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Pauliina Uusitalo

THE BOUND STATES IN THE QUANTUM WAVEGUIDES OF SHAPE Y, Z, AND C

UNIVERSITY OF OULU GRADUATE SCHOOL;
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FACULTY OF INFORMATION TECHNOLOGY AND ELECTRICAL ENGINEERING

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Abstract

In this thesis, we study quantum waveguides and their spectral properties. A quantum waveguide is a system of narrow strips or tubes. That is, the waveguide has large longitudinal but small transverse sizes. The study of quantum waveguides is essential in the semi-conductor industry, and the waveguides are used to model the electron behavior in these devices.

We consider two- and three-dimensional waveguides with sharp bends and question whether the quantum particle can propagate in the waveguide. It is well known that a certain type of bends and bulges cause the resonance phenomena, that is, at some energy levels the electron motion is localized in a finite area, and the propagation is disturbed. The study of waveguides leads to the interesting field of mathematics - the spectral analysis of differential operators. For a waveguide having high purity and a crystalline structure, the electron motion can be considered as a free particle motion with effective mass. This gives rise to the spectral problem, that is, the eigenvalue problem of the Laplace operator. On the boundary we set the Dirichlet conditions.

This thesis consists of three parts and in each part we study waveguides which form sharp bends in the junctions where two or three outlets are joined together. To be precise, we consider waveguides which resemble the letters Y, Z, and C. We study the discrete spectrum corresponding to these waveguides and the behavior of the bound modes when the geometry is slightly changed. For this, we apply the variational, numerical, and asymptotic methods.

For the Y-shaped waveguide, we let one outlet become wider than the others and found that a critical width exists, so that for smaller width values, exactly one bound state exists, but for larger values, no bound modes exist. We also let the angle between the strips to vary and found that the number of the bound modes highly depends on the opening angle of the outlets in the Y-shaped waveguide.

For the Z- and C-shaped waveguides, we let the height of the waveguide change. We saw that there may appear two bound states at most. Moreover, for the C-shaped waveguide, the first is monotone increasing as a function of height and the second eigenvalue is monotone decreasing. For the Z-shaped waveguide, we show that the lowest eigenvalue as a function of the height is not monotone.

Keywords: bound state, quantum waveguide, spectrum

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Tiivistelmä

Tässä väitöskirjassa tutkitaan kvanttiaaltojohteisiin liittyvää ominaisarvo-ongelmaa. Kvanttiaaltojohteessa aallon eteneminen on rajoitettu tiettyyn suuntaan, ja johde on poikittaissuunnassa nanokokoluokkaa. Kvanttiaaltojohteiden tutkimus on tärkeä osa nykyistä puolijohdeteknologiaa.

Tutkimuksessamme olemme keskittyneet kaksi- ja kolmiulotteisiin aaltojohteisiin, jotka geometrialtaan muistuttavat Y-, Z- tai C-kirjainta. Haluamme tietää millaisissa tilanteissa elektronin liike aaltojohteessa estyy. Yleisesti tiedetään, että aaltojohteessa olevat pullistumat ja mutkat johtavat niin sanottuun sidottuun tilaan, ts. tilanteeseen että tietyllä taajuudella tai energiatasolla oleva partikkeli jää lokalisoituun tilaan.

Aaltojohde rakentuu puhtaasta kiderakennemateriaalista, joka on kokoluokaltaan pieni poikittaissuunnassa, niin että elektronin liikettä voidaan kuvata vapaan elektronin mallilla Schrödingerin yhtälössä, jossa elektronilla on effektiivinen massa. Tämä johtaa Laplace-operaattorin ominaisarvo-ongelmaan, reunaehtoina on aaltojohteille käytetty Dirichlet nollareuna-arvoja. Tässä väitöstutkimuksessa on tutkittu kolmea erityyppistä aaltojohdetta, joiden geometriaa voidaan kuvata kirjainten Y, C ja Z avulla. Jokaisessa tapauksessa on tutkittu spektristä erityisesti diskreettiä osaa, ja erityisesti mahdollisia muutoksia diskreetissä spektrissä geometristen parametrien muuttuessa. Diskreetin spektrin tutkimiseen on käytetty variaatiomenetelmiä, asymptoottista analyysiä sekä numeerisista menetelmistä elementtimenetelmää.

Geometrialtaan kirjainta Y muistuttava aaltojohde koostuu kolmesta haarasta, joista yhden leveyden annetaan varioida. Tällöin voidaan löytää kriittinen raja, siten että jalan leveyden ollessa tätä rajaa pienempi on diskreetti spektri epätyhjä kun taas leveyden ollessa kriittistä rajaa suurempi, diskreetti spektri on tyhjä. Toisessa tapauksessa jalan leveydet pidetään samana, mutta annetaan kulman kahden haaran välillä muuttua. Voidaan nähdä, että diskreetissä spektrissä olevien ominaisarvojen lukumäärä riippuu aaltojohteen kulmasta siten että mitä pienempi kulma kahden haaran välillä, sitä enemmän ominaisarvoja on diskreetissä spektrissä.

Vastaavasti Z- ja C- aaltojohteissa, aaltojohteen korkeutta säädellään. Havaitaan, että korkeuden kasvaessa, voi aaltojohteessa esiintyä korkeintaan kaksi ominaisarvoa diskreetissä spektrissä. Lisäksi C-aaltojohteen ensimmäisen ominaisarvon voidaan havaita olevan kasvava aaltojohteen korkeuden funktiona kun taas toinen ominaisarvoista on vähenevä. Toisaalta taas Z-aaltojohteen pienin ominaisarvo korkeuden funktiona ei ole monotoninen.

Asiasanat: kvanttiaaltojohde, sidottu moodi, spektri

to my children

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Finally, I thank my family for their love and support.

List of original publications

This thesis consists of the following publications, which are referred to in the text by their Roman numerals (I–III):

I S. A. Nazarov, K. Ruotsalainen and P. Uusitalo, The Y-junction of quantum waveguides. Z. angew. Math. Mech. **94**(6) 477–486 (2014). doi: 10.1002/zamm.201200255

II P. Uusitalo, The bound states of 3D Y-junction waveguides, Ann. Acad. Sci. Fennicae 40(1), 329–341 (2015). doi: 10.5186/aasfm.2015.4023

III S. A. Nazarov, K. Ruotsalainen and P. Uusitalo, Bound states of waveguides with two right-angled bends, J. Math. Phys. 56, 021505 (2015). doi: 10.1063/1.4907559

Author's Contribution

- Publication I: Substantial part of writing and making the analysis.
- Publication II: Independent work by the author.
- Publication III: Substantial part of writing and making the analysis.

Contents

1 Introduction

Waveguides are systems to guide and transport waves. Such type of waveguides are, for example, water and acoustic channels, electromagnetic and quantum waveguides, for which we base this study on. According to the name, quantum waveguides have dimensions small enough that quantum effects dominate their electronic behavior.

The motivation to study quantum waveguides comes from the technical applications, where the importance to build nanometer-sized electronic devices is substantial. In particular, the need for building smaller and smaller gadgets has been a launch pad to the study of quantum waveguides. These kind of devices are important in electrical applications, because of their fast response, low consumption and small weight.

The aim is to study the propagation of the electron (or any other quantum particle) in the waveguide. It is assumed that these waveguides, in addition to small size, have a crystalline structure and high purity. Therefore, the scattering is unsubstantial, and this drives us to model the electron motion as a free particle in the infinite waveguide. A quantum waveguide can be built, for example, by combining different semiconductor materials. The wavefunction is restrained between the interfaces of these materials, and we set the zero Dirichlet condition on the boundaries. Thus, the problem can be modeled by a spectral Dirichlet boundary value problem for the Laplace operator.

The theory of self-adjoint operators in the Hilbert space indicates that the spectrum, σ, of the Laplace operator is a union of two disjoint sets, that is,

$$\sigma = \sigma_e \cup \sigma_d,$$

where σ_d is called a discrete spectrum, a set of the isolated eigenvalues of finite multiplicity. The essential spectrum, σ_e, contains the continuous spectrum, the eigenvalues of infinite multiplicity, and accumulation points (see [6, §3.7, §6.1, §9.1]). The essential spectrum of the operator is a closed set. This set can be as it is for example in papers I-III – a closed interval $\sigma_e = [\lambda_\dagger, \infty)$, where $\lambda_\dagger > 0$ is called a threshold. However, there exists, periodic waveguides and domains for which the essential spectrum is union of closed segments, and gaps, free of spectrum, may appear between these segments. This type of waveguides are studied, for example, in [39, 53].

The continuous spectrum is an energy band where electronic transport can occur, and these generalized eigenfunctions are often called propagating modes. Conversely, an eigenfunction u corresponding to the eigenvalue $\lambda \in \sigma_d$ belongs to the Sobolev space

$H_0^1(\Omega)$ and decays at infinity. These solutions are called localized waves or bound states. For these solutions, the probability of finding the particle is concentrated in a finite volume.

An electron at the energy of a bound mode does not move through the waveguide and strongly reduces the conductivity. The presence of such modes substantially changes the transmission properties, and therefore, an understanding of these modes is required for describing microelectronic, microwave, and optical systems.

For example, for the planar straight strip of constant unit width, $\sigma_e = [\pi^2, \infty)$, while the discrete spectrum is empty. Even a small perturbation, however, changes the situation, that is, any bulge, smooth or sharp bending of the equidistant strip causes the appearance of an eigenvalue in the discrete spectrum, see Fig. 1.

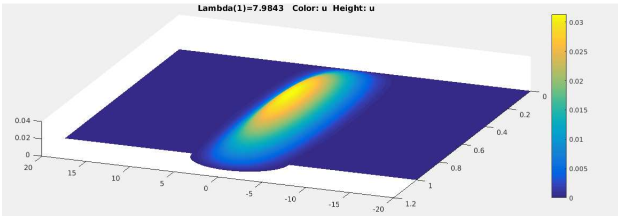

Fig. 1. The localized mode in the strip of unit width having small bulge.

Although we study quantum waveguides, for the acoustic channel with soft walls (i.e. Dirichlet boundary condition), the approach is the same. The bound states are then the vibration modes. In the Helmholtz equation

$$\Delta u + \lambda u = 0,$$

the spectral parameter has a naturally different physical meaning, in the case of the quantum waveguide, the parameter λ follows from the Hamiltonian and is $\lambda = \frac{2mE}{\hbar}$. For the acoustic channel, the parameter is then $\lambda = \frac{\omega^2}{c^2}$, where ω is the angular frequency and c – the speed of sound.

In the case of an acoustic waveguide with hard walls, the Dirichlet boundary conditions are replaced by the Neumann conditions. Then, the threshold of the essential spectrum is $\mu_\dagger = 0$, and clearly, there cannot be eigenvalues below the essential spectrum. However, localized modes belonging to the continuum may appear. For example, if the waveguide has an obstacle and is symmetric along the longitudinal axis, setting the Dirichlet condition along this axis, one can find so-called embedded modes, see e.g. [15, 17].

Moreover, setting the artificial Dirichlet conditions along the longitudinal axis for waveguides with Dirichlet boundary conditions may let one to find the embedded modes belonging to the continuum. Such an odd-parity mode was found in [48] for the cross-shaped waveguide, where the Dirichlet conditions were posed along the symmetry lines (see also [7, 36]). Also, localized modes can appear in the compressed waveguides; for example, consider a quantum waveguide of unit width and squeeze small parts from the strip, so that two small narrows arise. Then, the discrete spectrum is empty, but a localized mode may appear having its support between the narrows, see [5] and Fig. 2. In practice, all waveguides are of finite length, and therefore, these localized modes are in practice leaky modes, which propagate with small amplitude along the cylinders.

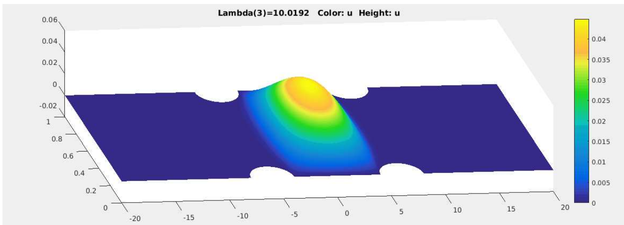

Fig. 2. The localized wave in the straight waveguide with two narrows.

The eigenvalue problems on the bounded regions with Neumann, Dirichlet, and Robin boundary conditions have been widely studied. The spectrum is purely discrete and, for some regions in particular, that is, for certain quadrilateral, triangular, and circular domains, the eigenvalues with the eigenfunctions can be thoroughly determined, see e.g. survey [24]. It should be noted that the existence of a localized eigenfunction may also appear in the bounded domains. The spectrum is purely discrete, but there may appear eigenfunctions whose support is located only in a small part of the region.

1.1 Background and research environment

The first examples of the existence of the trapped modes in unbounded media were made concerning the water channels. The existence of the trapped modes in surface water waves on channels was represented by Ursell in 1951, [49], and a few years later by Jones in [29]. For the acoustic waveguide, the experimental results of trapped modes were given by Parker [44] in 1966.

The pioneering work of the existence of bound states in the electromagnetic waveguides was carried out by Maslov in 1958, [32]. He considered a thin strip and found an asymptotic expression for the wave function corresponding to a bound state. In the work [18] of Exner and Šeba, it was shown that for a very narrow two-dimensional smoothly bend quantum waveguide, for which the curvature vanishes fast enough, the discrete spectrum is not empty. By the variational arguments, Goldstone and Jaffe had the same results concerning both two- and three-dimensional tubes, see [23], but without the restriction of the strip to be narrow, only of constant width. These results were improved, for example, in papers [47] and [16], where more general shapes were accepted, namely the curvature of the waveguide needed not be differentiable, and angular points were accepted.

The waveguides with angular points, especially the V- and L-shaped waveguides are extensively studied. The L-shaped waveguide was studied in [19] via the mode-matching technique, in other words, the domain was decomposed into subdomains and in each of these subdomains, the problem was solved by the separation of variables and required that the solutions fulfill the interface conditions between the subdomains. It was indicated that exactly one eigenvalue exists below the essential spectrum. This eigenvalue was computed to be approximately $0.93\pi^2$ for the L-shaped waveguide of unit width. Moreover, in paper [11], the bound state energy for the opening angle $\alpha = \frac{\pi}{2}$ with many other angles were found through experiments.

It was shown in [16] that when the tube of constant cross-section is slightly bent, only one bound state can appear. However, when the angle is small enough, it is possible to find even several eigenvalues below the threshold of the essential spectrum. Avishai with his co-workers showed that by setting a suitable rectangle inside the bend so that it has eigenvalues below the threshold $\lambda_\dagger$, by the domain monotonicity, at least the same number of eigenvalues lie in the discrete spectrum of the sharply bent waveguide (see [2]). In particular, a more detailed study was performed by Nazarov and Shanin in [43]. They found the critical angle α_*, so that if the angle is smaller than this critical value, the number of eigenvalues in the discrete spectrum exceeds one. Moreover, the asymptotic lower bound for the number of eigenvalues in the discrete spectrum was estimated as $\alpha \to +0$. The formal asymptotics for the eigenvalues as $\alpha \to +0$ were introduced in [13].

Most of the studies have concentrated on the waveguides in which the cross-sections in each branch remain the same outside the bend. The threshold $\lambda_\dagger$ of the essential spectrum crucially depends on the cross-section of the cylinder. That is, it is inversely proportional to the square of the area of the widest cylinder. Thus, when one branch widens and the rest remains of unit width, the essential spectrum occupies a larger interval which in turn means that the discrete spectrum may be located in a smaller interval.

This type of waveguides was studied, for example, in [37, 42], where a T-shaped waveguide was considered. The waveguide was composed of a strip of unit width and a semi-strip of width $H > 0$ perpendicular to the unit width strip. It was shown that there is a critical width H_*, so that whenever the widest branch is less than H_*, exactly one eigenvalue in the discrete spectrum appears, while for $H \geq H_*$, the discrete spectrum is empty. A similar approach was made in [36], where the cross-shaped waveguide with different branch width was explored.

In proportion, in [9], the problem of the domain of two semi-strips of slightly different widths connected by a small smooth bulge was studied, and the sufficient condition for the non-emptiness of the discrete spectrum was presented.

Systems with multiple bends have received much less attention. In [16], it was conjectured that if the bends are separated, so that the distance between the bends is large enough, a bound state exists associated with each bend. The double bend waveguides (as in III also) were studied in [10, 52]. These types of studies seem to be rare, except in the cases where the waveguide generates a periodic system, see e.g. [4, 39]. In the former, the band structure of the spectrum in the cross-shaped periodic waveguide and, in the latter, in the honeycomb-structure is studied. Moreover, in the latter, the periodicity cell is composed of two Y-shaped parts connected to each other, while in the former the periodicity cell is composed of T-shaped parts.

1.1.1 Physical Background

The electrons moving through the waveguide interact with the lattice atoms, impurities, boundaries, and external fields. Quantum waveguides are systems where the cross-sectional diameter is only up to some ten or hundred nanometers. The semiconductor material has a crystalline structure, and it is assumed that the material has high purity, so that the electron mean free path can even be some micrometers. Under these circumstances, electrons move in the lattice as free particles, only interacting with the boundaries. The influence of the lattice atoms and other electrons, that is, the potential caused by the lattice, can be neglected by replacing the mass of the electron m_e in the free particle Hamiltonian by the effective mass m^*, see e.g. [45]. The effective mass depends on the semiconductor materials; for Silicon (Si), the effective mass is $1.06m_e - 1.09m_e$, (depending on the temperature), while for Gallium Arsenide (GaAs), which is a typical semiconductor material, the effective mass is $0.067m_e$, (see e.g. [25, 34]).

The energy of the electron in the waveguide is

$$E = E_T + E_L,$$

where E_T is transverse, and E_L– longitudinal motion energy. The transverse motion energy is inversely proportional to the square of the cross-section. Thus, as the cross-section varies along the waveguide, the transverse motion and, therefore, also the longitudinal energy of the electron is changed. The cross-section of the junction (or the bulge) is larger than the cross-section of the branch, and therefore, the transverse energy in the branches is greater than in the junction. At the same time, since the total energy of the electron must remain the same, the longitudinal motion energy in the branches is decreased. Thus, the wave function may be trapped in the junction, and the electron transport is then disturbed (see e.g. [5]).

The same result is valid in the curved tubes with constant cross-section (see [23]). The bend itself allows for the increase of transverse energy, and this causes the waves to decay when being far from the junction.

1.2 Objectives and scope

In papers I-III, the sharply bent waveguide of the shape of letters Y, C, and Z is considered (see Figures 3 and 5). As discussed in Section 1.1, the width of the branches, also called arms, the number of bends, and the magnitude of the opening angle between the branches, have an impact on the structure of the discrete spectrum.

The natural question is to study under which circumstances the discrete spectrum is empty. For example, for the T-shaped waveguide mentioned in Section 1.1, the discrete spectrum is empty whenever the width of the widest branch is greater than $H_* \approx 1.35$.

Moreover, we examine whether there is only one or several eigenvalues belonging to the discrete spectrum, and furthermore, how the changes in the geometric parameters affect these eigenvalues. That is, does the number of eigenvalues in the discrete spectrum change? Does the eigenvalue increase or decrease as a function of this geometric parameter? These questions are motivated by the studies of the cranked V-shaped waveguides [43], where it has been shown how the eigenvalues in the discrete spectrum as a function of α, the magnitude of the opening angle, are monotone increasing.

In III, we let the height of the Z-shaped waveguide tend to 1, which means that the waveguide becomes a straight strip. The question about the behavior of the eigenvalue close to the limiting case $L \to 1+0$ is answered by computing the two-term asymptotics of the first eigenvalue. Similarly, the asymptotics of the first two eigenvalues, when the height tends infinity, are constructed.

2 Theoretical foundation

2.1 Operator formulation

Let $L^2(\Omega)$ be the usual space of square-integrable functions on $\Omega \subset \mathbb{R}^n$, and m – a non-negative integer. The Sobolev space $H^m(\Omega)$ (see e.g. [1]) is

$$H^m(\Omega) = \left\{u : \partial^\alpha u \in L^2(\Omega),\ |\alpha| \le m\right\}.$$

Here, $\partial^{|\alpha|} = \partial_1^{\alpha_1} \cdots \partial_n^{\alpha_n}$ with $\partial_j = \frac{\partial}{\partial x_j}$ and $|\alpha| = \alpha_1 + \cdots + \alpha_n$, where each α_j is a non-negative integer. Moreover, the space $H_0^1(\Omega)$ is the closure of $C_0^\infty(\Omega)$ in $H^1(\Omega)$, where $C_0^\infty(\Omega)$ is the space of infinitely differentiable functions having a compact support in Ω.

Let us consider the spectral Dirichlet boundary value problem for the Laplace operator:

$$\begin{aligned} -\Delta u &= \lambda u, \quad x \in \Omega, && (1)\\ u &= 0, \quad\ \ x \in \partial\Omega. && (2) \end{aligned}$$

Here, $\Omega \subset \mathbb{R}^n$, $n = 2,3$ is unbounded at least in one direction. It is often useful to study the problem in its variational form. That is, we multiply the equation (1) by a test function $v \in H_0^1(\Omega)$ and use Green's second identity with the given Dirichlet boundary condition (2) to derive

$$a(u,v) = \lambda b(u,v), \tag{3}$$

where a and b are bilinear forms defined by

$$\begin{aligned} a &: H_0^1(\Omega) \times H_0^1(\Omega) \to \mathbb{C}, \quad a(u,v) = \int_\Omega \nabla u \nabla \bar{v}\, \mathrm{d}x,\\ b &: L^2(\Omega) \times L^2(\Omega) \to \mathbb{C}, \quad\ \ b(u,v) = \int_\Omega u\bar{v}\, \mathrm{d}x. \end{aligned}$$

By [6, §10], each closed positive definite form is associated with a unique positive definite self-adjoint operator. Thus, the eigenvalue problem (1)-(2) is associated with an unbounded positive definite and self-adjoint operator A on the Hilbert space $L^2(\Omega)$.

2.2 The angular points on the boundary of the domain Ω

For the smooth boundary of the domain Ω, the domain $\mathscr{D}(A)$ of the Dirichlet-Laplacian is the space $H^2(\Omega) \cap H_0^1(\Omega)$, see for example [38]. When the boundary has some angular points, the solution may belong to the wider class of functions.

Due to the angular points, the solution is decomposed into a regular and a singular part, and the domain $\mathscr{D}(A)$ of operator A is

$$\mathscr{D}(A) = H^2(\Omega) \cap H_0^1(\Omega) \oplus \left\{ \chi(r_i) r_i^{\pi/\alpha} \sin\left(\frac{\pi}{\alpha}\phi_i\right) \right\}_i . \tag{4}$$

Here, (r_i, ϕ_i) is the polar coordinate system located at the non-convex angular point, and $\chi(r_i)$ is a smooth cut-off function with the value 1 for $|r_i| < \frac{1}{4}$ and vanishing for $|r_i| > \frac{1}{2}$. If at the point with the strongest singularity, the angle α is greater than π, then the second derivative of $r^{\pi/\alpha}$ will not be square-integrable, and therefore, the domain $\mathscr{D}(A)$ is wider than the space $H^2(\Omega) \cap H_0^1(\Omega)$.

The formulation (4) for the domain $\mathscr{D}(A)$ of operator A is based on the Kondratiev theory [31], (see also [26]) to ensure the behavior of the solution to be well-defined, even in the neighborhood of the boundary singularities.

2.3 Spectrum $\sigma(A)$ of the operator A

We follow the definition of the spectrum given in [6]. First, since operator A is self-adjoint and positive definite, the spectrum $\sigma(A) \subset \mathbb{R}_+$. The spectrum can be divided into several parts as follows.

Let $\mathrm{Ker}(A)$ be the null-space, and $\mathrm{R}(A)$ – the range of operator A. The point spectrum $\sigma_p(A)$ is defined as

$$\sigma_p(A) = \{\lambda \in \mathbb{R}_+ : \mathrm{Ker}(A - \lambda I) \neq \{0\}\}.$$

That is, the set of λ's for which there exists non-trivial $u \in \mathscr{D}(A)$, so that $Au = \lambda u$. The continuous spectrum $\sigma_c(A)$ is the set

$$\sigma_c(A) = \left\{ \lambda \in \mathbb{R}_+ : \mathrm{R}(A - \lambda I) \neq \overline{\mathrm{R}(A - \lambda I)} \right\}.$$

The essential spectrum $\sigma_e(A)$ is the union of the continuous spectrum, the eigenvalues from the point spectrum of infinite multiplicity, and accumulation points. The discrete spectrum $\sigma_d(A)$ is

$$\sigma_d(A) = \sigma(A) \setminus \sigma_e(A).$$

The following inclusions hold for the Dirichlet-Laplacian:

$$\sigma_d(A) \subset \sigma_p(A) \text{ and } \sigma_p(A) \setminus \sigma_d(A) \subset \sigma_c(A).$$

Since the domain Ω is unbounded, the embedding $H_0^1(\Omega) \subset L_2(\Omega)$ is not compact, and therefore, the spectrum of operator A has a non-empty continuous part. On the domain Ω with cylindrical outlets, that is, outside a ball of radius $R > 0$, the domain coincides with finite number of cylinders $\Pi_i,\ i = 1, \ldots, N$. In the local Cartesian system, the outlet is $\Pi_i = \omega_i \times \mathbb{R}$, where ω_i is the cross-section of the cylinder. The essential spectrum of operator A covers the ray

$$\sigma_e(A) = [\lambda_\dagger, +\infty),\ \text{where } \lambda_\dagger = \min_i \{\mu_i\},$$

and μ_i is the first eigenvalue of the Laplacian under the Dirichlet condition on ω_i.

2.4 Variational methods

The lower bound of the spectrum is found by

$$\underline{\sigma(A)} = \inf_{u \in H_0^1(\Omega)} \frac{\left\|\nabla u; L^2(\Omega)\right\|^2}{\left\|u; L^2(\Omega)\right\|^2}, \tag{5}$$

and by the max-min principle the nth eigenvalue belonging to the interval $(0, \lambda_\dagger)$ is

$$\lambda_n = \max_{E_n} \min_{u \in E_n \setminus \{0\}} \frac{\left\|\nabla u; L^2(\Omega)\right\|^2}{\left\|u; L^2(\Omega)\right\|^2}, \tag{6}$$

where E_n is a subspace of $H_0^1(\Omega)$ with co-dimension $n-1$, see [6, §10].

By finding a suitable test function, one can show the non-emptiness of the discrete spectrum, see e.g. [35] and III. That is, one builds up a function belonging to the space $H_0^1(\Omega)$ for which the right hand side of (5) is less than $\lambda_\dagger$, and hence, $\underline{\sigma(A)} \in \sigma_d(A)$.

For the Laplace eigenvalue problem under the Dirichlet boundary condition, so-called domain monotonicity (or comparison principle) holds, see e.g. [12, 54]. That is, the eigenvalues do not increase as the domain enlarges

$$\lambda_n(\Omega_0) \geq \lambda_n(\Omega) \text{ when } \Omega_0 \subseteq \Omega.$$

2.5 Finite element method

In several parts of the research, the numerical computations were introduced. Namely, we employ the finite element method for finding the estimates to the eigenvalues belonging to the discrete spectrum.

Let V_N be a finite-dimensional subspace of $H_0^1(\Omega)$, where $V_N = \text{span}\{\phi_1, \dots, \phi_N\}$. Then, the generalized eigenvalue problem is: find λ_h and u_h so that

$$Ku_h = \lambda_h M u_h,$$

where $K = [a(\phi_j, \phi_k)]_{j,k=1}^N$ is the stiffness and $M = [b(\phi_j, \phi_k)]_{j,k=1}^N$ – the mass matrix.

Since the domain Ω is unbounded, we truncate the waveguide into a bounded region $\Omega(R)$, where the branch length $R > 0$ is chosen as large enough. Since the bound state eigenfunction decays exponentially fast, the difference between λ_j and λ_j^R (corresponding to the problem in Ω and $\Omega(R)$, respectively) is small. More precisely, the difference is exponentially small and depends on the length R and on the difference between the searched eigenvalue λ_j and the threshold $\lambda_\dagger$. In addition, the significance of the posed boundary conditions on the ends of the outlets of the truncated domain is insubstantial, and therefore, we set Dirichlet boundary conditions on the entire boundary of $\Omega(R)$. Due to the comparison principle,

$$\lambda_j^R \geq \lambda_j,$$

and since the corresponding eigenfunctions decay exponentially fast, we obtain

$$\lambda_j^R < \lambda_\dagger,$$

when R is chosen to be large enough.

By the general theory of the finite element method, see e.g. [3], the convergence rate depends on the regularity of the eigenfunctions and the mesh size h. The approximate eigenvalue $\lambda_{j,h}^R$ satisfies the following inequality:

$$\lambda_j \leq \lambda_j^R \leq \lambda_{j,h}^R \leq \lambda_j^R + C\left(\lambda_j^R\right) h^{2\tau},$$

where $\tau \in (0,1]$ is a parameter which characterizes the regularity near the non-convex points of the domain $\Omega(R)$. Thus, since the singularity decreases the rate of convergence, more accurate solutions are obtained for example by refining the mesh in the neighborhood of the re-entrant corners.

Instead of using the Dirichlet condition on the boundaries of the truncated waveguide (as used in papers I and III), one may use for example Dirichlet to Neumann mapping, see e.g. [21] and [22]. The unbounded domain is split into a bounded region, where the computation is made, and into unbounded cylinders of constant cross-section. Between these disjoint domains, the artificial boundary conditions are defined by the relation between the unknown solution and its derivatives. The advantage of this is that the computation is less expensive, since the computations are made in a small region. However, one needs very specific boundary conditions on these boundaries. Since in the papers I and III the branches were long enough, and the decay of the eigenfunction is fast, the Dirichlet conditions on the outlets are sufficient.

2.6 Asymptotic analysis

The perturbation methods (see [30, 46]) are used to find the approximate solution for the problems, which slightly differ from a problem for which the solution is known. Consider an operator of the form

$$A(\varepsilon) = A + \varepsilon A',$$

where $0 < \varepsilon \ll 1$ is a small parameter, and $A(0) = A$ is the unperturbed operator, while $\varepsilon A'$ is the perturbation. The asymptotics of the eigenfunctions and eigenvalues belonging to the discrete spectrum may be found with the help of the formal asymptotic expansions. The two-term asymptotic expansion are

$$\begin{aligned} \lambda^{\varepsilon} &= \lambda + \varepsilon^{\alpha_1} \lambda' + \ldots, \\ u^{\varepsilon}(x) &= u(x) + \varepsilon^{\beta_1} v_1(x) + \ldots, \end{aligned}$$

where the pair $(\lambda,\ u)$ is the principal part, the solution of the limit problem ($\varepsilon = 0$), and the dots stand for the higher order terms. Moreover, λ is assumed to belong to the discrete spectrum. The second terms are multiplied with the integer or fractional power of ε.

Here, we consider the two-term asymptotic expansions, but the higher order terms are applied analogously. The second terms in the asymptotic series compensate the discrepancy between the limit and perturbed problem. Substituting the formal asymptotic solution into the problem and comparing the terms with equal power of ε, the coefficient λ' and the function $v_1(x)$ in the expansion can be solved.

In paper III, we consider singularly perturbed domain $\Omega(\varepsilon)$. The boundary may not be smooth even in the limit case. There are two methods to construct the expansion. These are the method of matched asymptotic [27, 50] and the method of compound asymptotic [5, 33, 51] expansions. In III, the former method is used for example during the study of the limiting case $L \to 1+0$.

In the method of matched asymptotic expansions [27, 50], one builds different asymptotic solutions concerning the inner and outer parts of the domain. In general, one takes new stretched inner variables $X = \frac{x}{\varepsilon}$ to find the solution close to the perturbed region, while for the outer solution, one uses the regular variables x. The inner solution is not valid in the outer zone and vice versa, but the solutions must coincide in some intermediate zone, connecting the inner and outer zones. Thus, the coefficients of the terms can be determined.

3 Results

The main results of papers I-III are summarized below. In each paper, the geometry of the waveguide is different, and these are illustrated in Figures 3 and 5. The main goal is to answer the question of how the geometry and small variations of the waveguide change the discrete spectrum. We also consider the eigenvalues belonging to the discrete spectrum as a function of some geometric parameter and study the monotonicity under the variations of the geometry.

3.1 Summary of findings

In paper I, the Y-shaped waveguide depicted in Fig. 3a is investigated. The waveguide is composed of three semi-strips, two of them having unit width, while for the lower semi-strip, the width is $H > 0$. The angle between the strips is fixed to be $2\pi/3$. The main result is the following.

Theorem 3.1.1. *There exists a critical width H_* so that for $H < H_*$, exactly one eigenvalue lies in the discrete spectrum; meanwhile, for $H \geq H_*$, the discrete spectrum is empty.*

Numerical results show that the critical width $H_* \approx 1.25$.

In II, the discrete spectrum of a three-dimensional Y-shaped waveguide is explored. The cross-sections of the cylinders are either squares with the unit side length or circles of radius $\frac{1}{2}$. Contrary to paper I, the outlets have constant width, but the angle 2α between two branches is not fixed and, therefore, $\alpha \in (0, \pi/2]$.

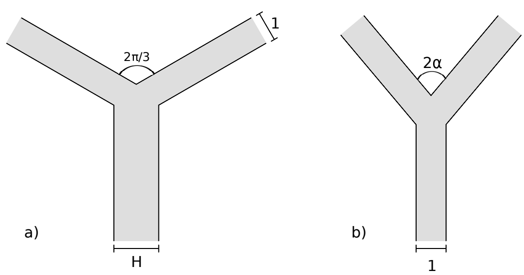

Fig. 3. The Y-shaped waveguide $\mathbb{Y}^H$ and $\mathbb{Y}^\alpha$, respectively.

For the waveguide with rectangular cylinders, the following results were obtained. Since in the rectangular case, the result is a consequence of the separation of variables, we obtain the same results for the two-dimensional waveguide as well.

Theorem 3.1.2. *The function* $\alpha \mapsto \lambda_p^\alpha$ *is strictly increasing when* $0 < \alpha \leq \pi/3$, *and strictly decreasing when* $\pi/3 < \alpha \leq \pi/2$.

Theorem 3.1.3. *There is a critical value* $\alpha_* \in (0, \arctan(3/4))$, *so that exactly one eigenvalue is located in the discrete spectrum when* $\alpha > \alpha_*$. *Moreover, when* $\alpha \leq \alpha_*$ *the number of eigenvalues belonging to the discrete spectrum exceeds one.*

In the case of the cross-section of the branches being a circle of radius $\frac{1}{2}$, the above result given in Theorem 3.1.3 is weaker. That is, there is exactly one eigenvalue in the discrete spectrum when $\alpha \in (0.326\pi, 0.342\pi)$. Thus, the critical value α_* belongs to the interval $(0, 0.326\pi)$.

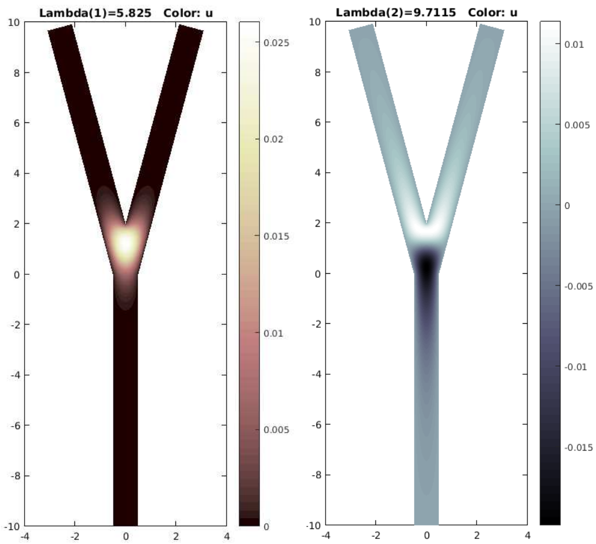

Fig. 4. The first and second eigenvalue of the Y-shaped waveguide with $\alpha = \frac{\pi}{12}$**.**

In III, the waveguides of two right-angled bends are studied. These waveguides form a shape of letter Z or C, see Fig. 5. This type of waveguides are composed of a rectangle with width H and height L and two semi-strips of unit widths connected to the rectangle. The parameters H and L vary and give rise to changes in the discrete spectrum. Here, in this summary, we set $H = 1$, while height L varies. The following results were obtained.

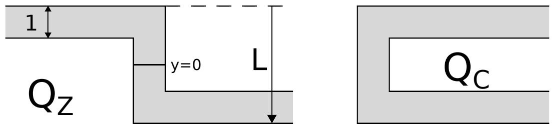

Fig. 5. The Z- and C-shaped waveguides, Q_Z and Q_C, respectively.

Theorem 3.1.4. *The number of eigenvalues in the discrete spectrum $\sigma_d(Q_Z)$ and $\sigma_d(Q_C)$ cannot exceed two.*

By the finite element method, we find that whenever $L \geq L_* \approx 2.55$, the number of eigenvalues belonging to the discrete spectrum equals two. We denote the first and second eigenvalue in $\sigma_d(Q_C)$ by $\lambda^N(L)$ and $\lambda^D(L)$ (here N and D stand for Neumann and Dirichlet, respectively). Similarly, the eigenvalues belonging to $\sigma_d(Q_Z)$ are denoted by $\lambda^S(L)$ and $\lambda^A(L)$ (i.e. symmetry and anti-symmetry). We obtain the following result.

Theorem 3.1.5. *Let $L \geq 2$. Then,*

$$\lambda^D(L) > \lambda^A(L) > \lambda^S(L) > \lambda^N(L).$$

In the absence of $\lambda^D(L)$ or both $\lambda^D(L)$ and $\lambda^A(L)$, all remaining inequalities hold.

For the C-shaped waveguide, these eigenvalues are shown to be monotone as functions of the height L.

Theorem 3.1.6. *The functions*

$$(2,\infty) \ni L \mapsto \lambda^P(L), \ P{=}N \text{ or } D$$

are monotone growing (P=N) and decreasing (P=D).

For the limit case in Q_Z as $L \to 1+0$ the first eigenvalue $\lambda^S(L)$ behaves as

$$\lambda^S(L) = \pi^2 - \pi^4(L-1)^2 + \mathscr{O}\left((L-1)^{\frac{5}{2}}\right). \tag{7}$$

As the height L tends to infinity, the eigenvalues differ only slightly from the eigenvalue of the L-shaped waveguide $\lambda_L \approx 0.93\pi^2$, and the split between these eigenvalues is exponentially small. That is,

$$\lambda^{\pm}(L) = \lambda_L \pm c\,\mathrm{e}^{-L\kappa} + \mathscr{O}\left(\mathrm{e}^{-2L\kappa}\right),$$

where $\kappa = \sqrt{\pi^2 - \lambda_L}$. Moreover, $\lambda^S(L)$ approaches λ_L from below, while $\lambda^A(L)$ approaches it from above. Therefore, for large L, the $\lambda^S(L)$ is increasing, and hence, by (7), the first eigenvalue of the Z-shaped waveguide is not monotone as a function of the height L.

3.1.1 Comparison with earlier work

As already discussed in Section 1, the question about the existence and the number of eigenvalues located in the discrete spectrum is dependent on the geometry of the waveguide, that is, the magnitude of the opening angle and the width of the branches. In the paper [16], it was seen that when the waveguide is slightly bent, there is only one eigenvalue in the discrete spectrum, and for the strongly bent waveguide, even more eigenvalues may appear. Furthermore, in papers [43] and [13], the number of eigenvalues are shown to be dependent on the inverse of the opening angle. In article I, the opening angle between the arms is large, and even though the waveguide is broken, the similar result given in [16] is valid. On the other hand, in paper II, where the opening angle is allowed to decrease, the number of bound states increases. This is analogous to the results of the broken V-shaped waveguides with a small opening angle.

In both studies [43] and [14], the monotonicity of the eigenvalues (or the Rayleigh quotient (6)) as a function of the angle in the V-shaped waveguides is shown. These conclusions coincide with the results given in paper II for $\alpha \in (0, \pi/3)$. Theorem 3.1.2 states that the lowest eigenvalue attains its maximum when angle $\alpha = \frac{\pi}{3}$. In paper [7], it is shown that for two straight waveguides which cross at the angle $\theta \in (0, \pi/2)$, the ground state is monotonously increasing as a function of the angle, and the maximum is attained when the system is symmetric. A similar result is obtained for the leaky star graphs with finitely many edges, that is, the maximum of the ground state is achieved when the star graph is fully symmetric, see [20].

Similarly to the study in I, in [37, 42], a T-shaped waveguide with different lower branch width was studied. The critical width was found to be $H_*^T \approx 1.35$. The reason for the difference of the values of the critical widths between the T-shaped and the Y-shaped waveguides follows from the fact that in the T-shaped waveguide, the bend is sharper than in the regular Y-shaped waveguide.

The Z-shaped waveguide of finite length was studied in [52]. It was shown by the mode-matching technique and numerical experiments that when the distance between the bends is large enough, there are two localized eigenfunctions, while for short distance, the number of localized eigenfunction is one. Our results in III concerning the unbounded Z-shaped waveguide, coincide with these results.

In [8], a planar strip of unit width with a small, smooth bulge was investigated. It was found that the asymptotic approximation for the first (and only) eigenvalue in the discrete spectrum is

$$\lambda(\varepsilon) = \pi^2 - \pi^4 |\Omega(\varepsilon) \setminus \Omega|^2 + \mathscr{O}\left(|\Omega(\varepsilon) \setminus \Omega|^3\right),$$

where $|\Omega(\varepsilon) \setminus \Omega|$ is the area of the bulge. In III, the perturbation is not local, but very similar asymptotics are obtained in formula (7), even though the Z-shaped waveguide does not satisfy the smoothness conditions. Corresponding results were obtained in [36], where the cross-shaped waveguides with lower semi-branch with width $h \to +0$ were investigated. Moreover, in paper [9], where the converging waveguide with a local small bulge was considered, the asymptotic expansion for the only eigenvalue located in the discrete spectrum is very similar to the results in [8] and (7).

3.2 Prospective studies

In the earlier studies concerning the Y-shaped waveguide, either the leg width or the angle between the arms changes. It would be interesting to study a case where both of these parameters vary simultaneously. Moreover, one may choose to study cases where each leg width would be slightly different, for example. The methods used in I-III can be applied to several different types of waveguides.

In each of these studies, we set the Dirichlet conditions on the boundary. Interesting results from applying Robin boundary conditions on a straight quantum waveguide are described in paper [28]. It was shown that under certain conditions, bound states appear. A study with a more complicated domains would be fascinating.

Furthermore, the results obtained for the Y-shaped waveguides can be used in a study of a hexagonal, double-periodic structure. Two Y-shaped models are connected to each other and define the periodicity cell. The main interest is to study the spectrum of a hexagonal graph when the width of the ligaments tends to zero. The asymptotics of the spectrum of the Dirichlet Laplacian is found in paper [39], see also papers [40] and [41].

For the Z-shaped waveguides, cases $L \to 1+0$ and $L \to \infty$ were examined. As was pointed out by the other pre-examiner it would be useful to study the case when $L \to 1-0$.

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