Im \Lambda(\xi + iy) = \Lambda'(\xi)y + o(y)$  as  $y \rightarrow +0$ . Thus,

$$\Lambda'(\xi) \leq 0. \quad (13)$$

For a given  $\xi \in \mathbf{R}$  the transformation  $\Lambda(\xi)$  exists iff  $\xi$  is not a point of the spectrum  $\sigma(l_{\mathcal{D}})$  of the selfadjoint operator  $l_{\mathcal{D}}$  in  $L^2(\Gamma_0)$  which has been considered above. On the other hand  $\Lambda^{-1}(\xi)$  exists iff  $\xi$  does not belong to the spectrum  $\sigma(l_{\mathcal{N}})$  of the selfadjoint operator  $l_{\mathcal{N}}$ . Moreover, these matrices are analytic functions on the set  $\mathbf{C} \setminus (\sigma(l_{\mathcal{D}}) \cup \sigma(l_{\mathcal{N}}))$  and the set  $\sigma(l_{\mathcal{D}}) \cap \sigma(l_{\mathcal{N}})$  is a set of their common singularities. One might expect that for some number  $\xi \in \sigma(l_{\mathcal{D}}) \cap \sigma(l_{\mathcal{N}})$  the corresponding proper subspaces of the operators  $l_{\mathcal{D}}$  and  $l_{\mathcal{N}}$  have a nontrivial common element (see Section 4.2 below). It means that for such  $\xi$  there is a localized eigenfunction of the operator  $\mathcal{L}$  with a support on  $\Gamma_0$ . Thus, let us introduce the following notation

$$\sigma_0 = \sigma_0(\mathcal{L}) := \{\xi \in \sigma(l_{\mathcal{D}}) \cap \sigma(l_{\mathcal{N}}) : \text{the corresponding proper subspaces of the operators } l_{\mathcal{D}} \text{ and } l_{\mathcal{N}} \text{ have a nontrivial common element}\}. \quad (14)$$

It is clear that the set  $\sigma_0$  may be empty. For instance, let us consider the operator  $\mathcal{L}$  on the graph  $\Gamma := (-\infty, 0] \cup [0, 1] \cup [1, +\infty)$  with  $q \equiv 0$  and smooth boundary conditions, i.e.,  $u(-0) = u(+0)$ ,  $u(1-0) = u(1+0)$ ,  $u'(-0) = u'(0)$ , and  $u'(1-0) = u'(1+0)$ . Then  $\sigma(l_{\mathcal{N}}) = \{\pi^2 n^2 : n = 0, 1, 2, \dots\}$  with eigenfunctions  $\cos \pi n x$  and  $\sigma(l_{\mathcal{D}}) = \sigma(l_{\mathcal{N}}) \setminus \{0\}$  with eigenfunctions  $\sin \pi n x$ .

## 4.1 Discrete spectrum

We now look at negative eigenvalues of the operator  $\mathcal{L}$ . Let us denote by  $I_N$  the unit matrix on  $\mathbf{C}^N$ . The following result follows from the definitions given above (cf. [2, 18]).

**Theorem 1.** *Let  $\sigma_0(\mathcal{L})$  be as in (14) and let  $E_0$  be a negative number such that  $E_0 \notin \sigma(l_{\mathcal{D}}) \cap \sigma(l_{\mathcal{N}}) \setminus \sigma_0(\mathcal{L})$ . Then  $E_0$  is an eigenvalue of the operator  $\mathcal{L}$  if and only if at least one of the following assertions holds:*

- $E_0 \in \sigma_0(\mathcal{L})$ ,

- $E_0 \notin \sigma(l_{\mathcal{D}})$  and  $\det(\sqrt{|E_0|}I_N + \Lambda(E_0)) = 0$ ,
- $E_0 \notin \sigma(l_{\mathcal{N}})$  and  $\det(I_N + \sqrt{|E_0|}\Lambda^{-1}(E_0)) = 0$ .

The multiplicity of the eigenvalue  $E_0$  of the operator  $\mathcal{L}$ ,  $E_0 \notin \sigma(l_{\mathcal{D}}) \cap \sigma(l_{\mathcal{N}})$ , coincides with the multiplicity of the eigenvalue  $-\sqrt{|E_0|}$  of the matrix  $\Lambda(E_0)$  (or  $-1/\sqrt{|E_0|}$  of the matrix  $\Lambda^{-1}(E_0)$ ).

*Proof.* First, let  $E_0$  be a negative eigenvalue of the operator  $\mathcal{L}$  with an eigenfunction  $F$ . It means that there is such a vector  $\vec{c} \in \mathbf{C}^N$  that

$$F_j(x) = c_j e^{-x\sqrt{|E_0|}}, \quad F'_j(x) = -\sqrt{|E_0|}c_j e^{-x\sqrt{|E_0|}}, \quad \vec{F} = \vec{c}, \quad \text{and} \quad \vec{F}' = -\sqrt{|E_0|}\vec{c}.$$

If  $\vec{c} = 0$  then  $F_0 \not\equiv 0$ ,  $l_0 F_0 = E_0 F_0$ , and  $F_j \equiv 0$ ,  $j \geq 1$ . Thus,  $E_0 \in \sigma_0$ . If  $\vec{c} \neq 0$  and  $E_0 \notin \sigma(l_{\mathcal{D}})$  (or  $E_0 \notin \sigma(l_{\mathcal{N}})$ ) then  $\vec{F}' = \Lambda(E_0)\vec{F}$  (or  $\Lambda^{-1}(E_0)\vec{F}' = \vec{F}$ ). Therefore the homogeneous equation

$$(\sqrt{|E_0|}I_N + \Lambda(E_0))\vec{x} = 0 \quad (\text{or} \quad (I_N + \sqrt{|E_0|}\Lambda^{-1}(E_0))\vec{x} = 0), \quad \vec{x} \in \mathbf{C}^N, \quad (15)$$

has a non-trivial solution  $\vec{x} = \vec{c}$ .

Conversely, if  $E_0 \in \sigma_0$  then there is such a function  $F \in D(\mathcal{L})$  that  $F_0 \not\equiv 0$ ,  $l_0 F_0 = E_0 F_0$ , and  $F_j \equiv 0$ ,  $j \geq 1$ . Hence,  $\mathcal{L}F = E_0 F$  and  $E_0$  is an eigenvalue of the operator  $\mathcal{L}$  with the eigenfunction  $F$ .

Now, let  $E_0 \notin \sigma(l_{\mathcal{D}})$  and let  $\vec{c} \in \mathbf{C}^N$  be a solution of the corresponding homogeneous equation (15). Matching numbers of numerical unknowns and linear homogeneous equations shows that the following boundary value problem:

$$\begin{cases} \text{find a solution } f \in W^{2,2}(\Gamma_0) \text{ of the equation } l_0 f = E_0 f \text{ such that} \\ \text{there is } F \in D(\mathcal{L}) \text{ with } F_0 = f \text{ and } \vec{F} = \vec{c} \end{cases} \quad (16)$$

has a solution for any  $\vec{c} \in \mathbf{C}^N$  because the solution should be unique since  $E_0$  does not belong to the spectrum of the operator  $l_{\mathcal{D}}$ . Finally, the function  $F$  will be an eigenfunction of the operator  $\mathcal{L}$  if we choose  $F_j(x) = c_j \exp(-x\sqrt{|E_0|})$ ,  $j \geq 1$ .

To compare the multiplicities we note that a finite set of functions  $\{F^{(\alpha)}\} \subset D(\mathcal{L})$  is linearly independent iff the corresponding vectors  $\vec{F}^{(\alpha)} \in \mathbf{C}^N$  are linearly independent.

The arguments just used may be applied also when  $E_0 \notin \sigma(l_{\mathcal{N}})$ . This concludes the proof of the theorem.  $\square$

It has been mentioned above that in such a case the operator  $\mathcal{L}$  has a finite number of negative eigenvalues of finite multiplicity. Further we will deal with one fixed negative eigenvalue  $E_0 \notin \sigma_0$ . We assume that  $E_0$  is a simple eigenvalue with an eigenfunction  $F \in D(\mathcal{L})$ .

**Remark 1.** We notice that the graph  $\Gamma_0$  can be replaced by a bounded domain  $\Omega$  in  $\mathbf{R}^3$  [13], in  $\mathbf{R}^2$  [10], or  $\Gamma_0 = \emptyset$  (see [7, 11, 12]). Then the operator extension scheme is used to attach a finite number of semi-infinite rays at contact points of the boundary  $\partial\Omega$ . Finally, we define the matrix  $\Lambda(z)$  in a similar way and Theorem 1 gives us description of the negative part of the spectrum of the corresponding operator. Moreover, Theorem 1 is valid in a non-selfadjoint case with  $E_0 \in \mathbf{C} \setminus [0, \infty)$  (cf. [12]).

## 4.2 Example

It is clear that for each  $z$  the matrices  $\Lambda(z) = \Lambda(z; \beta, a)$  and  $\Lambda^{-1}(z) = \Lambda^{-1}(z; \beta, a)$  are meaningless if  $\beta = 0$  or  $\beta = \infty$  (see Section 2.1). On the other hand if  $\beta \neq 0$ ,  $l_0 u_0 = \xi u_0$ , and  $u_j(0) = 0$  for any  $j$  then  $u_0(j) = 0$  and  $u_0 \equiv 0$  if  $\xi$  is not an eigenvalue of the Sturm-Liouville problem:  $-y'' - a^2 y = zy$ ,  $y(0) = y(1) = 0$ . Thus  $\Lambda(z)$  exists iff  $\beta \neq 0$  and  $z \notin \sigma(l_{\mathcal{D}}) = \{(\pi n)^2 - a^2, n = 1, 2, \dots\}$ . In the same way we get that in the case  $\beta \neq 0$  the transformation  $\Lambda^{-1}(z)$  exists iff  $z \notin \sigma(l_{\mathcal{N}}) = \{(\pi n/2)^2 - a^2, n = 0, 1, 2, \dots\}$ , where  $\sigma(l_{\mathcal{N}})$  is the spectrum of the following periodic problem on the ring:  $-y'' - a^2 y = zy$ ,  $y(0) = y(4)$  and  $y'(0) = y'(4)$ . Note that  $\sigma(l_{\mathcal{D}}) \subset \sigma(l_{\mathcal{N}})$ . Moreover, for any natural number  $n \geq 1$  the function  $u_0(x) = \sin \pi n x$  on the interval  $[0, 4]$  is a common eigenfunction of both operators  $l_{\mathcal{D}}$  and  $l_{\mathcal{N}}$ . Hence

$$\sigma_0 = \sigma_0(\mathcal{L}(\beta; a)) = \sigma(l_{\mathcal{D}}) = \sigma(l_{\mathcal{D}}) \cap \sigma(l_{\mathcal{N}}) = \{(\pi n)^2 - a^2 : n = 1, 2, \dots\}. \quad (17)$$

It is not difficult to check (see Appendix B for details) that

$$\Lambda^{-1}(z) = |\beta|^2 g(z) \quad (18)$$

with the matrix

$$g(z) := \{G(j, s; z)\}_{j,s=1}^4,$$

where

$$G(x, t; z) := -\frac{\cos \sqrt{a^2 + z}(2 - |x - t|)}{2\sqrt{a^2 + z} \sin 2\sqrt{a^2 + z}} \quad (19)$$

is the Green function of the operator  $l_{\mathcal{N}}$  with periodical conditions (see (9)) on the ring.

We now look at negative eigenvalues of the operator  $\mathcal{L}(\beta; a)$ , which, according to the estimation (7), lie in the interval  $[-a^2, 0)$ . By Theorem 1 any negative number from  $\sigma_0$  belongs to the spectrum of the operator  $\mathcal{L} = \mathcal{L}(\beta; a)$ . On the other hand a negative number  $E_0 \neq (\pi n/2)^2 - a^2, n = 1, 2, \dots$ , is an eigenvalue of the operator  $\mathcal{L}$  iff the number 1 is an eigenvalue of the matrix

$$\frac{\sqrt{|E_0|} |\beta|^2}{k \sin 2k} A(k)$$

where  $k := \sqrt{a^2 + E_0} \in (0, a)$  and

$$A(k) := \frac{1}{2} \begin{pmatrix} \cos 2k & \cos k & 1 & \cos k \\ \cos k & \cos 2k & \cos k & 1 \\ 1 & \cos k & \cos 2k & \cos k \\ \cos k & 1 & \cos k & \cos 2k \end{pmatrix}.$$

The eigenvalues  $\mu(k)$  of the matrix  $A(k)$  are  $\mu_{\pm} := \cos k(\cos k \pm 1)$ ,  $\mu_0 := -\sin^2 k$ . We note that  $\mu_+ \neq \mu_-$  and  $\mu_{\pm}$  are simple, but the multiplicity of  $\mu_0$  is equal to 2.

Finally, we will consider only the lowest eigenvalue  $E_0 = E_0(\beta; a) < 0$  of the operator  $\mathcal{L}(\beta; a)$  which corresponds to  $E_0(0; a) = -a^2$ . This eigenvalue exists for any  $a > 0$

and  $\beta \in \mathbf{C}$  and it is a solution of the following transcendental equation in the interval  $\xi \in (-a^2, 0)$ :

$$\frac{|\beta|^2 \sqrt{-\xi}}{\sqrt{a^2 + \xi} \sin 2\sqrt{a^2 + \xi}} \mu_+(\sqrt{a^2 + \xi}) = 1,$$

or

$$\tan \frac{\sqrt{a^2 + \xi}}{2} = \frac{|\beta|^2 \sqrt{-\xi}}{2\sqrt{a^2 + \xi}}. \quad (20)$$

It is clear that  $E_0(\beta; a) = (-a^2 + |\beta|^2 a)(1 + o(1))$ , as  $\beta \rightarrow 0$ . The corresponding solution of the equation (15), that is  $x_j = 1$ ,  $1 \leq j \leq 4$ , generates an eigenfunction  $F \in D(\mathcal{L})$ , i.e.,  $\mathcal{L}F = E_0 F$ , so that  $F_j(0) = x_j = 1$ ,  $j \geq 1$ , or just  $\vec{F} = \vec{x} = (1, 1, 1, 1)^t$ .

## 5 Dispersion equation for the Schrödinger operator on the periodic graph

Here we want to consider the Schrödinger operator  $\tilde{\mathcal{L}}_T$  on a periodic graph  $\tilde{\Gamma}_T$  constructed by using a cell-graph  $\Gamma_T$  where the latter looks like  $\Gamma_\infty$  with finite intervals  $[0, T/2]$  instead of the rays  $[0, +\infty)$  and with an even number of the rays, i.e., we have  $2N$  instead of  $N$ .

We assume a "cubic" placement of the cells in  $\mathbf{R}^N$  with smooth connection of the intervals  $[0, T/2]$  at common points  $T/2$ . It means that the problem is reduced to the spectral analysis of the family of operators on the fundamental subgraph  $\Gamma_T$  with the same selfadjoint conditions  $\gamma$  and quasiperiodical conditions at the boundary vertices, which correspond to the point  $T/2$  on each interval  $[0, T/2]$ . Due to the Floquet-Bloch theory the spectrum of the operator  $\tilde{\mathcal{L}}_T$  has a band structure in a regular case (see [11] for details).

Let  $\mathbf{p} = (p_1, p_2, \dots, p_N)$  be a vector from the cube  $[0, 2\pi)^N \subset \mathbf{R}^N$  and let  $D_T$  be a restriction of the space  $D(\mathcal{L})$  on the graph  $\Gamma_T$ ,  $T > 0$ . We will consider the family of operators  $\mathcal{L}_{\mathbf{p}, T}$  with domains  $D(\mathcal{L}_{\mathbf{p}, T}) \subset D_T$  and the following additional quasiperiodical conditions:

$$u_{2s}(T/2) = e^{ip_s} u_{2s-1}(T/2), \quad u'_{2s}(T/2 - 0) = -e^{ip_s} u'_{2s-1}(T/2 - 0), \quad s = 1, 2, \dots, N. \quad (21)$$

with a fixed quasi-momentum  $\mathbf{p} \in [0, 2\pi)^N$ . Then the spectrum  $\sigma(\tilde{\mathcal{L}}_T)$  of the operator  $\tilde{\mathcal{L}}_T$  has this following representation

$$\sigma(\tilde{\mathcal{L}}_T) = \bigcup_{\mathbf{p} \in [0, 2\pi)^N} \sigma(\mathcal{L}_{\mathbf{p}, T}), \quad (22)$$

where  $\sigma(\mathcal{L}_{\mathbf{p}, T})$  is the spectrum of the operator  $\mathcal{L}_{\mathbf{p}, T}$ . Usually the description of the band spectrum of a periodic operator is based on the analysis of the dispersion equation which allows us to express the energy as a multi-valued function of the quasi-momentum  $\mathbf{p}$  on the cube  $[0, 2\pi)^N$ . The second and third statements of Theorem 2(i), see below, give us the desired dispersion equations.

To the graph  $\Gamma_T \setminus \Gamma_0$  constructed of  $2N$  intervals  $[0, T/2]$  connected in pairs by conditions (21) there corresponds a Dirichlet-to-Neumann map  $\Lambda_{\mathbf{p},T} = \Lambda_{\mathbf{p},T}(z)$ , satisfying  $-\vec{u}' = \Lambda_{\mathbf{p},T}\vec{u}$  (cf. (10)), for any  $u_j \in W^{2,2}([0, T/2])$  with  $-u_j'' = zu_j$ ,  $1 \leq j \leq 2N$ . Clearly, the  $2N \times 2N$  matrix  $\Lambda_{\mathbf{p},T}$  has diagonal structure with  $2 \times 2$  blocks  $\lambda_{p_s,T}$ ,  $1 \leq s \leq N$ , on the principal diagonal. Note that  $\lambda_{p,T} = m^{-1}\lambda_{0,T}m$  where  $m = m(p) := \text{diag}[e^{ip}, 1]$ ,  $p \in \mathbf{R}$ . Then one can calculate the matrix  $\lambda_{0,T}$  using the general solution of the equation  $f'' + zf = 0$  on the interval  $[0, T]$ . Finally, for a given  $p \in [0, 2\pi)$  and  $z \in \mathbf{C}$  with  $\Im\sqrt{z} \geq 0$ , we get

$$\lambda_{p,T}(z) = \frac{\sqrt{z}}{\sin \sqrt{z}T} \begin{pmatrix} \cos \sqrt{z}T & -e^{-ip} \\ -e^{ip} & \cos \sqrt{z}T \end{pmatrix}$$

and

$$\Lambda_{\mathbf{p},T}(z) = \sum_{s=1}^N \lambda_{p_s,T}(z)P_s, \quad (23)$$

where  $P_s$  is the corresponding orthogonal projections in  $\mathbf{C}^{2N}$  onto two-dimension subspaces. We remark that  $\lambda_{p,T}(z)$  and  $\lambda_{p,T}^{-1}(z)$  are meromorphic matrix-valued functions on  $\mathbf{C}$  with the set

$$\sigma_{0,T} := \{(\pi n/T)^2 : n = 1, 2, \dots\} \quad (24)$$

of all of common singularities. At the same time  $\det \lambda_{p,T}(z) \equiv -z$  is a regular function on  $\mathbf{C}$ .

Choosing  $z = z_n := (\pi n/T)^2 \in \sigma_{0,T} \setminus (\sigma(l_{\mathcal{D}}) \cap \sigma(l_{\mathcal{N}}))$ , we see that  $z_n$  is the eigenvalue of the operator  $\mathcal{L}_{\mathbf{p},T}$ , i.e.,  $\mathcal{L}_{\mathbf{p},T}u = z_n u$  and  $0 \neq u \in D(\mathcal{L}_{\mathbf{p},T})$ , iff  $\Lambda(z_n)\vec{u} = \vec{u}'$  or  $\Lambda^{-1}(z_n)\vec{u}' = \vec{u}$ . In this case we have the following representation of the eigenfunction  $u$  on the intervals  $(x \in [0, T/2])$

$$\begin{aligned} u_{2s-1}(x) &= a_s \cos \frac{\pi n}{T}x + b_s \sin \frac{\pi n}{T}x, \\ u_{2s}(x) &= (-1)^n e^{ip_s} (a_s \cos \frac{\pi n}{T}x - b_s \sin \frac{\pi n}{T}x), \quad s = 1, 2, \dots, N. \end{aligned}$$

It means that

$$\begin{pmatrix} u_{2s-1}(0) \\ u_{2s}(0) \end{pmatrix} = a_s \begin{pmatrix} 1 \\ (-1)^n e^{ip_s} \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} u'_{2s-1}(+0) \\ u'_{2s}(+0) \end{pmatrix} = b'_s \begin{pmatrix} 1 \\ (-1)^{n+1} e^{ip_s} \end{pmatrix}$$

with  $b'_s := (\pi n b_s)/T$ . Now we note that  $\mathbf{C}^{2N} = H_+ \oplus H_-$  where  $H_{\pm} := \text{span}\{\mathbf{e}_s^{\pm}, s = 1, 2, \dots, N\}$  and the vectors  $\mathbf{e}_s^{\pm} := \{(\mathbf{e}_s^{\pm})_k\}_{k=1}^{2N}$  are defined to mean

$$(\mathbf{e}_s^{\pm})_k = 0, \text{ if } k \notin \{2s-1, 2s\}, \quad (\mathbf{e}_s^{\pm})_{2s-1} = 1, \quad \text{and} \quad (\mathbf{e}_s^{\pm})_{2s} = \pm e^{ip_s}. \quad (25)$$

Thus, if  $u$  is an eigenfunction of the operator  $\mathcal{L}_{\mathbf{p},T}$  with the eigenvalue  $z_n$  then  $\vec{u} \in H_{(-1)^n}$  and  $\vec{u}' \in H_{(-1)^{n+1}}$ . Hence, we have proved the second part of this following

**Theorem 2.** *Assume  $\mathbf{p} \in [0, 2\pi)^N$  and  $T > 0$ . Let  $\sigma_0(\mathcal{L})$  and  $\sigma_{0,T}$  be as in (14) and (24) respectively.*

*i) If  $E$  is a real number such that  $E \notin \sigma_{0,T}$  and  $E \notin (\sigma(l_{\mathcal{D}}) \cap \sigma(l_{\mathcal{N}})) \setminus \sigma_0(\mathcal{L})$ , then  $E$  is an eigenvalue of the operator  $\mathcal{L}_{\mathbf{p},T}$  if and only if at least one of the following assertions holds:*

- $E \in \sigma_0(\mathcal{L})$ ,
- $E \notin \sigma(l_{\mathcal{D}})$  and  $\det(\Lambda_{\mathbf{p},T}(E) + \Lambda(E)) = 0$ ,
- $E \notin \sigma(l_{\mathcal{N}})$  and  $\det(\Lambda_{\mathbf{p},T}(E)\Lambda^{-1}(E) + I_{2N}) = 0$ .

ii) Pick a positive integer  $n$  so that  $E := (\pi n/T)^2 \notin \sigma(l_{\mathcal{D}}) \cap \sigma(l_{\mathcal{N}})$ . Then  $E$  is an eigenvalue of the operator  $\mathcal{L}_{\mathbf{p},T}$  if and only if at least one of the following holds

- $E \notin \sigma(l_{\mathcal{D}})$  and for the even/odd  $n$ ,  $\det\{\langle \Lambda(E)\mathbf{e}_s^{+/-}, \mathbf{e}_t^{+/-} \rangle_{\mathbf{C}^{2N}}\}_{s,t=1}^N = 0$ ,
- $E \notin \sigma(l_{\mathcal{N}})$  and for the odd/even  $n$ ,  $\det\{\langle \Lambda^{-1}(E)\mathbf{e}_s^{+/-}, \mathbf{e}_t^{+/-} \rangle_{\mathbf{C}^{2N}}\}_{s,t=1}^N = 0$

with  $\mathbf{e}_s^{\pm}$  from (25).

*Proof.* The arguments used in the proof of Theorem 1 may also be applied here.  $\square$

**Remark 2.** First, we observe that the cubic configuration of the periodical graph  $\tilde{\mathcal{L}}_T$  means that its translation group has  $N$  generators. But if we split the set of indexes of the boundary conditions (21) on  $M$  subsets,  $1 \leq M < N$ , and assume that for each subset all components  $p_s$  are the same then we get a periodic graph with the group of translations which has only  $M$  generators (the case  $M = 1$  see in [3]).

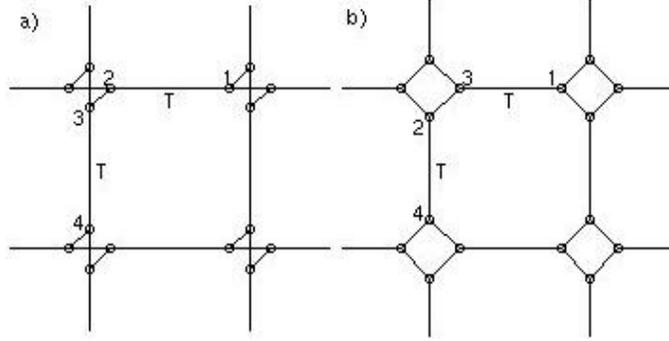
Further, we notice that in the general case of the graph  $\Gamma_0$  and the boundary conditions  $\gamma$ , by reindexing intervals  $[0, T/2]$  of the graph  $\tilde{\mathcal{L}}_T$  and by using (21), we get  $(2N - 1)!!$  different operators  $\mathcal{L}_{\mathbf{p},T}$  for any fixed  $\mathbf{p}$  and  $T > 0$ .

Finally, one may put  $T_s$ , which depends on  $s$ , instead of  $T$  in (21).

Suitable reformulations of Theorem 2 are obvious.

## 5.1 Example

Due to symmetry of the boundary conditions (4) and the ring one may construct only two different 2-periodical operators. The first operator  $\tilde{\mathcal{L}}_T^{(1)} = \tilde{\mathcal{L}}_T^{(1)}(\beta; a)$  corresponds to the pairs of indexes (1, 2)(3, 4) (figure 1a) and the second one  $\tilde{\mathcal{L}}_T^{(2)} = \tilde{\mathcal{L}}_T^{(2)}(\beta; a)$  does to (1, 3)(2, 4) (figure 1b, cf. [9]).



**Figure 1.** The periodical graphs from the example.

By Theorem 2 because  $\sigma_0 = \sigma(l_D) \cap \sigma(l_N)$  we have got a complete description of the sets  $\sigma(\tilde{\mathcal{L}}_T^{(j)})$ ,  $j = 1, 2$  (see Appendix C for details).

## 6 Asymptotics of localized spectral bands

In this section we establish an asymptotic formula of a localized band of the spectrum of the periodic operator  $\tilde{\mathcal{L}}_T$  as  $T \rightarrow +\infty$ , the band which associated with a simple eigenvalue  $E_0 < 0$  of the operator  $\mathcal{L}$  such that  $\Lambda(E_0)$  (or  $\Lambda^{-1}(E_0)$ ) exists. The following simple decomposition of the matrix  $\Lambda_{\mathbf{p}, T}$  will get us started (cf. [18]),

$$\Lambda_{\mathbf{p}, T}(-k^2) = k \left( I_{2N} - \frac{1}{\sinh kT} \sum_{s=1}^N \begin{pmatrix} 0 & e^{-ips} \\ e^{ips} & 0 \end{pmatrix} P_s + \frac{e^{-kT}}{\sinh kT} I_{2N} \right). \quad (26)$$

Thus  $\Lambda_{\mathbf{p}, T}(-k^2) \rightarrow kI_{2N}$  as  $T \rightarrow +\infty$ , for  $\Re k > 0$ . On the other hand by Theorem 1 we have  $(\sqrt{|E_0|}I_{2N} + \Lambda(E_0))\vec{F} = 0$  where  $F \in D(\mathcal{L})$  is the corresponding eigenfunction of the operator  $\mathcal{L}$ . Hence, one can expect that for any large  $T$  in a neighborhood of the point  $E_0$  there is only one solution  $z = E_{\mathbf{p}, T}$  of the equation  $\det(\Lambda_{\mathbf{p}, T}(z) + \Lambda(z)) = 0$  and that  $E_{\mathbf{p}, T} \rightarrow E_0$  as  $T \rightarrow +\infty$ . Then the second addend in (26) will give us an asymptotic description of the isolated spectral band

$$b(E_0, T) := \bigcup_{\mathbf{p} \in [0, 2\pi]^N} E_{\mathbf{p}, T}$$

of the operator  $\tilde{\mathcal{L}}_T$ . From this we have the following

**Theorem 3.** Let  $E_0 < 0$  be a simple eigenvalue of the operator  $\mathcal{L}$  such that  $\Lambda(E_0)$  exists and let  $F = \{F_j, j = 0, 1, \dots, 2N\}$  be the corresponding eigenfunction, i.e.,  $\mathcal{L}F = E_0F$ . Denote by  $d_0, d_0 \leq |E_0|$ , the distance from  $E_0$  to the set  $(\sigma(\mathcal{L}) \cup \sigma(l_{\mathcal{D}})) \setminus \{E_0\}$ , i.e.,

$$d_0 := \text{dist}(E_0, (\sigma(\mathcal{L}) \cup \sigma(l_{\mathcal{D}})) \setminus \{E_0\}).$$

Then

i) for any number  $r \in (0, d_0)$  there is a positive constant  $T_r$  such that for any  $T > T_r$  and  $\mathbf{p} \in [0, 2\pi]^N$  the closed disk  $D_r := \{z \in \mathbf{C} : |z - E_0| \leq r\}$  contains only one point  $E_{\mathbf{p},T}$  of the negative spectrum of the operator  $\mathcal{L}_{\mathbf{p},T}$ ;

ii) if  $T$  tends to infinity then the following asymptotic formula is valid

$$E_{\mathbf{p},T} = E_0 + \frac{8E_0 e^{-T\sqrt{|E_0|}}(1 + o(1))}{\|\vec{F}\|_{\mathbf{C}^{2N}}^2 - 2\sqrt{|E_0|}\langle \Lambda'(E_0)\vec{F}, \vec{F} \rangle_{\mathbf{C}^{2N}}} \Re \sum_{s=1}^N e^{ip_s} F_{2s-1}(0) \overline{F_{2s}(0)} \quad (27)$$

uniformly on  $\mathbf{p} \in [0, 2\pi]^N$  with  $\Lambda'(E_0) := (d/dz) \Lambda(z)|_{z=E_0}$  and  $\vec{F} = (F_1(0), F_2(0), \dots, F_{2N}(0))^t$ .

*Proof.* i) To prove the first part of the theorem we note that for a given positive  $r \in (0, d_0)$  the regular matrix valued function

$$A(z) := \sqrt{-z}I_{2N} + \Lambda(z)$$

with  $\Re\sqrt{-z} \geq 0$  has no zeros on  $D_r$  but  $z = E_0$  with the eigenvector  $\vec{F}$ , i.e.,  $A(E_0)\vec{F} = 0$ . Therefore

$$\alpha_r := \max_{|z-E_0|=r} \|A^{-1}(z)\|_{\mathbf{C}^{2N}} < \infty.$$

On the other hand the difference between  $A(z)$  and the regular matrix valued function

$$B(z) = B(z; \mathbf{p}, T) := \Lambda_{\mathbf{p},T}(z) + \Lambda(z)$$

is uniformly small on the disk  $D_r$  for any large  $T$ . Indeed, because of  $r < |E_0|$ , by (26) for any  $T > T_r$  with  $T_r$  such that  $\exp(-2T_r\sqrt{|E_0+r|}) \leq 1/2$  we have the following estimation

$$\begin{aligned} \max_{|z-E_0| \leq r} \|B(z) - A(z)\|_{\mathbf{C}^{2N}} &= \max_{|z-E_0| \leq r} \|\Lambda_{\mathbf{p},T}(z) - \sqrt{-z}I_{2N}\|_{\mathbf{C}^{2N}} \\ &\leq 2\sqrt{|E_0|} \max_{|z-E_0| \leq r} \frac{1 + |e^{-T\sqrt{-z}}|}{|\sinh T\sqrt{-z}|} \leq \frac{8\sqrt{|E_0|}e^{-T\sqrt{|E_0+r|}}}{1 - e^{-2T\sqrt{|E_0+r|}}} \leq 16\sqrt{|E_0|}e^{-T\sqrt{|E_0+r|}}. \end{aligned} \quad (28)$$

The latter means that one may choose a positive number  $T_r$  so that for any  $T > T_r$

$$\max_{|z-E_0|=r} (\|B(z) - A(z)\|_{\mathbf{C}^{2N}} \|A^{-1}(z)\|_{\mathbf{C}^{2N}}) < 1.$$

Thus, by Rouché's theorem [5] the regular matrix valued function  $B(z)$  has only one zero  $z = E_{\mathbf{p},T} \in D_r$  for any  $T > T_r$  and this zero is simple as is  $E_0$ . We note also that  $E_{\mathbf{p},T}$  is

an eigenvalue of the selfadjoint operator  $\mathcal{L}_{\mathbf{p},T}$ . Therefore,  $E_{\mathbf{p},T}$  is a real negative number. Moreover,

$$\lim_{T \rightarrow +\infty} E_{\mathbf{p},T} = E_0 \quad (29)$$

because one may put  $r \rightarrow 0$  as  $T \rightarrow +\infty$ .

ii) Now, let  $\Phi = \Phi(\mathbf{p}, T) \in D(\mathcal{L}_{\mathbf{p},T})$  be an eigenfunction of the operator  $\mathcal{L}_{\mathbf{p},T}$  which corresponds to the eigenvalue  $E_{\mathbf{p},T} \in D_r$  with  $T > T_r$ . Then, by Theorem 2  $B(E_{\mathbf{p},T})\vec{\Phi} = 0$ . Let us normalize  $\Phi$  by the following condition of orthogonality in  $\mathbf{C}^{2N}$

$$\vec{f} = \vec{f}(\mathbf{p}, T) := \vec{\Phi}(\mathbf{p}, T) - \vec{F} \perp \vec{F}.$$

Thus, there is a positive constant  $c_0$  independent of  $\mathbf{p}$  and  $T$  ( $T > T_r$ ) such that

$$\|A(E_0)\vec{f}\|_{\mathbf{C}^{2N}} \geq c_0 \|\vec{f}\|_{\mathbf{C}^{2N}}. \quad (30)$$

Then,

$$\|B(E_{\mathbf{p},T})\vec{f}\|_{\mathbf{C}^{2N}} \geq (c_0 - \|B(E_{\mathbf{p},T}) - A(E_0)\|_{\mathbf{C}^{2N}}) \|\vec{f}\|_{\mathbf{C}^{2N}}$$

and by the definitions of  $\vec{f}$  and  $\vec{F}$

$$\|B(E_{\mathbf{p},T})\vec{f}\|_{\mathbf{C}^{2N}} = \|-B(E_{\mathbf{p},T})\vec{F}\|_{\mathbf{C}^{2N}} \leq \|A(E_0) - B(E_{\mathbf{p},T})\|_{\mathbf{C}^{2N}} \|\vec{F}\|_{\mathbf{C}^{2N}}. \quad (31)$$

The matrix  $\Lambda(z)$  is a regular function on a neighborhood of the close disk  $D_r$ . Hence, one can choose a positive constant  $c_1 = c_1(r)$  such that

$$\|\Lambda(z) - \Lambda(E_0)\|_{\mathbf{C}^{2N}} \leq c_1 |z - E_0|, \quad z \in D_r. \quad (32)$$

From this, (29), and (31) we have the following estimation

$$\|\vec{f}\|_{\mathbf{C}^{2N}} \leq c_f (|\delta| + e^{-T\sqrt{|E_0+r|}}) \|\vec{F}\|_{\mathbf{C}^{2N}} \quad (33)$$

with  $\delta = \delta(\mathbf{p}, T) := E_{\mathbf{p},T} - E_0$  and a constant  $c_f$  independent of  $\mathbf{p}$  and  $T$ ,  $T > T_r$ .

Indeed, by (28) and (32) we get

$$\begin{aligned} \|B(E_{\mathbf{p},T}) - A(E_0)\|_{\mathbf{C}^{2N}} &\leq \left(16\sqrt{|E_0|}e^{-T\sqrt{|E_0+r|}} + \|A(E_{\mathbf{p},T}) - A(E_0)\|_{\mathbf{C}^{2N}}\right) \\ &\leq 16\sqrt{|E_0|}e^{-T\sqrt{|E_0+r|}} + |\delta|/\sqrt{|E_0|} + c_1|\delta| \leq c_2 \left(|\delta| + e^{-T\sqrt{|E_0+r|}}\right) \rightarrow 0, \end{aligned}$$

as  $T$  tends to infinity.

To get the asymptotic formula of the band  $b(\mathbf{p}, T)$  we suggest one considers the identity

$$\langle B(E_{\mathbf{p},T})\vec{\Phi}, \vec{F} \rangle_{\mathbf{C}^{2N}} \equiv 0$$

which can be re-written by the following way

$$\langle (B(E_{\mathbf{p},T}) - A(E_0))\vec{F}, \vec{F} \rangle_{\mathbf{C}^{2N}} + \langle (B(E_{\mathbf{p},T}) - \Lambda(E_0))\vec{f}, \vec{F} \rangle_{\mathbf{C}^{2N}} = 0. \quad (34)$$

Here we have used that  $\vec{f} \perp \vec{F}$ ,  $A(E_0)\vec{F} = 0$ ,  $\Lambda(E_0)\vec{F} = -\sqrt{|E_0|}\vec{F}$ , and that the matrix  $\Lambda(E_0)$  is selfadjoint.

Next we need the Taylor's formula

$$\Lambda(E_0 + \zeta) = \Lambda(E_0) + \zeta\Lambda'(E_0) + \zeta^2\Lambda_1(\zeta), \quad |\zeta| \leq r,$$

about the point  $E_0$  with a uniformly bounded matrix function  $\Lambda_1(\zeta)$  on the disk  $D_r = \{|\zeta| \leq r\}$ .

We see immediately from (26) that

$$\begin{aligned} B(E_{\mathbf{p},T}) - A(E_0) &= \delta\Lambda'(E_0) + \delta^2\Lambda_1(\delta) - \frac{\delta}{\sqrt{|E_{\mathbf{p},T}|} + \sqrt{|E_0|}}I_{2N} \\ &- \frac{2\sqrt{|E_{\mathbf{p},T}|}e^{-T\sqrt{|E_{\mathbf{p},T}|}}}{1 - e^{-2T\sqrt{|E_{\mathbf{p},T}|}}} \left( \sum_{s=1}^N \begin{pmatrix} 0 & e^{-ip_s} \\ e^{ip_s} & 0 \end{pmatrix} P_s - e^{-T\sqrt{|E_{\mathbf{p},T}|}}I_{2N} \right). \end{aligned}$$

From this with  $E_{\mathbf{p},T} = E_0 + \delta$  we have

$$\begin{aligned} \langle (B(E_0 + \delta) - A(E_0))\vec{F}, \vec{F} \rangle_{\mathbf{C}^{2N}} &= \frac{\delta}{2\sqrt{|E_0|}} (2\sqrt{|E_0|}\langle \Lambda'(E_0)\vec{F}, \vec{F} \rangle_{\mathbf{C}^{2N}} - \|\vec{F}\|_{\mathbf{C}^{2N}}^2) \\ &- 4\sqrt{|E_0|}e^{-T\sqrt{|E_0+\delta|}}\Re \sum_{s=1}^N e^{ip_s} F_{2s-1}(0)\overline{F_{2s}(0)} + o(|\delta| + e^{-T\sqrt{|E_0+\delta|}})\|\vec{F}\|_{\mathbf{C}^{2N}}^2. \end{aligned} \quad (35)$$

On the other hand, since the number  $\delta$  and the vector  $\vec{f}$  are small (see (30) and (33)) and  $\vec{f} \perp \vec{F}$ , by (26) we have

$$|\langle (B(E_0 + \delta) - \Lambda(E_0))\vec{f}, \vec{F} \rangle_{\mathbf{C}^{2N}}| = o(|\delta| + e^{-T\sqrt{|E_0+\delta|}})\|\vec{F}\|_{\mathbf{C}^{2N}}^2 \quad (36)$$

as  $T \rightarrow +\infty$ .

Notice that by (13)  $\Lambda'(E_0) \leq 0$ , thus,

$$2\sqrt{|E_0|}\langle \Lambda'(E_0)\vec{F}, \vec{F} \rangle_{\mathbf{C}^{2N}} - \|\vec{F}\|_{\mathbf{C}^{2N}}^2 < 0.$$

Therefore, the unique solution  $\delta = \delta(\mathbf{p}, T)$ ,  $|\delta| \leq r$ , of the equation

$$\langle B(E_0 + \delta)\vec{\Phi}, \vec{F} \rangle_{\mathbf{C}^{2N}} \equiv 0$$

can be estimated as follow  $|\delta| \leq c_\delta \exp(-T\sqrt{|E_0 + r|})$ ,  $T > T_r$ . It means that

$$\lim_{T \rightarrow +\infty} T \delta(\mathbf{p}, T) = 0 \quad (37)$$

uniformly with respect to  $\mathbf{p}$ . So, one can put  $E_0$  instead of  $E_{\mathbf{p},T} = E_0 + \delta$  in the formulae (35) and (36) because by (37) we have

$$e^{-T\sqrt{|E_0+\delta|}} = e^{-T\sqrt{|E_0|}}(1 + o(1)), \quad T \rightarrow +\infty. \quad (38)$$

After that the asymptotic formula (27) follows from (34).  $\square$

We now make some comments.

1. Using the equations  $\Lambda' = -\Lambda(\Lambda^{-1})'\Lambda$  and  $\Lambda(E_0)\vec{F} = -\sqrt{|E_0|}\vec{F}$  we get

$$\langle \Lambda'(E_0)\vec{F}, \vec{F} \rangle = -\langle (\Lambda^{-1})'(E_0)\Lambda(E_0)\vec{F}, \Lambda(E_0)\vec{F} \rangle = E_0 \langle (\Lambda^{-1})'(E_0)\vec{F}, \vec{F} \rangle.$$

Therefore, one may rewrite the formula (27) via Neumann-to-Dirichlet map  $\Lambda^{-1}(E_0)$ . Moreover, for any  $r \in (0, d_1)$  where  $d_1$  is the distance from  $E_0$  to the rest of spectrum, i.e.,

$$d_1 = \text{dist}(E_0, \sigma(\mathcal{L}) \setminus \{E_0\}),$$

because of  $\sigma_0(\mathcal{L}) \subset \sigma(\mathcal{L})$  there is a positive number  $T_r$  such that for any  $T > T_r$  in the disk  $D_r$  the operator  $\tilde{\mathcal{L}}_T$  has no spectral bands but  $b(E_0, T)$ . Thus, if the negative spectrum of the operator  $\mathcal{L}$  consists of  $M$  simple eigenvalues then for every large  $T$  the periodical operator  $\tilde{\mathcal{L}}_T$  has exactly  $M$  spectral bands.

2. Choosing in (27) suitable values of the parameters  $p_s$ ,  $s = 1, 2, \dots, N$ , one may get the following asymptotic formula of the width  $\Delta = \Delta(E_0, T)$  of the band  $b(E_0, T)$

$$\Delta = \frac{16|E_0|e^{-T\sqrt{|E_0|}}(1 + o(1))}{\|\vec{F}\|_{\mathbf{C}^{2N}}^2 - 2\sqrt{|E_0|}\langle \Lambda'(E_0)\vec{F}, \vec{F} \rangle_{\mathbf{C}^{2N}}} \sum_{s=1}^N |F_{2s-1}(0)F_{2s}(0)|, \quad T \rightarrow +\infty. \quad (39)$$

Small functions  $o(1)$  in (38) as well as in (27) and (39) have an order  $Te^{-T\sqrt{|E_0|}}$ . Hence, in the case

$$\sum_{s=1}^N |F_{2s-1}(0)F_{2s}(0)| = 0$$

we have only got an estimate of the width

$$\Delta = O(T e^{-2T\sqrt{|E_0|}}).$$

3. The main focus of interest at this paper is a multi-dimensional behavior of one-dimensional structures. Therefore we have considered only the simplest operator on joints. The suitable asymptotic formulae with  $q \neq 0$  and  $N = 1$  have been proved in [14], [15], and [16].

4. Finally we remark that the proof of Theorem 3 can be extended to a non-selfadjoint operator  $\mathcal{L}$  with  $E_0 = \zeta^2 \in \mathbf{C}$ ,  $\Im\zeta \geq 0$  (see [12] for  $N=1$ ). In this case we need to start with the identity  $\langle B(E_{\mathbf{p},T})\vec{\Phi}, \vec{F}^* \rangle_{\mathbf{C}^{2N}} \equiv 0$ , where  $\vec{F}^*$  is a unique solution, up to a constant, of the conjugate equation  $(\bar{\zeta}I_{2N} + \Lambda^*(\zeta^2))\vec{F}^* = 0$ .

## 6.1 Example

In Section 4.2 the lowest eigenvalue  $E_0 = E_0(\beta, a) < 0$  of the operator  $\mathcal{L}(\beta, a)$  has been found. It is simple and is a solution of the equation (20). For instance, if we choose  $\beta = 1$  and  $a = 4$  then  $E_0(1, 4) = -13.24$ .

For any  $\beta$  and  $a$  the corresponding eigenfunction  $F$  has the components  $F_j$  with  $F_j(0) = 1$ ,  $j = 1, 2, 3, 4$ . Therefore,

$$\|\vec{F}\|_{\mathbf{C}^{2N}}^2 = 4, \quad \Re \sum_{s=1}^2 e^{ip_s} F_{2s-1}(0) \overline{F_{2s}(0)} = \cos p_1 + \cos p_2, \quad \text{and}$$

$$g(z) := \langle \Lambda(z) \vec{F}, \vec{F} \rangle_{\mathbf{C}^{2N}} = -\frac{8\sqrt{a^2+z}}{|\beta|^2} \tan \frac{\sqrt{a^2+z}}{2}$$

with  $\Lambda(z)$  from Appendix B. Using the identity

$$g'(z) := \langle \Lambda'(z) \vec{F}, \vec{F} \rangle_{\mathbf{C}^{2N}},$$

together with the equation (20), that is,

$$\tan \frac{\sqrt{a^2+E_0}}{2} = \frac{|\beta|^2 \sqrt{|E_0|}}{2\sqrt{a^2+E_0}},$$

we have the following asymptotic formula of the band  $b(E_0, T)$  of the periodical operators  $\tilde{\mathcal{L}}_T^{(1)}(\beta; a)$  and  $\tilde{\mathcal{L}}_T^{(2)}(\beta; a)$

$$E_{(p_1, p_2), T}(\beta, a) = E_0 + \frac{8E_0|\beta|^2(a^2+E_0)e^{-T\sqrt{|E_0|}}(1+o(1))}{4|\beta|^2a^2+|E_0|^{3/2}|\beta|^4+4|E_0|^{1/2}(a^2+E_0)}(\cos p_1 + \cos p_2) \quad (40)$$

as  $T$  goes to infinity. Of course, using  $\Lambda^{-1}$  one has got the same result.

## 7 The case $T = 0$

In Section 6 we established results on the behavior of negative spectral bands of the periodic operator  $\tilde{\mathcal{L}}_T$  as  $T \rightarrow \infty$ . Here we will show how one can construct a periodic operator which is in a certain sense a limit of the operator  $\tilde{\mathcal{L}}_T$  as  $T \rightarrow 0$ .

Taking the limit, we obtain a new periodic graph  $\tilde{\Gamma}_0$  which is an infinite periodic set of replicas of the compact graph  $\Gamma_0$  connected to each other. Then the first question is: What are new boundary conditions at common points?

It just seems the natural thing to restrict the operator  $\tilde{\mathcal{L}}_T$  by imposing additional selfadjoint boundary conditions

$$f(0) = f(T) \quad \text{and} \quad f'(+0) = f'(T-0) \quad (41)$$

on each interval  $[0, T]$  which connects two cells in the graph  $\tilde{\mathcal{L}}_T$ . Indeed, if an interval  $[0, T]$  is small then for a component  $f$  of each wavefunction on the interval we have equations  $f(0) = f(T)(1+o(1))$  and  $f'(+0) = f'(T-0)(1+o(1))$ . The suitable procedure of restrictions is discussed in Appendix A and it will be illustrated by the following example.

## 7.1 Example

Let us test the conditions (41) for the operators  $\tilde{\mathcal{L}}_0^{(j)}$ ,  $j = 1, 2$  (see Sec. 5.1). At any node we have the boundary conditions (4) ( $\beta \neq 0, \infty$ ). Now we assume that on each interval  $[0, T]$  we have the conditions (41). One may eliminate all components  $f$  which correspond to the intervals. So, we get new graphs and operators with vertices of four edges and "zero-current" boundary conditions. The latter in particular means that the conditions are independent of the parameter  $\beta$ . Moreover, straightforward calculations show that all gaps of the spectrum of the operators  $\tilde{\mathcal{L}}_0^{(j)}$ ,  $j = 1, 2$ , are degenerate. Indeed, the corresponding dispersion equations are

$$8 \cos^2 \sqrt{a^2 + E} - 4(\cos p + \cos q) \cos \sqrt{a^2 + E} + \cos(p - q) - 1 = 0$$

and

$$2 \cos \sqrt{a^2 + E} + \cos \frac{p + q}{2} + \cos \frac{p - q}{2} = 0.$$

It should be notice that the same equations are derived from the dispersion equation (64) and (65) taking limit with  $T \rightarrow 0$ . The latter confirms that the conditions (41) might be correct for the limit operator in the general case.

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## 8 Appendix A

Here we give two alternative proofs (finite-dimensional and an abstract one) of the self-adjointness of the operators  $l_{\mathcal{D}}$  and  $l_N$  (see Section 3). We start with an observation that if we remove only one semi-infinite channel  $\mathbf{R}_+$  then we will still get a selfadjoint operator. After that the self-adjointness of the operator  $l_{\mathcal{D}}$  follows by induction on numbers of closed channels.

Let  $\Gamma'$  be  $\Gamma_\infty$  without the ray  $R_N = \mathbf{R}_+$  which corresponds to the last component  $u_N$  of a function  $u \in L^2(\Gamma_\infty)$ . So, for  $f \in L^2(\Gamma')$  we have the representation  $f = \{f_j, j = 0, 1, \dots, N-1\}$  with  $f_0 \in L^2(\Gamma_0)$  and  $f_j \in L^2(\mathbf{R}_+)$ ,  $j \geq 1$ . One may consider  $L^2(\Gamma')$  as a restriction of  $L^2(\Gamma_\infty)$  on  $\Gamma'$  and we say that any function  $f \in L^2(\Gamma')$  is a trace of some function  $F \in L^2(\Gamma_\infty)$  in the sense that  $F|_{\Gamma'} = f$ .

Now, let  $\mathcal{L}'$  be a part of the operator  $\mathcal{L}$  on the domain

$$D(\mathcal{L}') := \{f \in W^{2,2}(\Gamma') : \text{there is } F \in D(\mathcal{L}) \text{ with } F|_{\Gamma'} = f \text{ and } F_N(0) = 0\} \quad (42)$$

and the operator  $\mathcal{L}'$  acts on  $f \in D(\mathcal{L}')$  as

$$\mathcal{L}'f := (\mathcal{L}F)|_{\Gamma'}$$

with  $F$  from (42). We have to emphasize that  $F$  in (42) is subjected to the selfadjoint conditions  $\gamma$ .

It follows from the localization property of the operators  $l_0$  and  $-d^2/dx^2$  that the operator  $\mathcal{L}'$  is well-defined. On the other hand the set  $C_0^\infty(\Gamma')$  of smooth functions with compact support of each component is a subset of the domain  $D(\mathcal{L}')$ . Thus, the operator  $\mathcal{L}'$  is densely defined on  $L^2(\Gamma')$ . Moreover, just as in Sec. 3, the operator  $\mathcal{L}'$  is a symmetric operator because of the self-adjointness of the operator  $\mathcal{L}$ .

To prove self-adjointness of the operator  $\mathcal{L}'$ , we only need to consider boundary conditions on the functions  $f$  from  $D(\mathcal{L}')$  at a vertex  $n' \in \Gamma'$  which is the trace of the node  $n \in \Gamma_\infty$  common with the removed ray  $R_N$ . Let us denote by  $\vec{f} \in \mathbf{C}^m$  and  $\vec{f}' \in \mathbf{C}^m$  the boundary values of the function  $f \in D(\mathcal{L}')$  at the point  $n'$ . According to the representation (2) the self-adjointness of the boundary conditions  $\gamma$  at the node  $n$  means that there is a unique unitary matrix  $U = \{u_{st}\}_{s,t=1}^{m+1}$  such that for any  $F \in D(\mathcal{L})$  we have

$$(I_{m+1} + U)\vec{F} + i(I_{m+1} - U)\vec{F}' = 0, \quad (43)$$

where  $\vec{F}$  and  $\vec{F}'$  are the corresponding boundary values of the function  $F$  at the point  $n$ . In our case one may put

$$F = \begin{pmatrix} f \\ F_N \end{pmatrix}$$

and rewrite (43) as

$$(I_{m+1} + U) \begin{pmatrix} \vec{f} \\ a \end{pmatrix} + i(I_{m+1} - U) \begin{pmatrix} \vec{f}' \\ b \end{pmatrix} = 0, \quad (44)$$

where  $\{a, b\} \subset \mathbf{C}$ ,  $a := F_N(0)$ , and  $b := F'_N(+0)$ . We note that the general solution of the equation (44) has the following representation

$$\begin{pmatrix} \vec{f} \\ a \\ \vec{f}' \\ b \end{pmatrix} = \begin{pmatrix} i(I_{m+1} - U^*) \\ I_{m+1} + U^* \end{pmatrix} \vec{c}, \quad \vec{c} \in \mathbf{C}^{m+1}. \quad (45)$$

Therefore the condition  $f \in D(\mathcal{L}')$  implies  $a = 0$  or  $\vec{c}$  is orthogonal to the last column  $\vec{r} := \{\delta_{s,m+1} - u_{s,m+1}\}_{s=1}^{m+1}$  of the matrix  $I - U$ .

The simplest case  $\vec{r} = 0$  corresponds to the equations  $u_{s,m+1} = \delta_{s,m+1}$ ,  $s = 1, 2, \dots, m+1$ . It means that  $U = U' \oplus 1$  on  $\mathbf{C}^m \oplus \mathbf{C}$  with a unitary matrix  $U'$ . Therefore  $\mathcal{L} = \mathcal{L}' \oplus l^0$  on  $L^2(\Gamma_\infty) = L^2(\Gamma') \oplus L^2(R_N)$  where  $l^0 := -d^2/dx^2$  with Dirichlet boundary condition at the origin. Thus, a priori, we have the desired condition  $a = 0$  and the operators  $\mathcal{L}'$  and  $l^0$  are selfadjoint.

Similarly, the case  $U = U' \oplus (-1)$  leads to the selfadjoint decomposition  $\mathcal{L} = \mathcal{L}' \oplus l^\pi$  with Neumann boundary condition  $b = F'_N(+0) = 0$  at the origin on the ray  $R_N$ . If in addition we put  $a = F_N(0) = 0$  then the domain of the operator  $\mathcal{L}'$  does not change, but the corresponding restriction of the operator  $l^\pi$  on the subspace  $a = 0$  is not selfadjoint.

If  $u_{s,m+1} = e^{i\theta} \delta_{s,m+1}$ ,  $s = 1, 2, \dots, m+1$ ,  $\theta \in (0, \pi) \cup (\pi, 2\pi)$  then we have the mixed boundary condition

$$a \cos(\theta/2) + b \sin(\theta/2) = 0$$

at the origin on the ray  $R_N$  and again we get the orthogonal sum of selfadjoint operators  $\mathcal{L} = \mathcal{L}' \oplus l^\theta$ .

Now let us consider the general case.

**Lemma 1.** *The operator  $\mathcal{L}'$  is a selfadjoint operator. Let  $u_{m+1,m+1} \neq 1$  and let*

$$F = \begin{pmatrix} f \\ F_N \end{pmatrix} \in D(\mathcal{L}).$$

*Then  $f \in D(\mathcal{L}')$  if and only if the function  $f$  is subjected to the selfadjoint boundary conditions*

$$(I_m + U')\vec{f} + i(I_m - U')\vec{f}' = 0 \quad (46)$$

*at the vertex  $n' \in \Gamma'$ , where*

$$U' = \{u'_{st}\}_{s,t=1}^m := \left\{ u_{st} + \frac{u_{s,m+1}u_{m+1,t}}{1 - u_{m+1,m+1}} \right\}_{s,t=1}^m \quad (47)$$

*is a unitary matrix.*

*Proof.* The case  $\vec{r} = 0$  has been considered above. Thus we suppose that  $u_{m+1,m+1} \neq 1$  and put  $\kappa := 1/(1 - u_{m+1,m+1})$ .

First we assume that  $f \in D(\mathcal{L}')$ , i.e., there is such a function  $F_N \in W^{2,2}(R_N)$  on the ray that  $F_N(0) = 0$  and

$$\begin{pmatrix} f \\ F_N \end{pmatrix} \in D(\mathcal{L}).$$

The latter means that

$$(I_{m+1} + U) \begin{pmatrix} \vec{\xi} \\ 0 \end{pmatrix} + i(I_{m+1} - U) \begin{pmatrix} \vec{\eta} \\ F'_N(+0) \end{pmatrix} = 0,$$

where  $\vec{\xi} = \{\xi_t\}_{t=1}^{m+1} := \vec{f}$  and  $\vec{\eta} = \{\eta_t\}_{t=1}^{m+1} := \vec{f}'$ . Next, one may eliminate  $F'_N(+0)$  from the previous equation. Note that the last line ( $s = m + 1$ ) of the equation is

$$\sum_{t=1}^m u_{m+1,t} \xi_t - i \sum_{t=1}^m u_{m+1,t} \eta_t + i(1 - u_{m+1,m+1}) F'_N(+0) = 0.$$

Thus,

$$F'_N(+0) = \kappa \sum_{t=1}^m u_{m+1,t} (i\xi_t + \eta_t)$$

and for  $s = 1, 2, \dots, m$  we get

$$\sum_{t=1}^m (\delta_{st} + u_{st}) \xi_t + i \sum_{t=1}^m (\delta_{st} - u_{st}) \eta_t + \kappa u_{s,m+1} \sum_{t=1}^m u_{m+1,t} (\xi_t - i\eta_t) = 0,$$

or

$$\sum_{t=1}^m (\delta_{st} + u_{st} + \kappa u_{s,m+1} u_{m+1,t}) \xi_t + i \sum_{t=1}^m (\delta_{st} - u_{st} - \kappa u_{s,m+1} u_{m+1,t}) \eta_t = 0.$$

The latter coincides with the conditions (46).

Conversely, let  $f \in W^{2,2}(\Gamma')$  and let  $f$  satisfies the conditions (46). One may choose any function  $F_N \in W^{2,2}(R_N)$  such that  $F_N(0) = 0$  and

$$F'_N(+0) = \kappa \sum_{t=1}^m u_{m+1,t} (i\xi_t + \eta_t),$$

where  $\vec{\xi} = \vec{f}$  and  $\vec{\eta} = \vec{f}'$ . Then

$$F := \begin{pmatrix} f \\ F_N \end{pmatrix} \in D(\mathcal{L}).$$

Therefore  $f \in D(\mathcal{L}')$ .

To prove unitarity of the matrix  $U'$  on  $\mathbf{C}^m$ , i.e.,

$$\sum_{j=1}^m u'_{sj} \bar{u}'_{tj} = \delta_{st}, \quad s, t = 1, 2, \dots, m, \quad (48)$$

we will use the unitarity of the original matrix  $U$  on  $\mathbf{C}^{m+1}$ , that is

$$\sum_{j=1}^{m+1} u_{sj} \overline{u_{tj}} = \delta_{st}, \quad s, t = 1, 2, \dots, m+1.$$

One may rewrite the last equations as

$$S(s, t) = \delta_{st} - u_{s, m+1} \overline{u_{t, m+1}}, \quad s, t = 1, 2, \dots, m+1, \quad (49)$$

where

$$S(s, t) := \sum_{j=1}^m u_{sj} \overline{u_{tj}}.$$

We know that

$$u'_{st} = u_{st} + \kappa u_{s, m+1} u_{m+1, t}.$$

Thus, the left hand side  $L$  of the equation (48) is equal to

$$L = S(s, t) + \kappa u_{s, m+1} S(m+1, t) + \overline{\kappa u_{t, m+1}} S(s, m+1) + |\kappa|^2 u_{s, m+1} \overline{u_{t, m+1}} S(m+1, m+1).$$

By (49) we have

$$\begin{aligned} \delta_{st} - L &= u_{s, m+1} \overline{u_{t, m+1}} + \kappa u_{s, m+1} \overline{u_{t, m+1}} u_{m+1, m+1} + \overline{\kappa u_{s, m+1}} \overline{u_{t, m+1}} u_{m+1, m+1} \\ &+ |\kappa|^2 u_{s, m+1} \overline{u_{t, m+1}} (|u_{m+1, m+1}|^2 - 1) = u_{s, m+1} \overline{u_{t, m+1}} \{1 + \kappa u_{m+1, m+1} + \overline{\kappa u_{m+1, m+1}} \\ &+ |\kappa|^2 (|u_{m+1, m+1}|^2 - 1)\} = u_{s, m+1} \overline{u_{t, m+1}} (|1 + \kappa u_{m+1, m+1}|^2 - |\kappa|^2) = 0 \end{aligned}$$

with the last equality due to the equation  $\kappa = 1 + \kappa u_{m+1, m+1}$ . This concludes the proof of the lemma.  $\square$

Now the self-adjointness of the operator  $l_{\mathcal{D}}$  follows by induction on numbers of removed rays. Next we will show that similarly we get the self-adjointness of the operator  $l_{\mathcal{N}}$ .

**Remark 3.** For any unitary matrix  $U = \{u_{st}\}_{s, t=1}^{m+1}$  the matrix

$$U'_\theta := \left\{ u_{st} + \frac{u_{s, m+1} u_{m+1, t}}{e^{i\theta} - u_{m+1, m+1}} \right\}_{s, t=1}^m, \quad \theta \in [0, 2\pi), \quad u_{m+1, m+1} \neq e^{i\theta}, \quad (50)$$

is unitary because one may multiply the last column/row of the matrix  $U$  by any number  $e^{-i\theta}$ ,  $\theta \in \mathbf{R}$ , and the new matrix will be unitary and by Lemma 1 we have that  $U'_\theta = U'$  is a unitary matrix. Moreover, in the same way as in Lemma 1 for each  $\theta \in [0, 2\pi)$  we get the coincidence of the following two sets

$$\begin{aligned} &\{f \in W^{2,2}(\Gamma') : \exists F \in D(\mathcal{L}) \text{ with } F|_{\Gamma'} = f \text{ and } F_N(0) \cos(\theta/2) + F'_N(+0) \sin(\theta/2) = 0\} \\ &= \{f \in W^{2,2}(\Gamma') : (I + U'_\theta) \vec{f} + i(I - U'_\theta) \vec{f}^\dagger = 0\} \text{ if } \theta \in [0, 2\pi), \quad u_{m+1, m+1} \neq e^{i\theta}. \end{aligned}$$

The case  $u_{m+1, m+1} = e^{i\theta}$  has been considered above.

According to Remark we get the self-adjointness of the operator  $l_{\mathcal{N}}$  which corresponds to  $\theta = \pi$ .

**Example.** By (50) for the matrix  $U$  in (6) we get

$$U'_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad \text{and} \quad U'_\pi = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}.$$

## 8.1 Reducing of a unitary operator

Let  $U$  be a unitary operator on Hilbert space  $H = H_1 \oplus H_2$  and let  $V$  be a unitary operator on  $H_2$ . Let  $x, y \in H_1$  and  $\xi, \eta \in H_2$ . We denote the unit operators on  $H_j$  by  $I_j$ ,  $j = 1, 2$ . Then  $I := I_1 \oplus I_2$  is the unit operator on  $H$ . According to the decomposition  $H = H_1 \oplus H_2$  the operator  $U$  has the following representation

$$U = \begin{pmatrix} U_{11} & U_{12} \\ U_{21} & U_{22} \end{pmatrix} \quad (51)$$

where  $U_{11}$  is an operator on  $H_1$ . We suppose that the operator  $V - U_{22}$  is invertible on  $H_2$  and  $T_V := (V - U_{22})^{-1}$  is a bounded operator.

**Lemma 2.** *The operator*

$$U'_V := U_{11} + U_{12}T_V U_{21} \quad (52)$$

*is unitary.*

*Proof.* First we will show that  $U'_V(U'_V)^* = I_1$ . The condition  $UU^* = I$  for  $U$  reads

$$\begin{aligned} U_{11}U_{11}^* &= I_1 - U_{12}U_{12}^*, \\ U_{21}U_{11}^* &= -U_{22}U_{12}^*, \\ U_{11}U_{21}^* &= -U_{12}U_{22}^*, \\ U_{21}U_{21}^* &= I_2 - U_{22}U_{22}^*. \end{aligned}$$

Using each of these equations we get

$$\begin{aligned} U'_V(U'_V)^* &= (U_{11} + U_{12}(V - U_{22})^{-1}U_{21})(U_{11}^* + U_{21}^*(V^* - U_{22}^*)^{-1}U_{12}^*) \\ &= U_{11}U_{11}^* + U_{12}T_V U_{21}U_{11}^* + U_{11}U_{21}^*T_V^*U_{12}^* + U_{12}T_V U_{21}U_{21}^*T_V^*U_{12}^* \\ &= I_1 - U_{12}U_{12}^* - U_{12}T_V^*U_{22}U_{12}^* - U_{12}U_{22}^*T_V^*U_{12}^* + U_{12}T_V(I_2 - U_{22})U_{22}^*T_V^*U_{12}^* = I_1 - U_{12}J_1U_{12}^* \end{aligned}$$

where

$$J_1 := I_2 + T_V U_{22} + U_{22}^*T_V^* - T_V(I_2 - U_{22})U_{22}^*T_V^* = T_V J_2 T_V^*$$

with

$$J_2 := (V - U_{22})(V^* - U_{22}^*) + U_{22}(V^* - U_{22}^*) + (V - U_{22})U_{22}^* - I_2 + U_{22}U_{22}^* = VV^* - I_2 = 0.$$

Here the last equality follows from unitarity of  $V$ .

In the same way one may check that the second condition  $(U'_V)^*U'_V = I_1$  is a consequence of the relations  $U^*U = I$  and  $V^*V = I_2$ . This concludes the proof of the lemma.  $\square$

### 8.1.1 Reducing of boundary conditions

According to the theory of spaces of boundary values (see [6, 17]) any selfadjoint condition on a Hilbert space  $H$  of boundary values is determined by a unitary operator  $U$  as

$$(I + U)f + i(I - U)g = 0, \quad f, g \in H. \quad (53)$$

We suppose that  $H = H_1 \oplus H_2$ . Then for any  $f, g \in H$  we have

$$f = \begin{pmatrix} x \\ \xi \end{pmatrix}, \quad g = \begin{pmatrix} y \\ \eta \end{pmatrix}, \quad x, y \in H_1, \quad \xi, \eta \in H_2.$$

Let us consider some process of closing one of the channels by switching an additional boundary conditions

$$(I_2 + V)\xi + i(I_2 - V)\eta = 0. \quad (54)$$

We will show that restriction of an original operator on  $H_1$  is subjected to the following selfadjoint boundary conditions

$$(I_1 + U'_V)x + i(I_1 - U'_V)y = 0 \quad (55)$$

with the unitary operator  $U'_V$  from Lemma 2. We need the following

**Lemma 3.** *Any solution of the system*

$$\begin{pmatrix} x \\ \xi \end{pmatrix} + U \begin{pmatrix} y \\ \eta \end{pmatrix} = 0, \quad (56)$$

$$\xi + V\eta = 0, \quad (57)$$

has the following representation

$$\begin{cases} x = -U'_V y, \\ \xi = -V(V - U_{22})^{-1}U_{21}y, \\ \eta = (V - U_{22})^{-1}U_{21}y. \end{cases} \quad (58)$$

*Proof.* . One may rewrite the equation (56) as

$$\begin{cases} x + U_{11}y + U_{12}\eta = 0, \\ \xi + U_{21}y + U_{22}\eta = 0. \end{cases}$$

Then subtracting the equation (57) from the second line we get

$$\eta = (V - U_{22})^{-1}U_{21}y.$$

Finally by (56) and (57) we have

$$\xi = -V(V - U_{22})^{-1}U_{21}y$$

and

$$x = -U'_V y$$

with the unitary operator  $U'_V := U_{11} + U_{12}(V - U_{22})^{-1}U_{21}$  as in Lemma 2.  $\square$

**Theorem 4.** *The representation (55) is true.*

*Proof.* . First, we rewrite (53) and (54) in the form (56) and (57), i.e.,

$$\begin{pmatrix} x + iy \\ \xi + i\eta \end{pmatrix} + U \begin{pmatrix} ix + y \\ i\xi + \eta \end{pmatrix} = 0,$$

$$\xi + i\eta + V(ix + \eta) = 0.$$

Then by lemma 2 we have  $x + iy = -U'_V(ix + y)$  which corresponds to (55). □

## 9 Appendix B

In this appendix we will describe Dirichlet-to-Neumann map  $\Lambda(z)$  and the negative spectrum of the Schrödinger operator  $\mathcal{L}(\beta; a)$  on the star-like graph from our example (see Section 2.1).

First we note that the function  $G(x, t; z)$  in (19) is the Green function of the operator  $l_{\mathcal{N}}$  on the ring  $(x, t) \in [0, 4]^2$  because

- 1)  $G(0, 0; z) = G(4, 0; z)$ ;
- 2)  $-G''_{xx} - a^2 G \equiv zG$ ,  $t = 0$ ,  $x \in (0, 4)$ ;
- 3)  $G'_x(+0, 0; z) - G'_x(4 - 0, 0; z) = -1$ ;

with  $z \notin \sigma(l_{\mathcal{N}})$ . Therefore, any solution of the equation

$$-u''_0 - a^2 u_0 = z u_0$$

on the union of intervals  $x \in \bigcup_{j=1}^4 (j-1, j)$ , which is continuous on  $[0, 4]$ , can be represented as

$$u_0(x) := \sum_{s=1}^4 \alpha_s G(x, s; z).$$

Hence by the second part of the boundary conditions (4) we have

$$u_j(0) = \beta u_0(j) = \beta \sum_{s=1}^4 \alpha_s G(j, s; z)$$

and

$$u'_0(j+0) - u'_0(j-0) = -\alpha_j = -\bar{\beta} u'_j(+0).$$

It means that the following correspondence holds (cf. (18))

$$u_j(0) = |\beta|^2 \sum_{s=1}^4 G(j, s; z) u'_s(+0).$$

Thus we have got the following expressions

$$\Lambda^{-1}(z) = -\frac{|\beta|^2}{2\kappa \sin 2\kappa} \begin{pmatrix} \cos 2\kappa & \cos \kappa & 1 & \cos \kappa \\ \cos \kappa & \cos 2\kappa & \cos \kappa & 1 \\ 1 & \cos \kappa & \cos 2\kappa & \cos \kappa \\ \cos \kappa & 1 & \cos \kappa & \cos 2\kappa \end{pmatrix}$$

or

$$\Lambda(z) = -\frac{\kappa}{|\beta|^2 \sin \kappa} \begin{pmatrix} -2 \cos \kappa & 1 & 0 & 1 \\ 1 & -2 \cos \kappa & 1 & 0 \\ 0 & 1 & -2 \cos \kappa & 1 \\ 1 & 0 & 1 & -2 \cos \kappa \end{pmatrix} \quad (59)$$

and

$$\det \Lambda(z) = -\frac{16\kappa^4}{|\beta|^8} \cot^2 \kappa,$$

with  $\kappa = \kappa(z) := \sqrt{a^2 + z}$ ,  $\Im \kappa \geq 0$ . It is clear that  $\Lambda \Lambda^{-1} \equiv I_4$ .

By Theorem 1 the negative spectrum of the operator  $\mathcal{L}(\beta; a)$  consists of the set

$$\sigma_0^- := \{(\pi n)^2 - a^2 < 0, n = 1, 2, \dots\}$$

and of all negative solutions of the equation

$$\det(\sqrt{-\xi} I_4 + \Lambda(\xi)) = 0, \quad \xi < 0. \quad (60)$$

The eigenvalues of the matrix

$$M(c) := \begin{pmatrix} c & 1 & 0 & 1 \\ 1 & c & 1 & 0 \\ 0 & 1 & c & 1 \\ 1 & 0 & 1 & c \end{pmatrix}$$

are  $c$  and  $c \pm 2$  and

$$\Lambda(z) = -\frac{1}{|\beta|^2} \begin{cases} (\kappa/\sin \kappa)M(-2 \cos \kappa) & \text{if } z \neq -a^2, \\ M(-2) & \text{if } z = -a^2. \end{cases}$$

The number  $-a^2$  is not a solution of (60) because

$$\det(aI_4 + \Lambda(-a^2)) = a(a + 4/|\beta|^2)(a + 2/|\beta|^2)^2 > 0.$$

Therefore the equation (60) is equivalent to a set of the following equations ( $-a^2 < \xi < 0$ ):

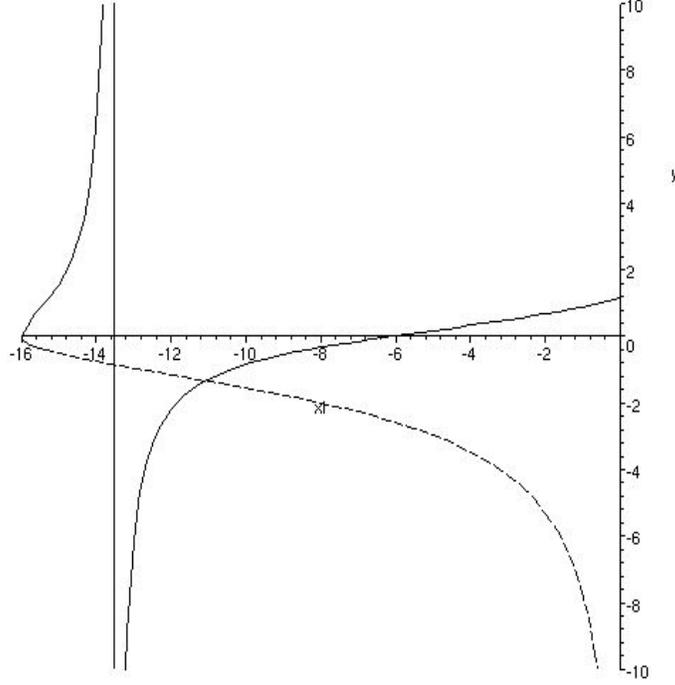
$$\tan \sqrt{a^2 + \xi} = -\frac{2\sqrt{a^2 + \xi}}{|\beta|^2 \sqrt{-\xi}}, \quad (61)$$

$$\tan \frac{\sqrt{a^2 + \xi}}{2} = -\frac{2\sqrt{a^2 + \xi}}{|\beta|^2 \sqrt{-\xi}}, \quad (62)$$

$$\tan \frac{\sqrt{a^2 + \xi}}{2} = \frac{|\beta|^2 \sqrt{-\xi}}{2\sqrt{a^2 + \xi}}. \quad (63)$$

We note that the equation (63) coincides with (20).

The equations (61) and (62) have solutions on the interval  $(-a^2, 0)$  iff  $a > \pi/2$  and  $a > \pi$  respectively. On the other hand the last one (63) is solvable for any  $a > 0$ . For example, if we put  $\beta = 1$  and  $a = 4$  then the negative spectrum of the operator  $\mathcal{L}(1; 4)$  consists of four points. The number  $\pi^2 - 16 \approx -6.13$  represents the set  $\sigma_0^-$  and the numbers  $-11.09$ ,  $-2.97$ , and  $-13.24$  are the unique negative solutions of the equations (61)-(63) respectively (see Fig 2). It is clear that all sets of solutions of the equations (61)-(63) and the set  $\sigma_0^-$  are mutually disjoint.



**Figure 2a.** The unique solution of the equation (61) is  $\xi = -11.09$ .

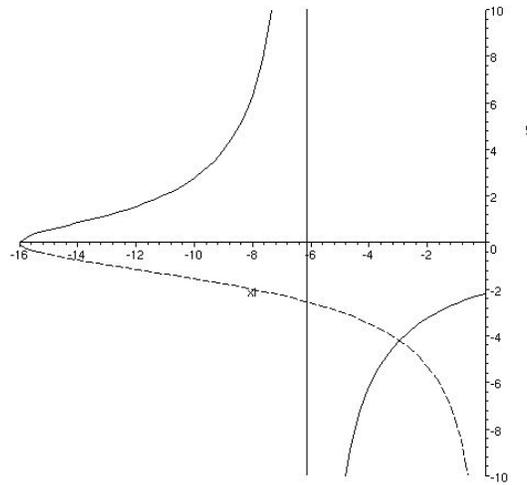
We will now describe eigenfunctions of the negative spectrum of the operator  $\mathcal{L}$ . First, as it has been mentioned above, the function, which is equal to  $\sin \pi n x$  on the compact part  $[0, 4]$  and vanishes on the rays, is an eigenfunction for any integer  $n \geq 1$ . Straightforward calculations show that the corresponding eigenvalue  $\pi^2 n^2 - a^2$  is simple.

Let  $\xi_0 < 0$  be a solution of the equation (60). Then the eigenfunction  $u(x) = u(x; \xi_0)$  has the following representation ( $j=1, 2, 3, 4$ )

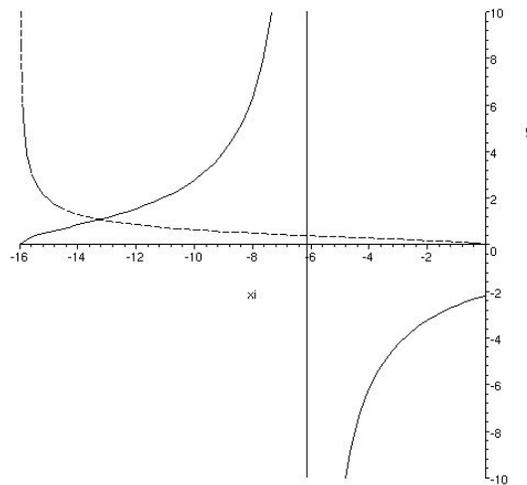
$$u_j(x) = c_j e^{-\sqrt{|\xi_0|x}},$$

$$u_0(x) = -\bar{\beta} \sqrt{|\xi_0|} \sum_{s=1}^4 G(x, s; \xi_0) c_s,$$

where the vector  $\vec{c} = \{c_s\}_{s=1}^4$  is an eigenvector of the matrix  $M(-2 \cos \sqrt{a^2 + \xi_0})$  which is  $(1, 0, -1, 0)$  or  $(0, 1, 0, -1)$  for the equation (61),  $(1, -1, 1, -1)$  in the case (62), and  $(1, 1, 1, 1)$  if  $\xi_0$  is a solution of (63).



**Figure 2b.** The unique solution of the equation (62) is  $\xi = -2.97$ .



**Figure 2c.** The unique solution of the equation (63) is  $\xi = -13.24$ .

## 10 Appendix C

We will now show how to describe the spectrum of the periodical operators from the example of Section 5.1 using Theorem 2.

Let us first note that the spectrum of the operator  $\tilde{\mathcal{L}}_T^{(1)}$  or  $\tilde{\mathcal{L}}_T^{(2)}$ , which is situated on the interval  $[-a^2, +\infty)$  because of (7), has the band structure with the exception of points of the set  $\sigma_0 = \{(\pi n)^2 - a^2 : n = 1, 2, \dots\}$  in (17), which are eigenvalues of infinite multiplicity.

By the definition (23) for the matrix  $\Lambda_{(p,q),T}(E)$  with  $0 \leq p, q \leq 2\pi$  and  $E \notin \sigma_{0,T} = \{(\pi n/T)^2 : n = 1, 2, \dots\}$  we have

$$\Lambda_{(p,q),T}(E) := \frac{\sqrt{E}}{\sin \sqrt{ET}} \begin{pmatrix} \cos \sqrt{ET} & -e^{-ip} & 0 & 0 \\ -e^{ip} & \cos \sqrt{ET} & 0 & 0 \\ 0 & 0 & \cos \sqrt{ET} & -e^{-iq} \\ 0 & 0 & -e^{iq} & \cos \sqrt{ET} \end{pmatrix}.$$

On the other hand the matrix  $\Lambda(E)$  is defined by (59) with  $\kappa = \sqrt{a^2 + E}$  and  $E \notin \sigma_0$ . Thus, according to Theorem 2 continuous spectra of the operators  $\tilde{\mathcal{L}}_T^{(1)}$  and  $\tilde{\mathcal{L}}_T^{(2)}$  coincide with sets

$$\sigma_{c,T}^{(1)} = \sigma_c(\tilde{\mathcal{L}}_T^{(1)}) := \bigcup_{p,q \in [0, 2\pi]} \{E : \det(\Lambda_{(p,q),T}(E) + \Lambda(E)) = 0\}$$

and

$$\sigma_{c,T}^{(2)} = \sigma_c(\tilde{\mathcal{L}}_T^{(2)}) := \bigcup_{p,q \in [0, 2\pi]} \{E : \det(\Lambda_{(p,q),T}(E) + J\Lambda(E)J) = 0\}$$

respectively, where

$$J := \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

Put  $|\beta| = 1$ . If we exclude singular points then straightforward calculations show that the dispersion equations  $\det(\Lambda_{(p,q),T}(E) + \Lambda(E)) = 0$  and  $\det(\Lambda_{(p,q),T}(E) + J\Lambda(E)J) = 0$  are respectively equivalent to

$$F_j(E, p, q; a, T) = 0, \quad j = 1, 2,$$

where

$$F_1 := A_1(\cos p + \cos q) + B_1 \cos(p - q) + C_1 \tag{64}$$

and

$$F_2 := A_2(\cos p + \cos q) + B_2 \cos p \cos q + C_2 \tag{65}$$

with

$$\begin{aligned} A_1 &:= 2((ES_\kappa^2 - 4c_\kappa^2)S_T - 4S_\kappa c_\kappa c_T); \quad B_1 := 2S_\kappa; \quad C_1 := 2S_\kappa(8c_\kappa^2 - 1) \\ &\quad + 8c_T c_\kappa S_T(4c_\kappa^2 - 2 - ES_\kappa^2) + S_\kappa S_T^2(E^2 S_\kappa^2 + 4E - 8c_\kappa^2(2\kappa^2 + 3E)); \end{aligned}$$

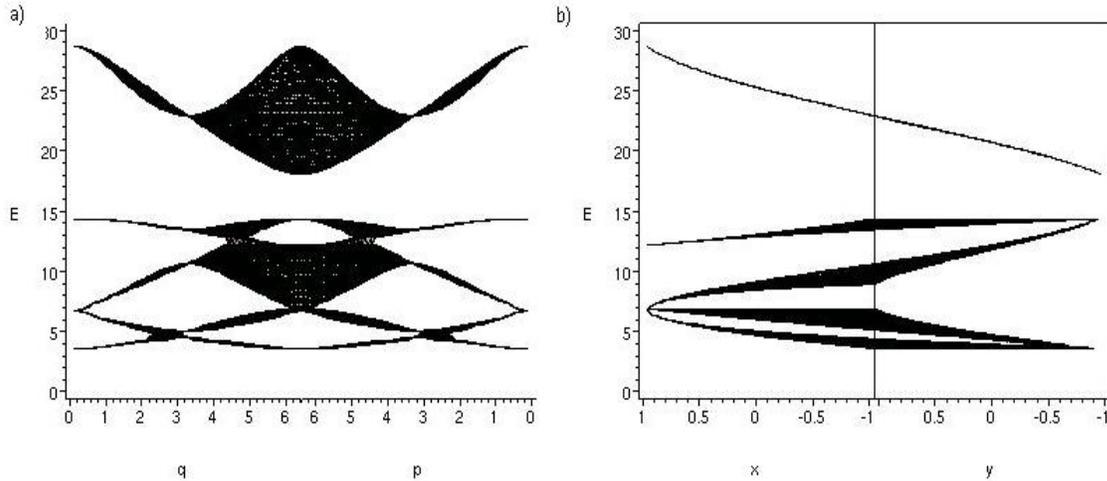
$$A_2 := 4(2c_\kappa S_T + c_T S_\kappa); \quad B_2 := 4S_\kappa; \quad C_2 := 2S_\kappa - C_1;$$

$$\kappa := \sqrt{a^2 + E}; \quad c_\kappa := \cos \kappa; \quad S_\kappa := \frac{\sin \kappa}{\kappa}; \quad c_T := \cos \sqrt{ET} \quad S_T := \frac{\sin \sqrt{ET}}{\sqrt{E}}.$$

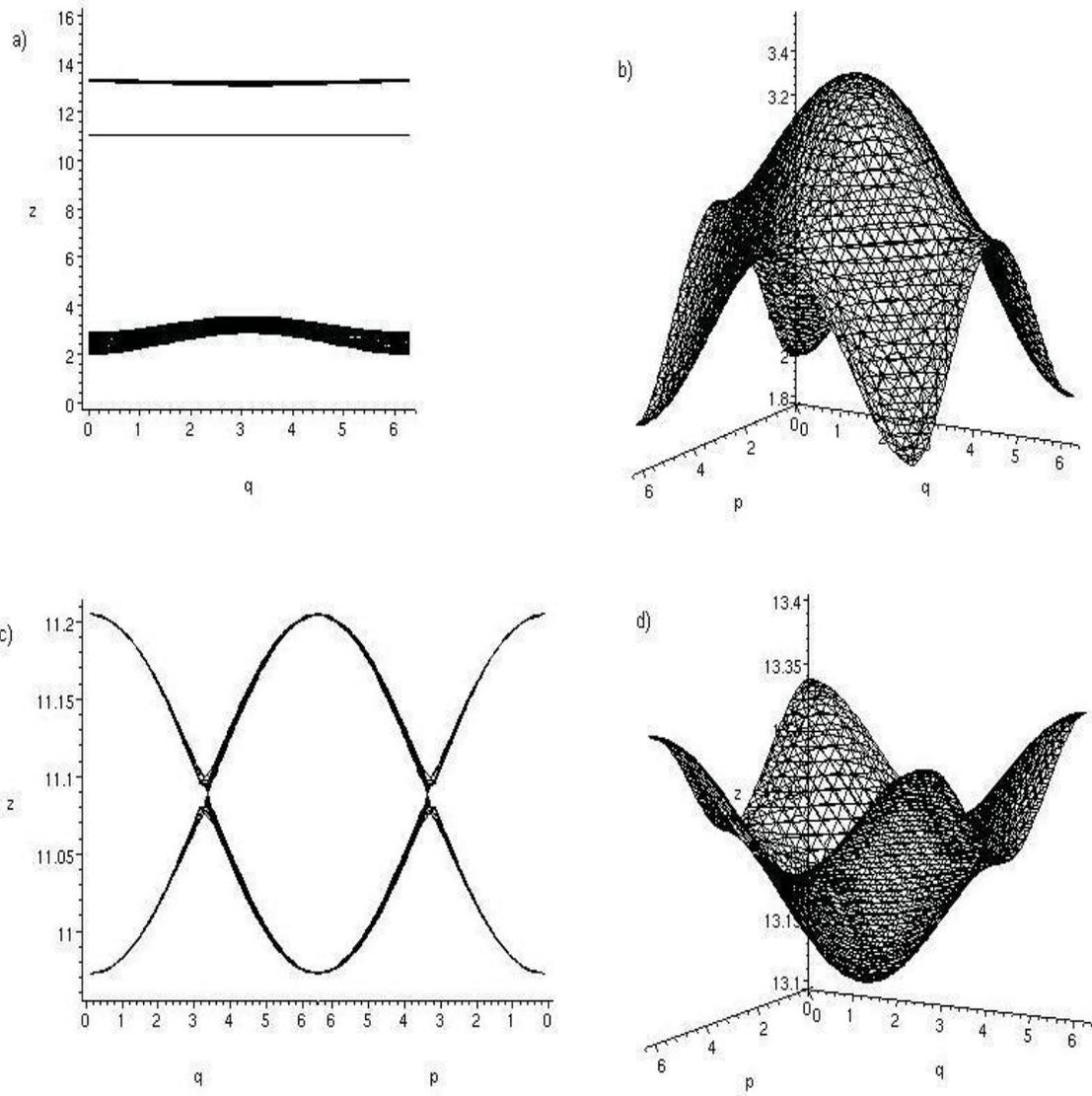
We note that  $F_j$  are entire functions with respect to  $E, p, q, a$  and  $T$ . It is straightforward to show that the asymptotic formula (40) follows from equations (64) and (65) with  $\beta = 1$ .

Now we will choose  $a = 4$  and  $T = 1$ . Then the dispersion equations  $F_j(E, p, q; 4, 1) = 0$  define many-sheeted functions  $E = E_j(p, q) \in \sigma_{c,1}^{(j)}$  with the domain  $(p, q) \in [0, 2\pi]^2$ ,  $j = 1, 2$ . Using the Maple function **implicitplot3d** which computes 3d-plot of an implicitly defined surface,  $E = E(p, q)$ , we will get a numerical description of the continuous spectrum of the periodical operators. Numerical results for  $E_j$  with  $T = 1$  plotted in Fig. 3a and Fig. 3b if  $0 < E \leq 30$  and in Fig. 4 - 5 if  $-16 \leq E < 0$ . Figures 4 and 5 show the localization of the negative spectrum. Figures 4c and 5c illustrate the difference between the spectral bands which corresponds to a non simple eigenvalue. For the small period  $T = 0.1$  the surface  $E_2(p, q)$  is painted on Figure 6.

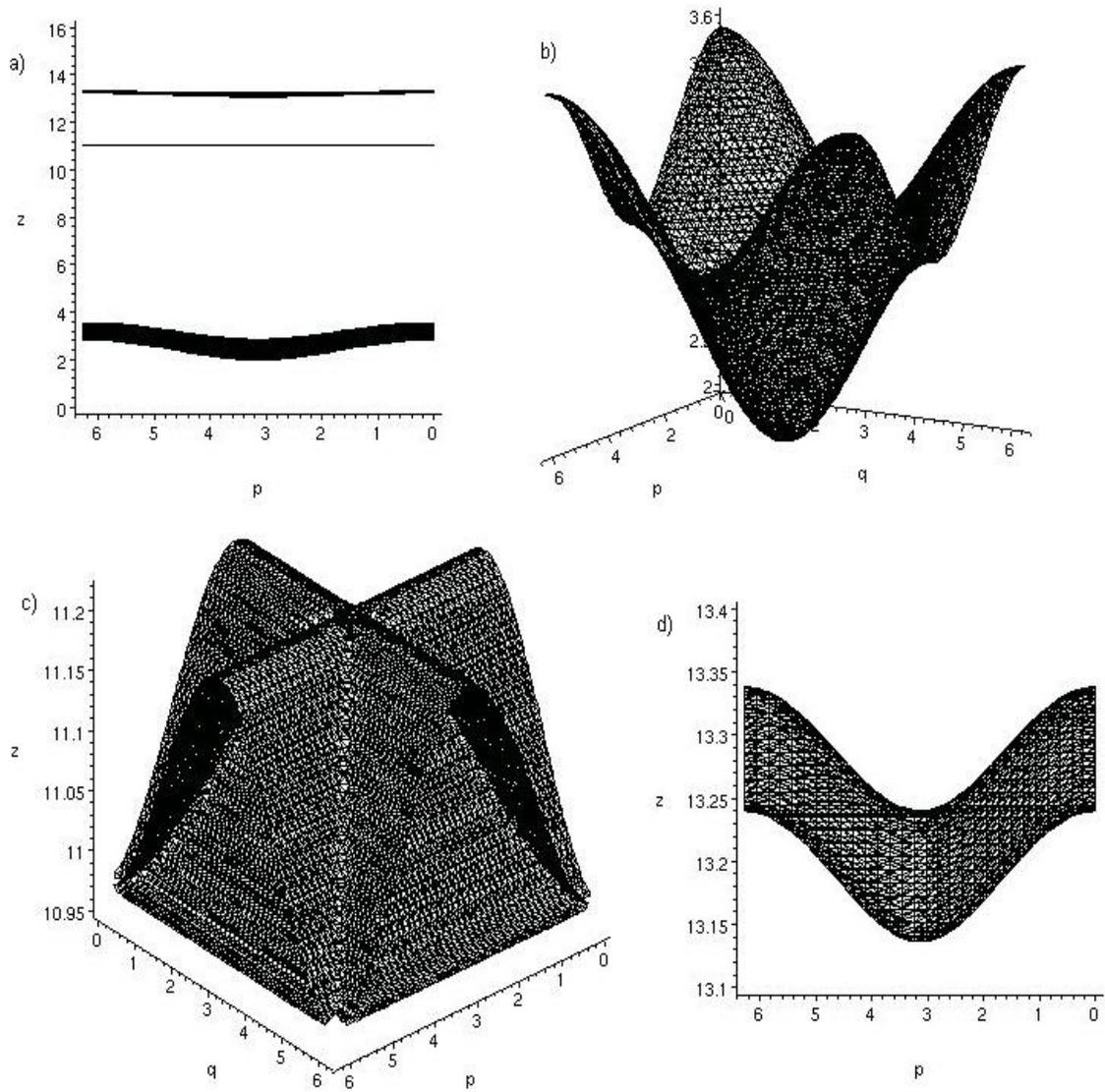
Notice that using the dispersion equation (65) it is amazing to observe how the pictures of Fig. 5 pass into Fig. 6, et cetera, as  $T$  goes from 1 to 0.1 and then down to zero. As follows from the results of Section 7.1 each point of the interval  $[-16, 0)$  belongs to the negative spectrum if  $T = 0$ . But the main surprising thing is that the energy surfaces  $E = E_j(p, q)$ ,  $j=1, 2$ , become nonsmooth with various singularities.



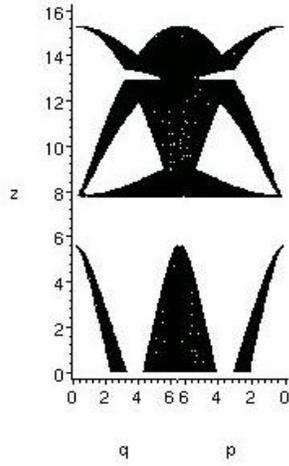
**Figure 3:** A projection of the surfaces a)  $E = E_1(p, q)$  on the plane  $p=q$  and b)  $E = E_2(x, y)$  where  $x = \cos p$  and  $y = \cos q$  on the plane  $x = y$  with  $T = 1$  and  $0 < E \leq 30$ .



**Figure 4:** The surface  $z = -E_1(p, q)$  with  $T = 1$ .



**Figure 5:** The surface  $z = -E_2(p, q)$  with  $T = 1$ .



**Figure 6:** A projection of the surface  $z = -E_2(p, q)$  with  $T = 0.1$  and  $0 < z \leq 16$  on the plane  $p = q$ .