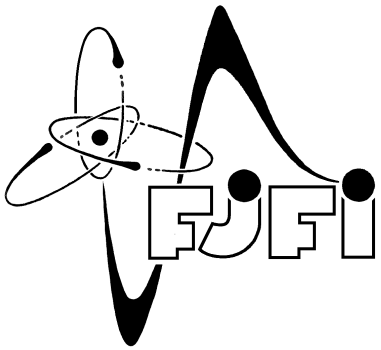
Czech Technical University in Prague
Faculty of Nuclear Sciences and Physical Engineering

Geometrically induced properties of the ground state of quantum mechanical Hamiltonians with contact interactions

Geometricky podmíněné vlastnosti základního stavu kvantově-mechanických hamiltoniánů s kontaktními interakcemi



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Prohlášení

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

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Abstract

In this work we discuss the ground state of Hamiltonians with contact interactions in dimension 1, 2 and 3. We study the relation between the ground state energy and the geometry of the support of the point interactions. We derive conditions under which the ground state energy increases with respect to the change of the geometry of the point interaction support. We show that for the systems with a simple topology such as a line, plane and three-dimensional Euclidian space, the increase in distance between point interaction sites results in an increase of the ground state energy. On the other hand, we show that this may not hold for systems with a more complex topology such as quantum graphs. We also present several examples of optimization of the ground state energy with respect to the position of the point interaction of systems with one point interaction and regular potential.

Key words

Point interaction operator, point interactions, ground state of the point interaction Hamiltonian, Krein's formula, generalized Birman-Schwinger formula, contact potential, quantum graphs

Abstrakt

V této práci se zabýváme Hamiltoniány s kontaktními potenciály v dimenzi 1, 2 a 3. Budeme zkoumat závislost mezi energií zakladního stavu a rozložením bodových interakcí v prostoru. Odvodíme podmínky, za kterých dojde ke zvýšení energie zakladního stavu v závislosti na změně vzájemné polohy bodových interakcí. Ukážeme, že pro systémy s jednoduchou topologií jako jsou přímka, rovina a třírozměrný Euklidovský prostor, zvýšení vzdálenosti mezi bodovými interakcemi vede ke zvýšení energie základního stavu. Dokážeme, že pro systémy se složitější topologií jako jsou kvantové grafy může být chování odlišné. Dále se budeme zabývat minimalizací energie základního stavu pro systémy jedné bodové interakce a regulárního potenciálu.

Klíčová slova

Operátor bodových interakcí, bodové interakce, základní stav operátoru bodových interakcí, Kreinova formule, zobecněná Birman-Schwingerova formule, kontaktní potenciál, kvantové grafy

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Chapter 1

Introduction

In this work we will discuss the properties of the ground state of several quantum systems. We will be interested in the ground state because it has natural importance as the most stable state with the lowest energy.

We will work with operators describing point interactions. These operators can be formally written as follows

$$\hat{H} = -\Delta + \sum_{y \in Y} \alpha_y \delta(x - y), \tag{1.1}$$

where $-\Delta$ denotes self-adjoint Laplacian with the domain $H^{2,2}(\mathbb{R}^d)$ for the dimension $d = 1, 2, 3$. Such an operator describes a quantum particle moving in the field of contact potentials placed at set of points Y in space with point interactions strengths α_y. These operators have the advantage that their spectral properties and scattering problem can be solved exactly. We can use them as approximations of more realistic physical systems, e.g. as description of short range interactions in atomic and nuclear physics, motion of nonrelativistic electron in crystal lattice of fixed atoms (so called Kronig-Penney model in solid state physics), propagation in dielectric media in electromagnetism, etc. A survey of such models is given in the monograph [1].

The next class of systems we will work with are quantum graphs. Under the term quantum graph we consider a graph, i.e. a finite number of edges connected into a network-like structure, equipped with a particular

differential operator. Quantum graphs can be used to describe one dimensional systems with more complex topological properties, where the particle is trapped on graph like structures. We will work with differential operator of the form

$$\hat{H} = -\Delta. \tag{1.2}$$

We need our operator to be self-adjoint. This is accomplished by introducing certain boundary conditions at the vertices. These conditions link the function values and values of first derivatives of the functions on the edges connected to each vertex. We will work with the conditions called attractive δ-coupling. Those conditions are generalization of point interactions on the line. These systems naturally occur as a simplification (due to reduction of dimension) of many models in mathematics and physics (for more details see [15]). They can be especially seen in situations where the wave moves though quasi one-dimensional systems, e.g. motion of a "free" electron in many systems in chemistry especially organic compounds, quantum chaos, quantum wires, theoretical model for nanotechnology, photonic crystals, etc. Quantum graph models have many advantages. Those include major simplification due to a reduction of the dimensionality, solvability of those systems by means of solving the spectral problem and scattering problem. Such simplification as are done with quantum graphs has also its drawbacks. The first one is the presence of parameters which describe how the functions are connected at the vertices. Another problem is the absence of tunneling outside the graph structure. Quantum graphs are discussed in great detail in the paper [7] or in the survey [9].

Next we will discuss systems where a singular potential is supported by a manifold of codimension one. The motivation for analyzing of such systems is twofold. The first one is that such an approach is a reasonable approximation for systems where the characteristic length of the particle, e.g. scattering length of the particle, is much larger then the range of the real interaction in the system. The second reason is the possibility of solving such models exactly. This is the result of the fact that the interaction support is "small" and outside of this support the free particle solution can be chosen leading so to an explicit solution. We will work with Hamiltonians which can be formally written as

$$\hat{H} = -\Delta - \mu(x)\delta(x - \Gamma), \tag{1.3}$$

where $\mu(x) > 0$ is a bounded positive function on the compact support Γ of

codimension one. We will work with such Hamiltonians in the dimension two and three. It is worth mentioning that for the dimension one the result we would obtain coincides with the point interaction on the line. These models can be used to describe so called "leaky" wires, where the particle is localized in the vicinity of Γ, however, with probability one in the classically forbidden region $\mathbb{R}^d \setminus \Gamma$, $d = 2, 3$. For more information we refer the reader to the paper [11] or to the review [12].

We will address one more topic concerning the ground state of Hamiltonians with a combination of a regular potential and a delta interaction in dimension one. The hamiltonian of such a system can be written as follows

$$\hat{H} = -\Delta + V(x) + \alpha\delta(x - y). \tag{1.4}$$

We will work with potential well, linear potential, monotonous potential and symmetric potential around point zero. Those models can be used to describe the system with the Hamiltonian in the form of $-\Delta + V(x)$ with either singular barrier added at the point y for the case of repulsive point interaction or a singular "well" for the case of attractive point interaction.

In our work we will be interested in the relation between geometry of the support of the singular interactions and the ground state energy. That is specifically, for point interactions we will look at the distances, for the quantum graphs the lengths of the edges. For the case of connected manifolds of the codimension one these are deformations maintaining the length of the curve or the area of the surface supporting the interaction. We consider Euclidian transformations of manifolds with respect to themselves for the case of separated manifolds. Finally for the point interaction and the potential we look at the position of point interaction with respect to the potential.

The reason we are interested in the ground state is the following. The ground state has a natural physical importance. While the isolated quantum system remains in a given state, in the real world we are not able to create a completely isolated system. Every system interacts with the surrounding which can act like a heat bath. For the case of quantum systems the interaction is usually by means of electromagnetic fields. Such an interaction usually results in an energy dissipation which leads the system to the most stable configuration which is the ground state-the minimal energy state.

Now let us briefly describe the content of this work. Chapter 2 serves mostly as reference, but some results, in particular, in Section 2.2.3 are original. In Chapter 2 we give a review of mathematical rigorous definitions of the operators we mentioned earlier as a self-adjoint extensions of symmetric operators on appropriate Sobolev spaces. We write down their basic spectral properties. We introduce the Krein's formula which relates the resolvents of two self-adjoint extensions of a certain symmetric operator usually by a finite rank operator. With help of Krein's formula we describe the point interactions for systems where different self-adjoint extensions of this kind exists, i.e. in the dimension one, two a three and also for quantum graphs. Next we introduce generalized Birman-Schwinger formula, which relates resolvents of two operators by their difference expressed as an integral operator. These operators differ by the multiplication operator defined by a bounded Borel measurable function and a positive Radon measure. By means of generalized Birman-Schwinger formula we are able to introduce contact potentials supported by manifolds of the codimension one, i.e. curves in $\mathbb{R}^2$ and surfaces in $\mathbb{R}^3$. We could by the same approach introduce point interactions for $\mathbb{R}$. It is a result of the fact that points have codimension one with respect to the line. However by this approach one would obtain same results as for the Krein's formula.

These two methods are both based on the same principle. They describe the difference between the resolvents of two self-adjoint operators which have a common contraction. The difference between these two methods is as follows. For the case of Krein's formula we describe self-adjoint operator via separated boundary conditions. By this approach we can introduce point interactions in the dimensions one, two and three. For the case of Birman-Schwinger formula we describe singular interactions supported by the codimension one.

In Chapter 3 we present the properties of the ground state energy with respect to the geometry of the point interactions sites for the dimension one. We will show that a decrease in distance between the attractive point interactions results in a decrease of the ground state energy for the case of the line and quantum graph without branching. We also show that the situation is more complex for the branched graphs. At the end of this chapter we present several examples.

Chapter 4 treats the case of point interactions on a plane and in a three-dimensional Euclidian space. We will show that the situation is similar to the case of attractive point interactions on the line, i.e. an increase in distance between point interactions results in an increase of the ground state energy.

In Chapter 5 we will present the situation of the ground state of the system with contact potential supported by the manifold of the codimension one on a plane and in a three-dimensional Euclidian space. The ground state energy behaves similarly for this case as for point interactions. The decrease of distance between the points of the manifold results in decrease of the ground state energy.

Chapter 6 is focused on examples of minimization of the ground state energy with respect to the position of point interaction along to several potential types. We will work with a rectangular potential well, a piecewise linear potential, a monotonous potential and a mirror-symmetric confining potential. We will show that for the case of symmetric potential the optimal position of the attractive point interaction is at the minimum of the potential. The situation is different for the asymmetric case where the optimal position is shifted from the minimum of the potential.

Chapter 2

Setting of the problem

In this chapter we introduce mathematically rigorous definition of the point interactions in one, two and three dimensions. We summarize basic properties of point interactions. We describe basic characteristics of such operators and properties necessary for proving relations between the ground state energy and distance between point interactions.

There are many ways how to introduce point interactions. We will be working with two mathematical constructs.

One of them is based on interpreting our operators as self-adjoint extension of appropriate densely defined symmetric operator. By this approach we can obtain operators which can be formally written as

$$H_{\alpha,Y} = -\Delta + \sum_{i=1}^{N} \alpha_j \delta(x - y_j), \tag{2.1}$$

where $N < \infty$. These operators describe a finite number of point interactions. Our review of the properties of these operators will be brief; for a more complete description we refer to the monograph [1].

We also introduce a different approach using the Birman-Schwinger argument. We describe interactions with the help of the measure. This approach allows us to introduce singular interactions supported on the manifold of codimension one. We will work with operators which can be formally written as

$$H = H_0 + \gamma m, \tag{2.2}$$

where γm represents a multiplication operator described by a bounded Borel measurable function γ and a positive Radon measure m. This approach is based on describing the resolvent of the desired operator H as a addition of the resolvent of H_0 and the integral operator depending on γ. For a complete description of this approach see [11].

2.1 Self-adjoint extensions of symmetric operators

One of possible ways how to introduce point interactions is as a self-adjoint extension of the symmetric operator obtained by restricting the free Hamiltonian to functions which vanish in the vicinity of the interaction support. In this subsection we present a brief review of some basic properties in the general setting including a very useful formula due to Krein.[1]

We start by self-adjoint extension of operator $\dot{A}$ which is densely defined, closed and symmetric in a Hilbert space $\mathscr{H}$ with deficiency indices $(1,1)$, this means that there exists functions ϕ_+ and ϕ_- which fulfill

$$\begin{aligned} \dot{A}^*\phi_+ &= i\phi_+, \\ \dot{A}^*\phi_- &= -i\phi_-, \end{aligned} \tag{2.3}$$

where i is the complex unit.

Theorem 2.1. *Let the operator $\dot{A}$ defined above fulfills*

$$\dot{A}^*\phi(z) = z\phi(z), \quad \phi(z) \in \mathscr{D}(\dot{A}^*), \quad z \in \mathbb{C} \setminus \mathbb{R}, \tag{2.4}$$

then all self-adjoint extensions A_θ of $\dot{A}$ may be parameterized by a real parameter $\theta \in [0, 2\pi)$ in the following way

$$\begin{aligned} \mathscr{D}(A_\theta) &= \{g + c\phi_+ + ce^{i\theta}\phi_- \mid g \in \mathscr{D}(\dot{A}), c \in \mathbb{C}\}, \\ A_\theta(g + c\phi_+ + ce^{i\theta}\phi_-) &= \dot{A}g + ic\phi_+ - ice^{i\theta}\phi_-, \quad 0 \le \theta < 2\pi, \end{aligned} \tag{2.5}$$

where

$$\phi_\pm = \phi(\pm i), \quad \|\phi_+\| = \|\phi_-\|. \tag{2.6}$$

Next we state Krein's formula which relates two self-adjoint extensions of the symmetric operator by a finite rank operator. Krein's formula for this case can be written according to [1, Appendix A] as follows.

Theorem 2.2 (Krein's formula)**.** *Let $\dot{A}$ be a symmetric operator and B and C denote two self-adjoint extensions of $\dot{A}$. Then for the resolvent we can write*

$$(B-z)^{-1}-(C-z)^{-1}=\lambda(z)(\phi(\overline{z}),\cdot)\phi(z),\quad z\in\rho(B)\cap\rho(C),\tag{2.7}$$

where λ and ϕ may be chosen to be analytical functions for all $z\in\rho(B)\cap\rho(C)$ and $\lambda(z)\neq 0\ \forall z\in\rho(B)\cap\rho(C)$. The vector function $\phi(z)$ satisfies

$$\phi(z)=\phi(z_0)+(z-z_0)(C-z)^{-1}\phi(z_0),\quad z\in\rho(C),\tag{2.8}$$

where $\phi(z_0)$ fulfills

$$\dot{A}^*\phi(z_0)=z_0\phi(z_0),\quad z_0\in\mathbb{C}\setminus\mathbb{R}.\tag{2.9}$$

If we choose $\phi(z)$ according to (2.8), $\lambda(z)$ satisfies

$$\lambda(z)^{-1}=\lambda(z')^{-1}-(z-z')(\phi(\overline{z}),\phi(z')),\quad z,z'\in\rho(B)\cap\rho(C).\tag{2.10}$$

Next we describe a more general case for which the operator $\dot{A}$ is densely defined, a closed symmetric operator in some Hilbert space $\mathscr{H}$ with deficiency indices (N,N), where $N\in\mathbb{N}$. Let the operators B and C be self-adjoint extensions of the operator $\dot{A}$. We denote by $\mathring{A}$ the maximal common part of B and C, in other words $\mathring{A}$ obeys $\mathring{A}\subseteq B$, $\mathring{A}\subseteq C$ and also $\mathring{A}$ extends any operator A' fulfilling $A'\subseteq B$, $A'\subseteq C$. We denote by M the deficiency index of $\mathring{A}$. We know that M fulfills $0\leq M\leq N$. The span of linearly independent vectors $\{\phi_1(z),\dots\phi_M(z)\}$ equals the deficiency subspace of $\mathring{A}$, i.e.:

$$\mathring{A}^*\phi_m(z)=z\phi_m(z),\quad \phi_m(z)\in\mathscr{D}(\mathring{A}^*),\quad m\in\hat{M},\quad z\in\mathbb{C}\setminus\mathbb{R}.\tag{2.11}$$

Theorem 2.3 (Krein's formula for deficiency indices $N\geq 1$)**.** *Let the operators $\dot{A}$, $\mathring{A}$, B and C be as above. Then*

$$(B-z)^{-1}-(C-z)^{-1}=\sum_{m,n=1}^{M}\lambda_{mn}(z)(\phi_n(\overline{z}),\cdot)\phi_m(z),\quad z\in\rho(B)\cap\rho(C),\tag{2.12}$$

where the matrix $\lambda_{mn}(z)$ is nonsingular for all $z\in\rho(B)\cap\rho(C)$ and $\lambda_{mn}(z)$ along with ϕ_m may be chosen analytically for all $m,n\in M$ and $z\in\rho(B)\cap\rho(C)$. We may define $\phi_m(z)$ as

$$\phi_m(z)=\phi_m(z_0)+(z-z_0)(C-z)^{-1}\phi_m(z_0),\quad m=1,\dots,M,\quad z\in\rho(C),\tag{2.13}$$

where $\phi_m(z_0)$ are linearly independent solutions of (2.11), where $z = z_0$. Then the matrix $\lambda_{mn}(z)$ can be written as

$$[(\lambda_{mn}(z))]^{-1}_{m,n} = [(\lambda_{mn}(z'))]^{-1}_{m,n} - (z - z')(\phi_n(\overline{z}), \phi_m(z')), \\ m, n \in \hat{M}, \quad z, z' \in \rho(B) \cap \rho(C). \tag{2.14}$$

We can also write Krein's formula in another basis as

$$(B - z)^{-1} - (C - z)^{-1} = \sum_{m,n=1}^{N} \widetilde{\lambda_{mn}}(z)(\widetilde{\phi_n}(\overline{z}), \cdot)\widetilde{\phi_m}(z), \quad z \in \rho(B) \cap \rho(C), \tag{2.15}$$

where $\widetilde{\phi_m}(z)$ $m \in N$ are linearly independent functions fulfilling the relation

$$\dot{A}^* \widetilde{\phi_m}(z) = z\widetilde{\phi_m}(z), \quad \widetilde{\phi_m}(z) \in \mathscr{D}(\dot{A}^*), \quad m \in \hat{M}, \quad z \in \mathbb{C} \setminus \mathbb{R}. \tag{2.16}$$

For such a case there is the possibility that $\forall z \det \widetilde{\lambda}(z) = 0$. For further reference we refer the reader to [1, Appendix A].

2.2 Point interactions as self-adjoint extensions

In this section we introduce point interactions as self-adjoint extension of symmetric operators. We start with symmetric operator to which we construct self-adjoint extensions differing by boundary conditions at the point interaction sites. Later on, with the help of Krein's formula, we construct the resolvents of such operators. From the resolvent of the operator we will be able to derive certain properties of the ground state. We will discuss point interactions in the dimension one, two and three. These models are discussed in great detail in [1]. We would like to mention that there is an alternative approach to the one of the self-adjoint extensions based on the Fourier transformation described in the monograph [1, Chapter II.1].

2.2.1 One point interaction on a line

We start by one point interaction on a line. As we mention earlier we employ self-adjoint extension of a suitable densely defined symmetric operator. We

start with a closed and nonnegative operator

$$\dot{H}_y = -\frac{d^2}{dx^2} \tag{2.17}$$

with the domain $\mathscr{D}(\dot{H}_y) = \{g \in H^{2,2}(\mathbb{R}) | g(y) = 0\}$. Its adjoint can be written as

$$\dot{H}_y^* = -\frac{d^2}{dx^2}. \tag{2.18}$$

Its domain is $\mathscr{D}(\dot{H}_y^*) = H^{2,2}(\mathbb{R} \setminus \{y\}) \cap H^{2,1}(\mathbb{R})$, where $H^{m,n}(\mathbb{R})$ are the corresponding Sobolev spaces. Solutions of the equation

$$\dot{H}_y^* \psi(k) = k^2 \psi(k) \tag{2.19}$$

are given by

$$\psi(k, x) = e^{ik|x-y|}, \tag{2.20}$$

where $\psi(k) \in \mathscr{D}(\dot{H}_y^*)$, $k^2 \in \mathbb{C} \setminus \mathbb{R}$ and $\Im k > 0$. From this we can infer that $\dot{H}_y$ has deficiency indices (1,1) which means that our operator has a one-parameter family of self-adjoint extensions.

Now according to [4, Section X.1] and by direct application of Theorem 2.2 to our operator $\dot{H}_y$ we are able to describe all self-adjoint extension of our operator $\dot{H}_y$ by the parameter $\theta \in [0, 2\pi)$ in the following manner. All self-adjoint extensions H_θ can be written as

$$\mathscr{D}(H_\theta) = \{g + c\psi_+ + ce^{i\theta}\psi_- | g(z) \in \mathscr{D}(\dot{H}_y), c \in \mathbb{C}\} \tag{2.21}$$

and the operator acts as

$$H_\theta(g + c\psi_+ + ce^{i\theta}\psi_-) = \dot{H}_y g + ic\psi_+ - ice^{i\theta}\psi_-, \tag{2.22}$$

where $\psi_\pm(x)$ are given by the relation (2.20) as

$$\begin{aligned} \psi_\pm(x) &= \psi(\pm i, x), \\ \|\psi_-\| &= \|\psi_+\|. \end{aligned} \tag{2.23}$$

We come to self-adjoint extensions $H_{\theta,y}$, whose functions of theirs domain are continuous at the point y and satisfy the condition

$$\begin{aligned} \lim_{\epsilon \downarrow 0}[(g + c\psi_+ + ce^{i\theta}\psi_-)'(y + \epsilon) - (g + c\psi_+ + ce^{i\theta}\psi_-)'(y - \epsilon)] = \\ -c(1 + e^{i\theta}) = \alpha[g(y) + c\psi_+(y) + ce^{i\theta}\psi_-(y)], \end{aligned} \tag{2.24}$$

where $\alpha = \frac{-2\cos\left(\frac{\theta}{2}\right)}{\cos\left(\frac{\theta}{2}-\frac{\pi}{4}\right)}$. It can be seen that α covers the real axis as a function of $\theta \in [0, 2\pi)$. We can thus parameterize the self-adjoint extensions using boundary conditions written as (2.24) in the following manner.

Theorem 2.4. *Let the operator $-\Delta_{\alpha,y}$ be defined as*

$$-\Delta_{\alpha,y} = -\frac{d^2}{dx^2} \tag{2.25}$$

with the domain

$$\mathscr{D}(-\Delta_{\alpha,y}) = \{g \in H^{2,1}(\mathbb{R}) \cap H^{2,2}(\mathbb{R}\backslash\{y\}) |\, g'(y+) - g'(y-) = \alpha g(y)\}, \tag{2.26}$$

where α satisfies $-\infty < \alpha \leq \infty$. Then all self-adjoint extensions of $\dot{H}_y$ coincide with $\{-\Delta_{\alpha,y} | -\infty < \alpha \leq \infty\}$. The special case $\alpha = 0$ leads to the kinetic energy operator in $L^2(\mathbb{R})$,

$$-\Delta_{0,y} = -\Delta = -\frac{d^2}{dx^2}, \quad \mathscr{D}(-\Delta) = H^{2,2}(\mathbb{R}). \tag{2.27}$$

Another particular case is $\alpha = \infty$, which corresponds to the situation of two separated halflines with Dirichlet boundary condition at y,

$$\begin{aligned} -\Delta_{\infty,y} &= (-\Delta_{D-}) \oplus (-\Delta_{D+}), \\ \mathscr{D}(-\Delta_{\infty,y}) &= \{g \in H^{2,1}(\mathbb{R}) \cap H^{2,2}(\mathbb{R} \setminus \{y\}) | g(y) = 0\} \\ &= H_0^{2,2}((-\infty, y)) \cup H_0^{2,2}((y, \infty)), \end{aligned} \tag{2.28}$$

where $-\Delta_{D\pm}$ is the Dirichlet Laplacian (for the definition of these operators see [3, Section XIII.15]) on $(-\infty, y)$ and (y, ∞), respectively.

Proof: Can be found in [1, Chapter I.3.1]

Now we write the resolvent of our operator $-\Delta_{\alpha,y}$ according to Krein's formula, i.e. we specify Theorem 2.2 to this particular case.

Theorem 2.5. *The resolvent of $-\Delta_{\alpha,y}$ is given by*

$$\begin{aligned} (-\Delta_{\alpha,y} - k^2)^{-1} = G_k - 2\alpha k(i\alpha + 2k)^{-1}(\overline{G_k(\cdot - y)}, \cdot)G_k(\cdot - y), \\ k^2 \in \rho(-\Delta_{\alpha,y}), \quad \Im k > 0, \quad -\infty < \alpha \leq \infty, \quad y \in \mathbb{R}, \end{aligned} \tag{2.29}$$

where

$$G_k(x-x') = (i/2k)e^{ik|x-x'|},\ \Im k > 0 \tag{2.30}$$

is the integral kernel of $(-\Delta - k^2)^{-1}$ *in* $L^2(\mathbb{R})$. *The integral kernel of the resolvent* $(-\Delta_{\alpha,y} - k^2)^{-1}$ *can be written explicitly as*

$$(-\Delta_{\alpha,y} - k^2)^{-1}(x,x') = (i/2k)e^{ik|x-x'|} + \alpha(2k)^{-1}(i\alpha + 2k)^{-1}e^{ik[|x-y|+|y-x'|]},$$
$$k^2 \in \rho(-\Delta_{\alpha,y}), \quad \Im k > 0, \quad x, x' \in \mathbb{R}. \tag{2.31}$$

Proof: Can be found in [1, Section I.3.1]

The next theorem specifies some spectral properties of our operator $-\Delta_{\alpha,y}$.

Theorem 2.6. *Let* $-\infty < \alpha \leq \infty$, $y \in \mathbb{R}$ *then the essential, absolutely continuous and singularly continuous spectrum of the operator* $-\Delta_{\alpha,y}$ *can be written as*

$$\sigma_{ess}(-\Delta_{\alpha,y}) = \sigma_{ac}(-\Delta_{\alpha,y}) = [0,\infty), \quad \sigma_{sc}(-\Delta_{\alpha,y}) = \emptyset. \tag{2.32}$$

If $-\infty < \alpha < 0$, *then* $-\Delta_{\alpha,y}$ *has one simple, negative eigenvalue, namely*

$$\sigma_p(-\Delta_{\alpha,y}) = \left\{ \frac{-\alpha^2}{4} \right\}. \tag{2.33}$$

Eigenfunction corresponding to this eigenvalue can be chosen strictly positive:

$$\psi(x) = (-\alpha/2)^{1/2}e^{\alpha|x-y|/2}. \tag{2.34}$$

If $0 \leq \alpha \leq \infty$, *then the operator* $-\Delta_{\alpha,y}$ *has no eigenvalues, i.e.*

$$\sigma_p(-\Delta_{\alpha,y}). \tag{2.35}$$

Proof: Can be found in [1, Section I.3.1]

2.2.2 Finite number of point interactions on a line

Now we generalize the previous case of one point interaction of the last subsection to finitely many point interactions on the line. Our procedure

will be strictly analogous to that used for one point interaction. We start by defining the minimal operator $\dot{H}_Y$ as

$$\begin{aligned} \dot{H}_Y &= -\frac{d^2}{dx^2}, \\ \mathscr{D}(\dot{H}_Y) &= \{g \in H^{2,2}(\mathbb{R}) |\, g(y_j) = 0, y_j \in Y, j = 1, \dots N\}, \\ Y &= \{y_1, \dots, y_N\}, N \in \mathbb{N}. \end{aligned} \tag{2.36}$$

As before the operator $\dot{H}_Y$ is closed and nonnegative. Its adjoint operator $\dot{H}_Y^*$ can be written as

$$\begin{aligned} \dot{H}_Y^* &= -\frac{d^2}{dx^2}, \\ \mathscr{D}(\dot{H}_Y^*) &= H^{2,2}(\mathbb{R} \setminus \{Y\}) \cap H^{2,1}(\mathbb{R}). \end{aligned} \tag{2.37}$$

We find the solution of the eigenvector equation

$$\dot{H}_Y^* \psi(k) = k^2 \psi(k) \tag{2.38}$$

for $\psi(k) \in \mathscr{D}(\dot{H}_Y^*)$, $k^2 \in \mathbb{C} \setminus \mathbb{R}$, $\Im k > 0$, in the form

$$\psi_j(k, x) = e^{ik|x - y_j|},\ y_j \in Y,\ j = 1, \dots, N. \tag{2.39}$$

From this result we can conclude that $\dot{H}_Y$ has deficiency indices at least (N, N). The result that deficiency indices are exactly (N, N) comes from the fact that there are no other linearly independent solution of (2.38) than those written as (2.39). Consequently, all the self-adjoint extensions of our operator $\dot{H}_Y$ form a N^2-parameter family of self-adjoint operators. We restrict ourselves to the case of *local* boundary conditions, i.e. coupling of the boundary values at each point y_j, $j = 1, \dots, N$ separately. Similarly as for one point interaction we characterize the self-adjoint extension of $\dot{H}_Y$ as

$$\begin{aligned} -\Delta_{\alpha,Y} &= -\frac{d^2}{dx^2}, \\ \mathscr{D}(-\Delta_{\alpha,Y}) &= \{g \in H^{2,1}(\mathbb{R}) \cap H^{2,2}(\mathbb{R} \setminus Y) | \\ & g'(y_j+) - g'(y_j-) = \alpha_j g(y_j), j = 1, \dots, N\}, \end{aligned} \tag{2.40}$$

where $\alpha = (\alpha_1, \dots, \alpha_n)$, $-\infty < \alpha_j \leq \infty$, $j = 1, \dots, N$. The operator $-\Delta_{\alpha,Y}$ is self-adjoint ([1, Section II.2.1]). The special case $\alpha_i = 0$ for all $i \in \hat{N}$ leads

to the kinetic energy operator $-\Delta$ on $H^{2,2}(\mathbb{R})$. The case that $\alpha_i = 0$ for certain point interactions sites $i \in \{i_1, \ldots, i_m\}$ leads to the case of $N - m$ point interactions on the line. The case $\alpha_{j_0} = \infty$ leads to the Dirichlet boundary condition at y_{j_0}, which means, $g(y_{j_0}+) = g(y_{j_0}-) = 0$. According to [1, Section II.2.2] we can approximate the operator $-\Delta_{\alpha,Y}$ by the one parametric set of operators

$$H_{\epsilon,Y} = -\frac{d^2}{dx^2} + \epsilon^{-1} \sum_{j=1}^{N} V_j(\frac{\cdot - y_j}{\epsilon}). \tag{2.41}$$

It can be proven that the operator $H_{\epsilon,Y}$ converge to the operator $-\Delta_{\alpha,Y}$ in the norm resolvent sense and $\alpha_j = \int_{\mathbb{R}} dx\, V_j(x - y_j)$ for all $j = 1, \ldots, N$. From this we infer that $-\Delta_{\alpha,Y}$ describes N δ-point interactions located at points $y_j \in Y$ with strength equal to α_j, where $j = 1, \ldots, N$.

Let us formulate several basic properties of $-\Delta_{\alpha,Y}$. We start by restating Krein's formula introduced in Theorem 2.3 for our operator $-\Delta_{\alpha,Y}$.

Theorem 2.7. *Let $\alpha_j \neq 0$, $j = 1, \ldots, N$. Then the resolvent of the operator $-\Delta_{\alpha,Y}$ is given by*

$$\begin{gathered}(-\Delta_{\alpha,Y} - k^2)^{-1} = G_k + \sum_{j,j'=1}^{N} [\Gamma_{\alpha,Y}(k)]^{-1}_{jj'} (\overline{G_k(\cdot - y_{j'})}, \cdot) G_k(\cdot - y_j), \\ k^2 \in \rho(-\Delta_{\alpha,Y}),\ \Im k > 0,\ -\infty < \alpha_j \leq \infty,\ y_j \in Y,\ j = 1, \ldots, N.\end{gathered} \tag{2.42}$$

Inverse of the matrix $[\Gamma_{\alpha,Y}(k)]^{-1}$ is given by

$$[\Gamma_{\alpha,Y}(k)]_{jj'} = -[\alpha_j^{-1}\delta_{jj'} + G_k(y_j - y_{j'})]_{j,j'=1}^{N}, \tag{2.43}$$

where G_k is the free resolvent kernel given by (2.30)*, which can be explicitly written as*

$$G_k(y_j - y_{j'}) = \frac{i}{2k} e^{ik|y_j - y_{j'}|}. \tag{2.44}$$

Proof: Can be found in [1, Section II.2.1]

The following important theorem gives all the eigenvalues of our operator in implicit form.

Theorem 2.8. *Let $\alpha_j \neq 0$, $y_j \in Y, j \in \{1, 2, ..., N\}$. Assume that there is at most one index $j = j_0$ for which $\alpha_{j_0} = \infty$. Then $-\Delta_{\alpha,Y}$ has at most N eigenvalues which are all negative and simple. If $\alpha_j = \infty$ for at least two different values $j \in \{1, 2, ..., N\}$, then $-\Delta_{\alpha,Y}$ has at most $N - 2$ negative eigenvalues (counting multiplicity) and infinitely many eigenvalues embedded in $[0, \infty)$ accumulating at ∞. In particular, $k^2 \in \sigma_p(-\Delta_{\alpha,Y}) \cap (-\infty, 0)$ if $\det[\Gamma_{\alpha,Y}(k)] = 0$, $\Im k > 0$, and the multiplicity of eigenvalue $k^2 < 0$ equals the multiplicity of the eigenvalue zero of the matrix $\Gamma_{\alpha,Y}(k)$. Moreover, if $E_0 = k_0^2 < 0$ is an eigenvalue of $-\Delta_{\alpha,Y}$, the corresponding eigenfunctions are of the form*

$$\psi_0 = \sum_{j=1}^{N} c_j G_{k_0}(x - y_j), \quad \Im k_0 > 0, \tag{2.45}$$

where $(c_1, c_2, ..., c_N)$ are eigenvectors of the matrix $\Gamma_{\alpha,Y}(k_0)$ corresponding to the eigenvalue zero. If $-\Delta_{\alpha,Y}$ has a ground state (the lowest isolated eigenvalue) it is nondegenerate and the corresponding eigenfunction can be chosen to be strictly positive, i.e. the associated eigenvector $(c_1, c_2, ..., c_N)$ fulfills $c_j > 0$, $j \in \{1, 2, ..., N\}$.

Proof: Can be found in [1, Section II.2.1]

2.2.3 Point interactions on quantum graphs

In this subsection we describe a quantum particle living on a graph $\mathbb{G}$. Quantum graphs are to some extend a generalization of one-dimensional quantum mechanics. The particle on the quantum graph is still trapped on a one-dimensional structure. However graphs offer more complex topological properties than the line. For the operators to be self-adjoint on quantum graphs we have to impose boundary conditions at the vertices. We will use conditions which are called attractive δ coupling. These conditions are analogous to those we impose on the line for the case of point interactions.

We will not consider general graphs. We restrict ourselves to finite ones, i.e. constructed from p vertices and q edges, where $p, q \in \mathbb{N}$. We represent the lengths of the edges by the vector $L = \{l_i \mid i \in \hat{q}\}^T$, where $l_i \in \mathbb{R}^+ \cup \{+\infty\}$, which means that we allow both finite and infinite edges. We construct our space $L^2(\mathbb{G})$ on the graph $\mathbb{G}$, where we defined the Lebesgue measure dx in

the natural way, from classes of equivalence of measurable functions on each edge. Thus our space is an orthogonal sum of $L^2(0, l_i)$, that is

$$L^2(\mathbb{G}) = \bigoplus_{i=1}^{q} L^2(0, l_i). \tag{2.46}$$

In other words functions from our Hilbert space $L^2(\mathbb{G})$ can be written as $\Psi = \{\psi_i \mid \psi_i \in L^2(0, l_i), i \in \hat{q}\}^T$. We can write the condition on integrability of functions as

$$\|\Psi\|^2_{L^2(\mathbb{G})} = \sum_{i=1}^{q} \|\psi_i\|^2_{L^2(0,l_i)} < \infty. \tag{2.47}$$

We will be working with the operator which acts on the edges of our graph as negative second derivative, i.e.

$$H\psi_i = -\psi_i''. \tag{2.48}$$

It can be seen that such operator will be symmetric for the domain $\mathscr{D}(H) = \{\{\psi_i \mid \psi_i \in L^2(0, l_i), i \in \hat{q}\}^T \mid \lim_{x\to 0} \psi_i(x) = \lim_{x\to l_i} \psi_i(x) = 0\}$. However our operator has to be self-adjoint. We accomplish this by choosing its self-adjoint extension characterized by certain boundary conditions at each vertex. General conditions for the vertex of the degree k can be written in the matrix form according to [8] as

$$A_j\Psi_j + B_j\Psi_j' = 0, \tag{2.49}$$

where Ψ_j and Ψ_j' are vectors of functional values and values of outwards derivatives at the particular vertex of the degree k and the matrices $A_j, B_j \in \mathbb{C}^{k\times k}$ fulfill

$$\begin{aligned} \operatorname{rank}(A_j \mid B_j) &= k, \\ A_jB_j^* &\text{ is self adjoint.} \end{aligned} \tag{2.50}$$

It is not hard to see that the matrices A_j and B_j are not unique. Boundary conditions generated by the two sets of matrices (A_j, B_j) and (CA_j, CB_j), where C is a nonsingular matrix, are the same. We would like to have a set of matrices A_j and B_j which would generate unique boundary conditions. One suitable choice of the matrices is the following

$$A_j = U_j - I, \quad B_j = i(U_j + I), \tag{2.51}$$

where I is identity matrix and U_j is a unitary one.

Because we are interested in an analogy to δ-point interactions on graphs we will work with the conditions similar to those we had on the line. To write them down we can, without loss of generality, assume that the edges have fixed parametrization. This will help us to write down all the conditions at once more easily. Such conditions can be written as

$$\begin{aligned} \psi_{j_g}(0) = \psi_{j_h}(0) = \psi_{k_m}(l_{k_m}) = \psi_{k_n}(l_{k_n}) \quad \forall g, h \in \hat{m}_y \quad \forall m, n \in \hat{n}_y, \\ \sum_{i=1}^{m_y} \psi'_{j_i}(0+) - \sum_{i=1}^{n_y} \psi'_{k_i}(l_{k_i}-) = \alpha_y \psi_{j_1}(0) \end{aligned} \tag{2.52}$$

for all y where m_y and n_y are numbers of edges that in our given parametrization have at the vertex point either $x = 0$ or $x = l_i$ respectively. Our conditions (2.52) are the only ones from the general case (2.49), which have the wave functions continuous at the vertices. Now we can define a Hamiltonian on the domain $H^{2,2}(\mathbb{G})$ where all functions have to fulfill the condition (2.52). We should note that for the vertex with only one edge this condition is the same as the Robin condition when $\alpha \neq 0$ and Neumann condition for $\alpha = 0$. We rewrite the conditions (2.52) into matrix form for each vertex as

$$\begin{aligned} A_i \Psi_i + B_i \Psi'_i = 0, \\ A_i = \begin{pmatrix} 1 & -1 & 0 & \ddots & 0 \\ 0 & 1 & -1 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & 0 \\ 0 & \ddots & 0 & 1 & -1 \\ \alpha_i & 0 & \cdots & 0 & 0 \end{pmatrix}, \\ B_i = \begin{pmatrix} 0 & 0 & \cdots & 0 \\ 0 & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & 0 \\ 1 & \cdots & 1 & 1 \end{pmatrix}, \end{aligned} \tag{2.53}$$

where $i \in \hat{p}$ numbers the vertices, $A_i \in \mathbb{R}^{k \times k}$, $B_i \in \mathbb{R}^{k \times k}$ and $m_i + n_i = k$. Another choice of matrices A_i and B_i with the help of the unitary matrix U_i is

$$\begin{aligned} A_i &= U_i - I, \\ B_i &= i(U_i + I), \end{aligned} \tag{2.54}$$

where I is the identity matrix and $U_i = \frac{2}{d+i\alpha_i} J - I$ where d is the degree of the vertex and J is a matrix having all entries equal to 1.

Working with a set of conditions for each vertex separately is impractical. That is the reason why we restate our problem in terms of a different graph $\mathbb{G}_0$ obtained from $\mathbb{G}$ by identifying all its vertices. This graph has only one vertex. We encode the boundary conditions together with the topology of the original graph to the boundary condition of the new vertex as it is described in [9]. The space of the new graph $\mathbb{G}_0$ and original one are isomorphic. This is the result of the fact that the new graph $\mathbb{G}_0$ and the original one have the same lengths of corresponding edges. The operator on the new graph act the same as the operator on the original graph. We transfer the conditions (2.52) on a new graph in the following way

$$A\Psi + B\Psi' = 0, \tag{2.55}$$

where A and B are block diagonal matrices fulfilling

$$\begin{gathered} \operatorname{rank}(A \mid B) = \sum_{i=1}^{p} d_i, \\ AB^* \text{ is self-adjoint,} \end{gathered} \tag{2.56}$$

where the number d_i in the degree of the i-th vertex. We construct those matrices A and B as direct sums of A_i and B_i, $i \in \hat{p}$ respectively. This can be written as

$$A = \bigoplus_{i=1}^{q} A_i = \begin{pmatrix} A_1 & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & A_p \end{pmatrix}, \tag{2.57}$$

and

$$B = \bigoplus_{i=1}^{q} B_i = \begin{pmatrix} B_1 & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & B_p \end{pmatrix}. \tag{2.58}$$

At this point we are ready to write down the operator which describes the so called δ-coupling on graphs. Our operator acts as second derivative, i.e.

$$(-\Delta_{\mathbb{G},\alpha,L}\Psi)_i = -(\Psi'')_i. \tag{2.59}$$

Our operator has the domain of the form $\mathscr{D}(-\Delta_{\mathbb{G},\alpha,L}) = \{\Psi \in \bigoplus_{j=1}^{q} H^{2,2}(l_i) \mid A\Psi + B\Psi' = 0\}$ where $\alpha = (\alpha_1, \ldots, \alpha_p)$ describes "point interaction strengths" and matrices A and B enter the conditions (2.52) and they can be written as (2.57) and (2.58). For proofs of certain statements it is practical to associate the quadratic form with our operator $-\Delta_{\mathbb{G},\alpha,L}$. This quadratic form can be expressed as

$$d[\Psi] = (\Psi, -\Delta_{\mathbb{G},\alpha,L}\Psi) = \sum_{i=1}^{q} \int_0^{l_i} |\psi_i'(x)|^2 dx + \sum_{i=1}^{p} \alpha_i |\psi_i(0)|^2, \tag{2.60}$$

where $\psi_i(0)$ are the values of the function at the i-th vertex and $\psi_i'(x)$ are the values of the first derivative at the i-th edge. The domain of our quadratic form consists of functions $\Psi \in L^2(\mathbb{G})$ which fulfills $\Psi \in H^{1,2}(\mathbb{G})$ on the edges and are continuous at each vertex of the graph. Now we give some properties of the ground state of our operator $-\Delta_{\mathbb{G},\alpha,L}$ defined above. First we state under what circumstances our operator has the ground state [6].

Theorem 2.9. $\inf(\sigma(-\Delta_{\mathbb{G},\alpha,L})) < 0$ *if* $\alpha_i \leq 0$ *holds for all* $i \in \hat{q}$ *and* $\sum_{i=1}^{q} \alpha_i < 0$.

Proof. We will separate the proof of this statement into two parts. We start with a proof for graphs with no semi-infinite edges and then we generalize this procedure for a graph with semi-infinite edges. We want to find test function Ψ which fulfills

$$d[\Psi] < 0, \quad \Psi \in \mathscr{D}(d). \tag{2.61}$$

For the graph with finite edges we can choose constant function $\psi_i = C$ on all the edges which belongs to the form domain because

$$\int_\Gamma |C|^2 dx = |C|^2 \int_\Gamma dx < \infty. \tag{2.62}$$

For such function Ψ we get

$$d[\Psi] = |C|^2 \sum_{i=1}^{q} \alpha_i \leq \min_j \alpha_j |C|^2 < 0. \tag{2.63}$$

For the graph with one or more semi-infinite edges we choose the test function equal to constant for the finite edges $\psi_i = C$ and $\psi_j = C\exp(-\kappa x)$ for the semi-infinite ones. For such function we obtain

$$d[\Psi] \leq \left(\min_j \alpha_j + \frac{\kappa}{2} K\right) |C|^2, \tag{2.64}$$

where K is the number of semi-infinite edges. This expression is negative for κ chosen sufficiently small which completes the proof. □

The next theorem deals with basic properties of the ground state of our operator [6].

Theorem 2.10. *Let the graph $\mathbb{G}$ be connected, then the bottom of the spectrum $\lambda_0 = \inf \sigma(-\Delta_{\mathbb{G},\alpha,L})$ is a simple isolated eigenvalue. The corresponding eigenfunction Ψ^0 can be chosen strictly positive on $\mathbb{G}$ being convex on each edge.*

Proof. To prove the first part of the theorem let us consider the graph $\mathbb{G}'$. This graph differs from the original one $\mathbb{G}$ by boundary conditions at each vertex. We changed those conditions to the Dirichlet boundary condition which results in a fully disjoined graph. The spectral problem for the graph $\mathbb{G}'$ can be solved exactly. We know that the graph $\mathbb{G}'$ has either positive discrete spectrum, for the case when the graph $\mathbb{G}'$ has only finite edges, or the spectrum is equal to $\mathbb{R}^+$ for the graph with some semi-infinite edges. Now we use Krein's formula ([7, Proposition 1.3]) on the operators acting on the graph $\mathbb{G}$ and the graph $\mathbb{G}'$. Krein's formula connects these operators by finite rank operator in the resolvent. This formula has similar properties as we mentioned earlier for the operators of on the line. According to Weyl's theorem the essential spectra of the operators are the same and the negative discrete spectrum of the operator on the graph $\mathbb{G}$ is created by a finite number of eigenvalues with finite multiplicity. According to Theorem 2.9 negative discrete spectrum is non-empty and the ground state exists which completes the first part of the proof.

Ground state positivity follows from the modified Courant theorem [14]. Convexity of the ground state comes from

$$(\psi_j)'' = -\lambda_0 \psi_j > 0, \tag{2.65}$$

where ψ_j is the ground state eigenfunction and $\lambda_0 < 0$ is the ground state eigenvalue. Positivity of the previous expression is a direct result of the positivity of the ground state and the fact that each eigenfunction is twice differentiable at the edges except the vertices. □

2.2.4 One point interaction on a plane

In this subsection we will discuss one point interaction in two dimensions. We define the operator describing point interaction centered at point y. We start with nonnegative operator in $L^2(\mathbb{R}^2)$ which can be written as

$$H_y = -\Delta \mid_{C_0^\infty(\mathbb{R}^2\setminus\{y\})}, \tag{2.66}$$

where $y \in \mathbb{R}^2$. The closure of this operator is denoted by $\dot{H}_y$ in $L^2(\mathbb{R}^2)$. The domain of its closure equals to

$$\mathscr{D}(\dot{H}_y) = H_0^{2,2}(\mathbb{R}^2 \setminus \{y\}). \tag{2.67}$$

The adjoint operator $\dot{H}_y^*$ of the operator $\dot{H}_y$ can be written as

$$\dot{H}_y^* = -\Delta, \quad \mathscr{D}(\dot{H}_y^*) = \{g \in H_{loc}^{2,2}(\mathbb{R}^2 \setminus \{y\}) \cap L^2(\mathbb{R}^2) \mid \Delta g \in L^2(\mathbb{R}^2)\}. \tag{2.68}$$

By a simple calculation we are able to find solution of the equation

$$\dot{H}_y^*\psi(k) = k^2\psi(k), \quad \psi(k) \in \mathscr{D}(\dot{H}_y^*), \quad k^2 \in \mathbb{C} \setminus \mathbb{R}, \quad \Im k > 0, \tag{2.69}$$

in the form

$$\psi(k,x) = \frac{i}{4}H_0^{(1)}(k|x-y|), \quad x \in \mathbb{R}^2 \setminus \{y\}, \quad \Im k > 0, \tag{2.70}$$

where $H_0^{(1)}(\cdot)$ denotes Hankel function of the first kind and zeroth order, for more information about such functions see [10]. This implies that our operator $\dot{H}_y^*$ has deficiency indices $(1,1)$. Now, to obtain all self-adjoint extensions of our operator $\dot{H}_y^*$, we decompose $L^2(\mathbb{R}^2)$ with respect to angular momenta as

$$L^2(\mathbb{R}^2) = L^2((0,\infty); r \cdot dr) \bigotimes L^2(S^1), \tag{2.71}$$

where S^1 represents a unit circle on a plane. The basis for $L^2(S^1)$ can be chosen as $\{Y_m(\omega) \mid m \in \mathbb{Z}, 0 \le \theta < 2\pi\}$ with $Y_m(\omega) = \frac{\exp(im\theta)}{\sqrt{2\pi}}$ and $\omega = (\cos(\theta), \sin(\theta))$. We use the unitary transformation

$$\widetilde{U} : L^2((0,\infty); r \cdot dr) \longrightarrow L^2([0,\infty); dr), \quad (\widetilde{U})(r) = r^{\frac{1}{2}}f(r) \tag{2.72}$$

and we rewrite (2.71) as

$$L^2(\mathbb{R}^2) = \bigoplus_{m=-\infty}^{\infty} \widetilde{U}^{-1}L^2((0,\infty); dr) \bigotimes [Y_m]. \tag{2.73}$$

We use this decomposition and rewrite $\dot{H}_y$ as

$$\dot{H}_y = T_y^{-1} \left\{ \bigoplus_{m=-\infty}^{\infty} \widetilde{U}^{-1} \dot{h}_m \widetilde{U} \bigotimes 1 \right\} T_y, \quad y \in \mathbb{R}^2, \tag{2.74}$$

where the operator T_y acts as

$$(T_y g)(x) = g(x+y), \quad g \in L^2(\mathbb{R}^2) \tag{2.75}$$

and $\dot{h}_m$ acts as

$$\dot{h}_m = -\frac{d^2}{dr^2} + \frac{m^2 - \frac{1}{4}}{r^2}, \quad r > 0, \quad m \in \mathbb{Z}. \tag{2.76}$$

The domain of the operator $\dot{h}_0$ can be written as follows

$$\begin{aligned} \mathscr{D}(\dot{h}_0) = \{\phi \in L^2(\mathbb{R}^+) \mid \phi', \phi \in AC_{loc}(\mathbb{R}^+); \\ \overline{\phi(0+)}\phi'_{\pm}(0+) - \overline{\phi'(0+)}\phi_{\pm}(0+) = 0, \dot{h}_0\phi \in L^2(\mathbb{R}^+)\} \end{aligned} \tag{2.77}$$

and the domains for the operators $\dot{h}_m$ as

$$\mathscr{D}(\dot{h}_m) = \{\phi \in L^2(\mathbb{R}^+) \mid \phi', \phi \in AC_{loc}(\mathbb{R}^+); \dot{h}_m\phi \in L^2(\mathbb{R}^+)\}, \quad m \in \mathbb{Z} \setminus \{0\}, \tag{2.78}$$

where $AC_{loc}(\mathbb{R}^+)$ denotes locally absolutely continuous function on $\mathbb{R}^+$ and $\phi_{\pm}(x)$ denotes

$$\phi_{\pm}(x) = r^{\frac{1}{2}} H_0^{(1)}((\pm i)^{\frac{1}{2}} r). \tag{2.79}$$

According to [1, Chapter 1.5] $\dot{h}_m$ are all self-adjoint for $m \neq 0$ and $\dot{h}_0$ is symmetric with deficiency indices $(1,1)$. Also according to [1, Chapter 1.5] we are able to parameterize all self-adjoint extensions of $\dot{h}_0$ as follows

$$\begin{aligned} \dot{h}_{0,\alpha} = -\frac{d^2}{dr^2} - \frac{1}{4r^2}, \quad r > 0, \\ \mathscr{D}(h_{0,\alpha}) = \{\phi \in L^2(\mathbb{R}^+) \mid \phi', \phi \in AC_{loc}(\mathbb{R}^+); \\ 2\pi\alpha\phi_0 + \phi_1 = 0, \dot{h}_{0,\alpha}\phi \in L^2(\mathbb{R}^+)\}, \end{aligned} \tag{2.80}$$

where $-\infty < \alpha \leq \infty$ and the generalized boundary values ϕ_0 and ϕ_1 are defined as

$$\phi_0 = \lim_{r\to 0} [r^{\frac{1}{2}} \ln r]^{-1} \phi(r), \quad \phi_1 = \lim_{r \to 0} r^{-\frac{1}{2}} [\phi(r) - \phi_0 r^{\frac{1}{2}} \ln r], \tag{2.81}$$

where $\phi', \phi \in \mathscr{D}(\dot{h}_0^*)$. From this we are able to conclude this theorem.

Theorem 2.11. *All self-adjoint extensions of $\dot{H}_y$ can be written as*

$$-\Delta_{\alpha,y} = T_y^{-1}\left\{\left[\widetilde{U}^{-1}h_{0,\alpha}\widetilde{U} \oplus \bigoplus_{m=-\infty,m\neq 0}^{\infty} \widetilde{U}^{-1}\dot{h}_m\widetilde{U}\right]\otimes 1\right\}T_y, \qquad -\infty < \alpha \leq \infty, \quad y \in \mathbb{R}^2. \tag{2.82}$$

The special case $\alpha = \infty$ leads to the Hamiltonian of free particle, i.e.

$$-\Delta_{\infty,y} = -\Delta, \quad \mathscr{D}(-\Delta) = H^{2,2}(\mathbb{R}^2). \tag{2.83}$$

Proof: Can be found in [1, Chapter I.5]

The operator $-\Delta_{\alpha,y}$ provides us with the description of a point interaction located at y for $|\alpha| < \infty$. It is worth mentioning that according to [1, Chapter I.5] the expression $-\frac{1}{2\pi\alpha}$ represents the scattering length of the operator $-\Delta_{\alpha,y}$. The following theorem is an application of Krein's formula (Theorem 2.2) to our operator $-\Delta_{\alpha,y}$.

Theorem 2.12. *The resolvent of our operator $-\Delta_{\alpha,y}$ can be written as*

$$(-\Delta_{\alpha,y} - k^2)^{-1} = G_k + 2\pi\left[2\pi\alpha - \Psi(1) + \ln\frac{k}{2i}\right]^{-1}(\overline{G_k(\cdot - y)}, \cdot)G_k(\cdot - y), \tag{2.84}$$

where $k^2 \in \rho(-\Delta_{\alpha,y})$, $\Im k > 0$, $-\infty < \alpha \leq \infty$, $y \in \mathbb{R}^2$ and $\Psi(\cdot)$ is the digamma function. The integral kernel of the resolvent of $-\Delta_{\alpha,y}$ can be thus written as

$$(-\Delta_{\alpha,y} - k^2)^{-1}(x,x') = \frac{i}{4}H_0^{(1)}(k|x-x'|) - \frac{\pi}{8}\left[2\pi\alpha - \Psi(1) + \ln\frac{k}{2i}\right]^{-1} \cdot \cdot H_0^{(1)}(k|x-y|)H_0^{(1)}(k|y-x'|), \qquad k^2 \in \rho(-\Delta_{\alpha,y}), \quad \Im k > 0, \quad x, x' \in \mathbb{R}^2, x' \neq x \neq y \neq x', \tag{2.85}$$

where $\frac{i}{4}H_0^{(1)}(k|x-x'|)$ is the integral kernel of $(-\Delta - k^2)^{-1}$ for $\Im k > 0$, $x, x' \in \mathbb{R}^2$ and $x \neq x'$.

Proof: Can be found in [1, Chapter I.5]

Remark 1. *For more information about the digamma function see [10]. In our case* $\Psi(1)$ *can be written as* $\Psi(1) = \Gamma'(1) = -\int_1^\infty \left(\frac{1}{\lfloor x \rfloor} - \frac{1}{x}\right) dx$*, where* $\lfloor x \rfloor$ *represents the lower integer part of* x*, i.e.* $\lfloor x \rfloor \in \mathbb{Z}$ *and* $x - 1 < \lfloor x \rfloor \leq x$*.*

The next theorem specifies spectral properties of our operator.

Theorem 2.13. *Let* $-\Delta_{\alpha,y}$ *be the operator defined above with* $\alpha \in (-\infty, \infty]$ *and* $y \in \mathbb{R}^2$*. Then the spectrum of our operator satisfies*

$$\sigma_{ess}(-\Delta_{\alpha,y}) = \sigma_{ac}(-\Delta_{\alpha,y}) = [0, \infty), \quad \sigma_{sc}(-\Delta_{\alpha,y}) = \emptyset. \tag{2.86}$$

The point spectrum of our operator can be written as

$$\sigma_p(-\Delta_{\alpha,y}) = \{-4e^{2[-2\pi\alpha + \Psi(1)]}\}, \text{ for } \alpha \in \mathbb{R}. \tag{2.87}$$

The eigenvector to this eigenvalue can be chosen strictly positive in the form

$$G_{2i\exp[-2\pi\alpha+\Psi(1)]}(x - y) = \frac{1}{4} i H_0^{(1)}(2ie^{-2\pi\alpha+\Psi(1)}|x - y|), \quad x \neq y. \tag{2.88}$$

Proof: Can be found in [1, Chapter I.5]

2.2.5 Finite number of point interactions on a plane

In this section we discuss finite number of point interactions in two dimensions. Let us briefly describe the process of self-adjoint extension in dimension two. For more details we refer to [1, Chapter II.4].

We start from the nonnegative operator acting on $L^2(\mathbb{R}^2)$ as

$$-\Delta \mid_{C_0^\infty(\mathbb{R}^2 \setminus Y)}, \tag{2.89}$$

where $Y = \{y_1, \ldots, y_n\} \subset \mathbb{R}^2$. Its closure $\dot{H}_Y$ acts on $L^2(\mathbb{R}^2)$ with the domain $\mathscr{D}(\dot{H}_Y) = H_0^{2,2}(\mathbb{R}^2 \setminus Y)$. The adjoint operator of $\dot{H}_Y$ can be written as

$$\dot{H}_Y^* = -\Delta, \quad \mathscr{D}(\dot{H}_Y^*) = \{g \in H_{loc}^{2,2}(\mathbb{R}^2 \setminus Y) \cap L^2(\mathbb{R}^2) \mid \Delta g \in L^2(\mathbb{R}^2)\}. \tag{2.90}$$

We are interested in solution of the equation

$$\dot{H}_Y^* \psi(k) = k^2 \psi(k), \quad \psi(k) \in \mathscr{D}(\dot{H}_Y^*), \quad k^2 \in \mathbb{C} \setminus \mathbb{R}, \quad \Im k > 0. \tag{2.91}$$

The solution can be written as

$$\psi_j(k,x) = \frac{i}{4}H_0^{(1)}(k \mid x - y_j \mid). \tag{2.92}$$

for $x \in \mathbb{R}^2 \setminus \{y_j\}$, $\Im k > 0$, $y_j \in Y$ and $j = 1, \ldots, N$. The operator $\dot{H}_Y^*$ has deficiency indices (N, N). Thus we have N^2-parameter family of self-adjoint operators of the symmetric operator $\dot{H}_Y$. In general we can obtain all self-adjoint extensions $H_{U,Y}$ of $\dot{H}_Y$ as

$$\begin{aligned} H_{U,Y}\left(g + \sum_{j=1}^{N} c_j \left(\psi_{j+} + \sum_{j'=1}^{N} U_{jj'}\psi_{j'-}\right)\right) = \\ \dot{H}_Y g + i\sum_{j=1}^{N} c_j \left(\psi_{j+} - \sum_{j'=1}^{N} U_{jj'}\psi_{j'-}\right) \end{aligned} \tag{2.93}$$

with the domain

$$\mathscr{D}(H_{U,Y}) = \left\{ g + \sum_{j=1}^{N} c_j \left[\psi_{j+} + \sum_{j'=1}^{N} U_{jj'}\psi_{j'-}\right] \mid g \in \mathscr{D}(\dot{H}_Y), j = 1, \ldots, N \right\}, \tag{2.94}$$

where $U_{jj'}$, $j, j' = 1, \ldots, N$ are elements of unitary matrix in $\mathbb{C}^N$, $c_j \in \mathbb{C}$ and the functions $\psi_{j\pm}$ can be written as

$$\begin{aligned} \psi_{j\pm} = \psi_j(\sqrt{\pm i}, x) = \frac{1}{4} i H_0^{(1)}(\sqrt{\pm i}|x - y_j|), \\ x \in \mathbb{R}^2 - \{y_j\}, \quad \Im\sqrt{\pm i} > 0. \end{aligned} \tag{2.95}$$

The functions $\psi_{j\pm}$ provide a basis set of the deficiency subspaces $\ker[\dot{H}_Y^* \mp i]$. It can be seen that the case $U = -1$ leads to the operator of kinetic energy in $L^2(\mathbb{R}^2)$. Now if we follow the procedure mentioned in [1, Chapter II.4] and use of Theorem 2.3 we come to the following theorem.

Theorem 2.14. *Let $-\Delta_{\alpha,Y}$ be the self-adjoint operator describing point interactions in two dimensions. Then its resolvent can be written as*

$$(-\Delta_{\alpha,Y} - k^2)^{-1} = G_k + \sum_{j,j'=1}^{N} [\Gamma_{\alpha,Y}(k)]^{-1}_{jj'}(\overline{G_k(\cdot - y_j)}, \cdot)G_k(\cdot - y_j). \tag{2.96}$$

Matrix $[\Gamma_{\alpha,Y}(k)]$ *can be written as*

$$[\Gamma_{\alpha,Y}(k)]_{jj'} = \left\{ \frac{1}{2\pi} \left[2\pi\alpha_j - \Psi(1) + \ln\left(\frac{k}{2i}\right) \right] \delta_{jj'} - \tilde{G}_k(y_j - y_{j'}) \right\}_{j,j'=1}^{N}, \tag{2.97}$$

where $\Psi(1) = \Gamma'(1) = -\int_1^\infty \left(\frac{1}{\lfloor x \rfloor} - \frac{1}{x} \right) dx$. *The function* $\tilde{G}_k(x)$ *can be written as*

$$\tilde{G}_k(x) = \begin{cases} 0 & x = 0 \\ G_k(x) & x \neq 0, \end{cases} \tag{2.98}$$

where $G_k(x) = \frac{i}{4} H_0^{(1)}(k|x|)$. *We can rewrite the expression also using the so-called MacDonald function as* $G_k(x) = \frac{2}{\pi} K_0^{(1)}(\kappa|x|)$.

Proof: Can be found in [1, Chapter II.4]

At this point it is worth mentioning what happens in the case when some of the point interactions have its coefficient equal to $\alpha_j = \infty$. If $\alpha_{j_0} = \infty$ then one simply deletes the j_0-th row and line in the matrix $[\Gamma_{\alpha,Y}(k)]$. Now we turn our attention to the domain of the operator $-\Delta_{\alpha,Y}$.

Theorem 2.15. *Let* $\alpha_j \in \mathbb{R}$, $y_j \in Y$ *for* $j \in \hat{N}$. *Then the domain of the operator* $-\Delta_{\alpha,Y}$ *can be written as*

$$\mathscr{D}(-\Delta_{\alpha,Y}) = \{\psi(x) = \phi_k(x) + \sum_{j=1}^{N} [\Gamma_{\alpha,Y}(k)]^{-1}_{jj'} \phi_k(y'_j) G_k(x - y_j)\}, \tag{2.99}$$

where $\phi_k(x) \in \mathscr{D}(-\Delta) = H^{2,2}(\mathbb{R}^2)$, $y_j \in Y$, $\alpha_j \in \mathbb{R}$, $k^2 \in \rho(-\Delta_{\alpha,Y})$, $\Im k > 0$. *Such a decomposition is unique and every* $\psi \in \mathscr{D}(-\Delta_{\alpha,Y})$ *fulfills*

$$(-\Delta_{\alpha,Y} - k^2)^{-1}\psi(x) = (-\Delta - k^2)^{-1}\phi_k(x). \tag{2.100}$$

Furthermore $\psi \in \mathscr{D}(-\Delta_{\alpha,Y})$ *fulfilling* $\psi = 0$ *in an open set* $U \subseteq \mathbb{R}^2$ *satisfies* $-\Delta_{\alpha,Y}\psi = 0$ *in* U.

Proof: Can be found in [1, Chapter II.4].

Next we mention some basic properties of the eigenvalues of the operator $-\Delta_{\alpha,Y}$ in two dimensions.

Theorem 2.16. *Let $-\Delta_{\alpha,Y}$ be the operator defined above, where $y_j \in Y \subset \mathbb{R}^2$ and $\alpha_j \in \mathbb{R}$ for $j \in \hat{N}$. Then the spectrum of $-\Delta_{\alpha,Y}$ fulfills*

$$\begin{aligned} \sigma_{ess}(-\Delta_{\alpha,Y}) = \sigma_{ac}(-\Delta_{\alpha,Y}) = [0, +\infty), \\ \sigma_{sc}(-\Delta_{\alpha,Y}) = \emptyset,\ \sigma_p(-\Delta_{\alpha,Y}) \subset (-\infty, 0). \end{aligned} \tag{2.101}$$

Furthermore $1 \leq \operatorname{card} \sigma_p(-\Delta_{\alpha,Y}) \leq N$ counting multiplicity. Let $\Im k > 0$, then

$$k^2 \in \sigma_p(-\Delta_{\alpha,Y}) <=> \det[\Gamma_{\alpha,Y}(k)] = 0. \tag{2.102}$$

Multiplicity of the eigenvalue 0 of the matrix $\Gamma_{\alpha,Y}(k)$ equals the multiplicity of the eigenvalue k^2 of the operator $-\Delta_{\alpha,Y}$. Moreover, let $E_0 = k_0^2 < 0$ be an eigenvalue of our operator $-\Delta_{\alpha,Y}$. For this eigenvalue we have the corresponding eigenvector in the form

$$\psi_0(x) = \sum_{j=1}^{N} c_j G_{k_0}(x - y_j), \quad \Im k_0 > 0, \tag{2.103}$$

where $C = (c_1, ..., c_N)$ are eigenvectors belonging to the eigenvalue 0 of the matrix $\Gamma_{\alpha,Y}(k_0)$. The operator $-\Delta_{\alpha,Y}$ has the ground state which is non-degenerate and the corresponding eigenvector can be chosen strictly positive, which can be restated as that the eigenvector C can be chosen strictly positive, i.e. $c_j > 0$ for all $j \in \hat{N}$.

Proof: Can be found in [1, Chapter II.4]

2.2.6 One point interaction in three dimensions

In this subsection we describe one point interaction in dimension three. In the following subsection we describe generalization for a finite number of point interactions. Our approach will be analogous to that used in two dimensions. We start from the nonnegative operator

$$-\Delta \mid_{C_0^\infty(\mathbb{R}^3 \setminus \{y\})}, \tag{2.104}$$

where $-\Delta$ denotes the Laplacian operator on $L^2(\mathbb{R}^3)$ and $y \in \mathbb{R}^3$. The closure of such an operator can be written as

$$\dot{H}_y = -\Delta, \quad \mathscr{D}(\dot{H}_y) = H_0^{2,2}(\mathbb{R}^3 \setminus \{y\}), \tag{2.105}$$

where $H_0^{2,2}$ denotes the corresponding Sobolev space. Its adjoint can be expressed as

$$\begin{gathered}\dot{H}_y^* = -\Delta, \\ \mathscr{D}(\dot{H}_y^*) = \{g \in H_{loc}^{2,2}(\mathbb{R}^3 \setminus \{y\}) \cap L^2(\mathbb{R}^3) \mid -\Delta g \in L^2(\mathbb{R}^3)\},\end{gathered} \tag{2.106}$$

where $H_{loc}^{2,2}$ denotes the local Sobolev space (for the definition see [3, Section XIII.14]). A simple calculation shows that the solution of the equation

$$\dot{H}_y^* \psi(k) = k^2 \psi(k), \quad \psi(k) \in \mathscr{D}(\dot{H}_y^*), \quad k^2 \in \mathbb{C} \setminus \mathbb{R}, \quad \Im k > 0 \tag{2.107}$$

is given in the form

$$\psi(k, x) = \frac{\exp(ik|x-y|)}{|x-y|}, \quad x \in \mathbb{R}^3 \setminus \{y\}, \quad \Im k > 0. \tag{2.108}$$

A consequence of this result is that the operator $\dot{H}_y^*$ has deficiency indices $(1, 1)$. Now we decompose $L^2(\mathbb{R}^3)$ with respect to angular momenta. In other words we introduce spherical coordinates centered around the point y. This can be written as

$$L^2(\mathbb{R}^3) = L^2((0, \infty); r^2 \cdot dr) \bigotimes L^2(S^2), \tag{2.109}$$

where S^2 represents unit sphere in $\mathbb{R}^3$. Basis of the $L^2(S^2)$ is provided by the set of spherical harmonics $\{Y_{l,m} \mid l \in \mathbb{N}_0, m \in \{-l, \ldots, l\}\}$. Using the unitary transformation

$$U : L^2((0, \infty); r^2 \cdot dr) \longrightarrow L^2([0, \infty); dr), \quad (U)(r) = rf(r) \tag{2.110}$$

we rewrite (2.109) as

$$L^2(\mathbb{R}^3) = \bigoplus_{l=0}^{\infty} U^{-1} L^2((0, \infty); dr) \bigotimes [Y_{l,-l}, \ldots, Y_{l,l}]_\lambda, \tag{2.111}$$

where the notation $[Y_{l,-l}, \ldots, Y_{l,l}]_\lambda$ denotes a linear span of the set of vectors $Y_{l,-l}, \ldots, Y_{l,l}$. We introduce the operator T_y which acts as a translation by the vector y, i.e.

$$(T_y g)(x) = g(x + y), \quad g \in L^2(\mathbb{R}^3). \tag{2.112}$$

Now we are ready to rewrite $\dot{H}_y$ as

$$\dot{H}_y = T_y^{-1} \left\{ \bigoplus_{l=}^{\infty} U^{-1} \dot{h}_l U \bigotimes 1 \right\} T_y, \quad y \in \mathbb{R}^3. \tag{2.113}$$

The operator $\dot{h}_l$ acts as

$$\dot{h}_l = -\frac{d^2}{dr^2} + \frac{l(l+1)}{r^2}, \quad r > 0, \quad l \in \mathbb{N}_0 \tag{2.114}$$

with the domain

$$\begin{aligned} \mathscr{D}(\dot{h}_0) = \{\phi \in L^2(\mathbb{R}^+) \mid \phi', \phi \in AC_{loc}(\mathbb{R}^+); \\ \phi(0+) = \phi'(0+) = 0; \phi'' \in L^2(\mathbb{R}^+)\} = H_0^{2,2}(\mathbb{R}^+), \\ \mathscr{D}(\dot{h}_l) = \{\phi \in L^2(\mathbb{R}^+) \mid \phi', \phi \in AC_{loc}(\mathbb{R}^+); \dot{h}_l \phi \in L^2(\mathbb{R}^+)\} \end{aligned} \tag{2.115}$$

for $l \in \mathbb{N}$ where $AC_{loc}(\mathbb{R}^+)$ denotes locally absolutely continuous function on $\mathbb{R}^+$. According to [4, Section X.1] the operators $\dot{h}_l$ are all self-adjoint for $l > 0$ and the operator $\dot{h}_0$ is symmetric with deficiency indices $(1, 1)$. The operator $\dot{h}_0$ can be extended to a self-adjoint operator $\dot{h}_{0,\alpha}$ according to [1, Section 1.1] as

$$\begin{aligned} \dot{h}_{0,\alpha} = -\frac{d^2}{dr^2}, \\ \mathscr{D}(h_{0,\alpha}) = \{\phi \in L^2(\mathbb{R}^+) \mid \phi', \phi \in AC_{loc}(\mathbb{R}^+); \\ -4\pi\alpha\phi(0+) + \phi'(0+) = 0; \phi'' \in L^2(\mathbb{R}^+)\} \end{aligned} \tag{2.116}$$

for $-\infty < \alpha \leq \infty$. Now we are ready to formulate the theorem concerning all self adjoint extensions of $\dot{H}_y$.

Theorem 2.17. *All self-adjoint extensions of $\dot{H}_y$ are given in the form*

$$-\Delta_{\alpha,y} = T_y^{-1} \left\{ \left[U^{-1} h_{0,\alpha} U \oplus \bigoplus_{l=1}^{\infty} U^{-1} \dot{h}_l U \right] \otimes 1 \right\} T_y, \tag{2.117}$$

where $-\infty < \alpha \leq \infty$ and $y \in \mathbb{R}^3$. The special case $\alpha = \infty$ leads to the operator of kinetic energy, i.e.

$$-\Delta_{\infty,y} = -\Delta, \quad \mathscr{D}(-\Delta) = H^{2,2}(\mathbb{R}^3). \tag{2.118}$$

Proof: Can be found in [1, Chapter I.1]

The operator $-\Delta_{\alpha,y}$ gives us the description of the point interaction located at y for $|\alpha| < \infty$. According to [1, Chapter I.1] the expression $-\frac{1}{4\pi\alpha}$ represents the scattering length of the operator $-\Delta_{\alpha,y}$. Next we turn our attention to the resolvent of $-\Delta_{\alpha,y}$.

Theorem 2.18. *The resolvent of our operator $-\Delta_{\alpha,y}$ is given in the form*

$$(-\Delta_{\alpha,y} - k^2)^{-1} = G_k + (\alpha - ik(4\pi)^{-1})^{-1}(\overline{G_k(\cdot - y)}, \cdot)G_k(\cdot - y), \quad (2.119)$$

where $k^2 \in \rho(-\Delta_{\alpha,y})$, $\Im k > 0$, $-\infty < \alpha \leq \infty$, $y \in \mathbb{R}^3$. The integral kernel of the resolvent $-\Delta_{\alpha,y}$ can be written explicitly as

$$\begin{aligned}(-\Delta_{\alpha,y} - k^2)^{-1}(x, x') = \frac{\exp(ik|x - x'|)}{4\pi|x - x'|} + (\alpha - ik(4\pi)^{-1})^{-1} \cdot \\ \cdot \frac{\exp(ik|x - y|)}{4\pi|x - y|} \frac{\exp(ik|x' - y|)}{4\pi|x' - y|}\end{aligned} \quad (2.120)$$

for $k^2 \in \rho(-\Delta_{\alpha,y})$, $\Im k > 0$, $x, x' \in \mathbb{R}^3$, $x' \neq x \neq y \neq x'$ where $\frac{\exp(ik|x-x'|)}{4\pi|x-x'|}$ is the resolvent kernel of the free particle Hamiltonian $(-\Delta - k^2)^{-1}$ for $\Im k > 0$, $x, x' \in \mathbb{R}^3$ and $x \neq x'$.

Proof: Can be found in [1, Chapter I.5]

Now we collect additional information concerning spectral properties of our operator.

Theorem 2.19. *Let $-\Delta_{\alpha,y}$ be the operator defined above for $\alpha \in (-\infty, \infty]$ and $y \in \mathbb{R}^3$. The essential, absolutely continuous and singularly continuous spectrum of our operator is given by*

$$\sigma_{ess}(-\Delta_{\alpha,y}) = \sigma_{ac}(-\Delta_{\alpha,y}) = [0, \infty), \quad \sigma_{sc}(-\Delta_{\alpha,y}) = \emptyset. \quad (2.121)$$

The point spectrum of the operator $-\Delta_{\alpha,y}$ can be written for $\alpha \in (-\infty, 0)$ as

$$\sigma_p(-\Delta_{\alpha,y}) = \{-(4\pi\alpha)^2\} \quad (2.122)$$

with the normalized strictly positive eigenvector in the form

$$4\pi\sqrt{-\alpha}G_{-(4\pi\alpha)^2}(x - y) = \frac{\exp(4\pi\alpha \mid x - y \mid)}{\sqrt{-\alpha} \mid x - y \mid}, \quad (2.123)$$

where $x \neq y$.

Proof: Can be found in [1, Chapter I.1]

2.2.7 Finite number of point interactions in three dimensions

In this section we give rigorous meaning to the expression

$$H = -\Delta - \sum_{k=1}^{N} \beta_j \delta(\cdot - y_j) \tag{2.124}$$

which formally describes N point interactions located at distinct points $y_1, \ldots, l_N$ in $\mathbb{R}^3$. In this section we will briefly summarize basic properties of such operators. We start from the closed symmetric operator as in the previous cases.

Theorem 2.20. *Let $\dot{H}_Y$ be a closed symmetric operator*

$$\begin{aligned} \dot{H}_Y &= -\Delta \mid_{\mathscr{D}_Y}, \\ \mathscr{D}_Y &= \{\theta \in H^{2,2}(\mathbb{R}^3) \mid \theta(y_j) = 0, y_j \in Y, j \in \hat{N}\}, \end{aligned} \tag{2.125}$$

where $Y = \{y_1, \ldots, y_N\}$. The operator $\dot{H}_Y$ has deficiency indices (N, N) and the deficiency subspaces can be written as

$$\mathscr{K}_{\pm} = Ran(\dot{H}_Y \pm i)^{\perp} = [G_{\sqrt{\pm i}}(\cdot - y_1), \ldots, G_{\sqrt{\pm i}}(\cdot - y_N)], \quad \Im\sqrt{\pm i} > 0, \tag{2.126}$$

where $G_k(x)$ denotes the integral kernel of the free particle Hamiltonian.

Proof: Can be found in [1, Chapter II.1]

From the theory we obtain N^2-parameter family of self-adjoint extensions belonging to the operator $-\Delta \mid_{\mathscr{D}_Y}$. However we are not interested in all of those extensions. We restrict ourselves to so-called separated boundary conditions at the points y_i, $i = \hat{N}$. These local conditions can be described by N-parameter family defined by the resolvent in the form

$$(-\Delta_{\alpha,Y} - k^2)^{-1} = G_k + \sum_{j,j'=1}^{N} [\Gamma_{\alpha,Y}(k)]^{-1}_{jj'} (\overline{G_k(\cdot - y_j)}, \cdot) G_k(\cdot - y_j), \tag{2.127}$$

where $G_k(x) = \frac{\exp(ik|x|)}{4\pi|x|}$ and

$$[\Gamma_{\alpha,Y}(k)]_{jj'} = \left[\left(\alpha_j - \frac{ik}{4\pi}\right)\delta_{jj'} - \tilde{G}_k(y_j - y_{j'})\right]_{j,j'=1}^{N}. \tag{2.128}$$

$\tilde{G}_k(x)$ represents the function

$$\tilde{G}_k(x) = \begin{cases} 0 & x = 0 \\ G_k(x) & x \neq 0. \end{cases} \tag{2.129}$$

In the next theorem we give the explicit characterization of the domain and locality of the operator $-\Delta_{\alpha,Y}$.

Theorem 2.21. *The domain $\mathscr{D}(-\Delta_{\alpha,Y})$ of the operator can be written as $-\Delta_{\alpha,Y}$*

$$\mathscr{D}(-\Delta_{\alpha,Y}) = \{\psi(x) = \phi_k(x) + \sum_{j=1}^{N} a_j G_k(x - y_j)\}, \quad x \in \mathbb{R}^3 \setminus Y, \tag{2.130}$$

where $\phi_k(x) \in \mathscr{D}(-\Delta) = H^{2,2}(\mathbb{R}^3)$, $y_j \in Y$, $-\infty < \alpha_j \leq \infty$ and $k^2 \in \rho(-\Delta_{\alpha,Y})$, $\Im k > 0$. The coefficients a_j are given by

$$a_j = \sum_{j'=1}^{N} [\Gamma_{\alpha,Y}(k)]^{-1}_{jj'} \phi(y'_j), \tag{2.131}$$

where $j \in \hat{N}$. Also this decomposition is unique and the function ψ fulfills

$$(-\Delta_{\alpha,Y} - k^2)^{-1}\psi(x) = (-\Delta - k^2)^{-1}\phi_k(x). \tag{2.132}$$

Furthermore if $\psi \in \mathscr{D}(-\Delta_{\alpha,Y})$ fulfils $\psi = 0$ in an open set $U \subseteq \mathbb{R}^3$ then $-\Delta_{\alpha,Y}\psi = 0$ in U.

Proof: Can be found in [1, Chapter II.1]

Generally we expect the Hamiltonian $H = -\Delta + V$ where V is multiplication operator to be local in the sense

$$\psi(x) = 0 \ \forall x \in M \subset \mathbb{R}^3 \Rightarrow H\psi(x) = 0 \ \forall x \in M,$$

where M is an open subset in $\mathbb{R}^3$. We expect that such operators as H to have no singular continuous spectrum and no positive embedded eigenvalues. This is also true for point interactions Hamiltonians. Properties of the spectrum of our operator $\Delta_{\alpha,Y}$ as well as the way how to calculate the eigenvalues and eigenvectors from the zero eigenvalues of the $N \times N$ matrix are the content of following theorem.

Theorem 2.22. *Let $-\Delta_{\alpha,Y}$ be the operator defined above, where $y_j \in Y$ and $-\infty < \alpha_j \leq \infty$ for $j \in \hat{N}$. Then the essential spectrum of the operator $-\Delta_{\alpha,Y}$ is purely absolutely continuous and fulfills*

$$\sigma_{ess}(-\Delta_{\alpha,Y}) = \sigma_{ac}(-\Delta_{\alpha,Y}) = [0, +\infty), \quad \sigma_{sc}(-\Delta_{\alpha,Y}) = \emptyset. \tag{2.133}$$

Furthermore

$$\sigma_p(-\Delta_{\alpha,Y}) \subset (-\infty, 0) \tag{2.134}$$

and negative point spectrum of the operator $-\Delta_{\alpha,Y}$ has at most N eigenvalues counting multiplicity. Let $\Im k > 0$, then

$$\begin{aligned} k^2 \in \sigma_p(-\Delta_{\alpha,Y}) <=> \\ <=> \det[\Gamma_{\alpha,Y}(k)] = \det\left[\left(\alpha_j - \frac{ik}{4\pi}\right)\delta_{jj'} - \tilde{G}_k(y_j - y_{j'})\right] = 0. \end{aligned} \tag{2.135}$$

Multiplicity of the eigenvalue 0 of the matrix $\Gamma_{\alpha,Y}(k)$ is equal to the multiplicity of the eigenvalue k^2 of the operator $-\Delta_{\alpha,Y}$. Moreover, let $E_0 = k^2 < 0$ be an eigenvalue of our operator $-\Delta_{\alpha,Y}$. For this eigenvalue we have the corresponding eigenvector in the form

$$\psi_0(x) = \sum_{j=1}^{N} c_j G_{k_0}(x - y_j), \quad \Im k_0 > 0, \tag{2.136}$$

where $C = (c_1, ..., c_N)$ are eigenvectors belonging to the eigenvalue 0 of the matrix $\Gamma_{\alpha,Y}(k_0)$. If the operator $-\Delta_{\alpha,Y}$ has a ground state then it is non-degenerate and the corresponding eigenvector can be chosen strictly positive, which can be restated as the eigenvector C can be chosen strictly positive i.e. $c_j > 0$ for all $j \in \hat{N}$.

Proof: Can be found in [1, Chapter II.1]

2.3 Birman-Schwinger formula

In this subsection we introduce a different way how to address Hamiltonians with singular interactions. The approach sketched in this section is based on the Birman-Schwinger formula. This approach is similar to the Krein's formula in the way that the resolvent of the desired operator is expressed as a sum of the resolvent of the free particle Hamiltonian and another operator. The main differences between the Krein's formula and the Birman-Schwinger formula are the following. By means of the Krein's formula we describe point interaction supported by points. Such interactions can be well defined up to the dimension three. The Birman-Schwinger formula can be used for the operators, where singular interactions are supported by a manifold of codimension one and it can be used even to dimensions higher than three. We note that for the dimension one both approaches give the same result, because the points are the "manifolds" of codimension one on the line. The operator describing the difference between the operators for the case of the Birman-Schwinger formula is the integral operator, for the case of Krein's formula it is usually finite rank operator described by a matrix.

We will present facts which were derived in [11]. First we show that such operators can be defined with the help of associated quadratic forms. We define operators which can be written in the following form

$$H = -\Delta + \gamma m, \tag{2.137}$$

where m is a positive Radon measure on $\mathbb{R}^d$, $d = 1, 2, 3$. The Radon measure r is a measure defined on a Hausdorff space which is finite on compact sets and inner regular, i.e. $r(A) = \sup\{r(V) \mid V \text{ compact subset of A}\}$, where A is a Borel set. The function $\gamma : \mathbb{R}^d \to \mathbb{R}$ is a bounded Borel measurable function chosen in such a way that the following relation holds

$$\int_{\mathbb{R}^d} |f(x)|^2(1 + |\gamma(x)|^2)m(dx) \leq a \int_{\mathbb{R}^d} |\nabla f(x)|^2 dx + b \int_{\mathbb{R}^d} |f(x)|^2 dx, \tag{2.138}$$

where $f \in \mathscr{S}(\mathbb{R}^d)$ and $a < 1$ and b are constants. We introduce a linear bounded transformation

$$\begin{aligned} I_m := H^{1,2}(\mathbb{R}^d) \to L^2(\mathbb{R}^d, m) =: L^2(m), \\ I_m f = f \quad \forall f \in (\mathbb{R}^d). \end{aligned} \tag{2.139}$$

The existence of such a transformation follows from the fact that the Schwartz space $\mathscr{S}(\mathbb{R}^d)$ is dense in the Sobolev space $H^{1,2}(\mathbb{R}^d)$. We note that we will use the notation where f denotes continuous function from dx-equivalence class, i.e. $f \in L^2(\mathbb{R}^d, dx)$, and also function from m-equivalence class, i.e. $f \in L^2(m)$. It can be seen that the inequality (2.138) holds for all functions from $f \in H^{1,2}(\mathbb{R}^d)$ as long as we replace f on the left-hand side by $I_m f$. We define the quadratic form $\mathscr{E}_{\gamma m}$ as

$$\mathscr{E}_{\gamma m}(f,g) = \int_{\mathbb{R}^d} \overline{\nabla f(x)} \nabla g dx + \int_{\mathbb{R}^d} I_m \overline{f(x)} I_m g(x) \gamma(m) m(dx) \tag{2.140}$$

for all $f, g \in \mathscr{D}(\mathscr{E}_{\gamma m}) = H^{1,2}(\mathbb{R}^d)$. According to [13, Theorem 5.37] we can associate with the quadratic form $\mathscr{E}_{\gamma m}$ the self-adjoint operator $H_{\gamma m}$. The special case H_0, i.e. $\gamma m = 0$ corresponds to the Hamiltonian of the free particle on $\mathbb{R}^d$. Furthermore the inequality (2.138) is fulfilled if the measure m belongs to the generalized Kato class and γ is a bounded Borel measurable function.

Remark 2. *The measure m belongs to the generalized Kato class if*

$$\begin{aligned} \sup_{x\in\mathbb{R}} m([x,x+1]) < \infty \quad & \textit{for } d = 1, \\ \lim_{\epsilon\to 0+} \sup_{x\in\mathbb{R}^2} \int_{B(x,\epsilon)} |\ln(|x-y|)| m(dy) = 0 \quad & \textit{for } d = 2, \\ \lim_{\epsilon\to 0+} \sup_{x\in\mathbb{R}^3} \int_{B(x,\epsilon)} \frac{1}{|x-y|} m(dy) = 0 \quad & \textit{for } d = 3, \end{aligned} \tag{2.141}$$

where d denotes dimension and $B(x,\epsilon)$ is the sphere with the radius ϵ and center x.

At this point it is worth mentioning that a lower semi-bounded operator $H_0 + V$ consisted of the Laplacian and the multiplication operator V can be written as $H_{\gamma m}$, if the measure $m = |V|dx$ is from the Kato class and the function γ is equal to $\gamma = \operatorname{sgn} V$.

We denote $G_k(x)$, which for the $k \in \{x \in \mathbb{C} \mid \Im k > 0\} =: \mathbb{C}^+$ coincides with the integral kernel of the Hamiltonian of free particle H_0 on $L^2(\mathbb{R}^d)$. We have already met these functions in the previous part of this chapter when introducing the Krein's formula. They can be written depending on

the dimension d as:

$$\begin{aligned} G_k(x) &:= \frac{i}{2k}\exp(ik|x|) \quad d=1, x\in\mathbb{R}, \\ G_k(x) &:= \frac{2}{\pi}K_0^{(1)}(-ik|x|) \quad d=2, x\in\mathbb{R}^2\setminus\{0\}, \\ G_k(x) &:= \frac{\exp(ik|x|)}{4\pi|x|} \quad d=3, x\in\mathbb{R}^3\setminus\{0\}, \end{aligned} \tag{2.142}$$

where $k \in \mathbb{C}\setminus\{0\}$ and $K_0^{(1)}$ denotes the modified Bessel function of the second kind and zeroth order usually called MacDonald function. Let μ, ν be arbitrary Radon measures on $\mathbb{R}^d$, which satisfies $\mu(\{a\}) = \nu(\{a\}) = 0$ $\forall a \in \mathbb{R}^d$ for $d \geq 2$. For the Borel measurable functions $f, h : \mathbb{R}^d \to \mathbb{C}$ we define the expression $f * g\mu(x)$ as

$$f * g\mu(x) := \int_{\mathbb{R}^d} f(x-y)g(y)\mu(dy), \tag{2.143}$$

always when the right-hand side of the equation is defined. Furthermore we denote the integral operator $R_{\mu,\nu}(k) : L^2(\mu) \to L^2(\nu)$ with its kernel $G_k(x-y)$.

$$R_{\mu,\nu}(k)h = G_k * h\mu \quad \nu - \text{a.e.} \tag{2.144}$$

for all $h \in (R_{\mu,\nu}(k)) \subset L^2(\mu)$. According to [11] we can write the resolvent of our operator $H_{\gamma m}$ as $R(k) = (H_{\gamma m} - k^2)^{-1}$ for $k^2 \in \rho(H_{\gamma m})$ as follows

$$R(k) := R_0(k) - R_{m,dx}(k)[I + \gamma I_m R_{m,dx}(k)]^{-1}\gamma I_m R_0(k), \tag{2.145}$$

where $R_0(k)$ is the resolvent of Dirichlet Laplacian on $L^2(\mathbb{R}^d)$. The expression is valid when the right hand side of the equation is well defined, i.e. the operator $I + \gamma I_m R_{m,dx}(k)$ on $L^2(\mathbb{R}^d)$ is invertible. In the next lemma we give a different form of the previous expression and certain spectral properties of our operator $H_{\gamma m}$. The form we will present is more suitable for the analysis of singular interactions as well as for the use of Birgman-Schwinger principle for the analysis of point spectra.

Lemma 2.1. *a) For $\mu \in \{m, dx\}$ and $k \in \mathbb{C}^+$ we can write the equality $I_m R_{\mu,dx}(k) = R_{\mu,m}(k)$.*
b) There is a positive real number κ_0 so that the operator $I + \gamma R_{m,m}(i\kappa)$ on $L^2(m)$ has everywhere defined a bounded inverse for all $\kappa_0 \leq \kappa \leq \infty$.
c) Let $k \in \mathbb{C}^+$. Suppose that $I + \gamma R_{m,m}(k)$ is invertible and the operator

$$R(k) := R_0(k) - R_{m,dx}(k)[I + \gamma R_{m,m}(k)]^{-1}\gamma R_{dx,m}(k) \tag{2.146}$$

is everywhere defined on $L^2(\mathbb{R}^d)$. *Then the resolvent of* $H_{\gamma m}$ *for* $k^2 \in \rho(H_{\gamma m})$ *can be written as* $(H_{\gamma m} - k^2)^{-1} = R(k)$.
d) Let $k \in \mathbb{C}^+$ *then* $\dim\ker(H_{\gamma m} - k^2) = \dim\ker(I + \gamma R_{m,m}(k))$.

Proof: Can be found in [11]

2.3.1 Singular interactions using Birman Schwinger argument

We start this subsection by mentioning certain useful properties which are generally valid for the operators in the form (2.137). For a more complete reference we refer the reader to [11] or [12]. Later on we will apply these lemmas to our problem which can be formally described by the operator

$$H_{\mu,\Gamma} = -\Delta - \mu(x)\delta(x - \Gamma), \tag{2.147}$$

where $\mu(x) \geq 0$ is bounded Borel measurable function on Γ and Γ is the manifold of the codimension one. But first we will state one lemma and two more theorems for the general case Hamiltonian $H_{\gamma m}$.

Lemma 2.2. *Let* $k \in \mathbb{C}^+$ *and suppose that the measure* m *is finite. Then the operator* $R_{m,dx}(k)$ *is compact.*

Proof: Can be found in [11]

The next theorem deals with the essential spectrum of our operator.

Theorem 2.23. *Let the measure* $|\gamma|m$ *be finite, then the essential spectrum of the operator* $H_{\gamma m}$ *is* $\sigma_{ess}(H_{\gamma m}) = [0, \infty)$.

Proof: Can be found in [11]

The next theorem gives us a description of the continuous part of the spectrum for the case the measure m belongs to the generalized Kato class and m is finite.

Theorem 2.24. *Let the measure* $|\gamma|m$ *have compact support and let it belong to generalized Kato class. Then the following claims are valid:*
a) the singular continuous spectrum of the operator $H_{\gamma m}$ *is* $\sigma_{sc}(H_{\gamma m}) = \emptyset$,
b) the set of all positive eigenvalues of the operator $H_{\gamma m}$ *is discrete,*
c) absolutely continuous spectrum of the operator $H_{\gamma m}$ *is* $\sigma_{ac}(H_{\gamma m}) = [0, \infty)$.

Proof: Can be found in [11]

Now we sum up the important properties about our operator $H_{\mu,\Gamma}$ which we can formally write as (2.147).

Theorem 2.25. *Let $\mu : \Gamma \to \mathbb{R}$ be any bounded Borel measurable function. We define the quadratic form as*

$$E_{\mu,\Gamma}(f,g) := \int_{\mathbb{R}^d} \nabla\overline{f}(x)\nabla g(x)dx + \int_{\Gamma} \overline{f(x)}g(x)\mu(x)vol_{d-1}(dx) \qquad (2.148)$$

for all the $f, g \in \mathscr{D}(E_{\mu,\Gamma}) := C_0^\infty(\mathbb{R}^d)$. The quadratic form is lower semi-bounded and closable on $L^2(\mathbb{R}^d)$. Lower semi-bounded self-adjoint operator $H_{\mu,\Gamma}$ associated with the closure $\overline{E_{\mu,\Gamma}}(f,g)$ of $E_{\mu,\Gamma}(f,g)$ has the following properties:
a) $\sigma_{ess}(H_{\mu,\Gamma}) = [0,\infty)$ if $\int_\Gamma \overline{f(x)}g(x)|\mu(x)|vol_{d-1}(dx) < \infty$ and
b) $\sigma_{ac}(H_{\mu,\Gamma}) = [0,\infty)$, $\sigma_{sc}(H_{\mu,\Gamma}) = \emptyset$ if $\mu(x) = 0$ outside of a compact set.

Proof: Can be found in [11]

If we want to apply this theorem to the operator in the form (2.137) where m is a Dirac measure supported by a graph Γ in $\mathbb{R}^2$ we need several additional conditions on the graph. According to [12] we have to employ conditions in the following way:
a) edge smoothness: each edge of our graph Γ is C^1 a function $\gamma_j : I_j \to \mathbb{R}^2$, where I_j is finite, semi-finite or infinite interval. Additionally we want to be able to parametrize the edges by arc length,
b) cusp absence: edges meet at vertices at nonzero angles,
c) local finiteness: each compact subset of $\mathbb{R}^2$ contains at most a finite number of edges and vertices of Γ.
These conditions can be generalized for higher dimensions. We just need to employ analogous versions of them for $(d-1)$-dimensional manifolds embedded in $\mathbb{R}^d$.

Remark 3. *There exists alternative way of introducing the operators $H_{\mu,\Gamma}$ with singular interactions. This approach was described in [11]. We define the operator $H_{\nu,\Gamma}$ with the help of boundary condition. This operator will act on the space $\mathscr{D}(H_{\nu,\Gamma}) = \{f \in H^{1,2}(\mathbb{R}^d) \cap C_0(\mathbb{R}^d), |f| \in H^{2,2}(\mathbb{R}^d) \cap C^\infty(\mathbb{R}^d) \mid \forall x \in \Gamma : \partial_{n_+} f(x) - \partial_{n_-} f(x) = \nu(x)f(x)\}$ where $\partial_{n\pm} f(x)$ denotes a derivative of the function f in the direction of the normal vector of the manifold Γ. This approach describes δ point interactions at the points of the manifold.*

Chapter 3

Properties of the ground state for the one dimensional case

In this chapter we give a review of the properties of the ground state for point interactions on a line and for a more general case of quantum graphs presented in [5] and [6].

3.1 Ground state on the line

The property we will show for the ground state on the line for the operator (1.1) is the following: an increase in distance between attractive point interactions results in an increase of the ground state energy. There is more than one way how to prove this property. One of them is to employ the proof based on singularity of the resolvent. Another approach is based on so called Neumann bracketing.

The method of the Neumann bracketing([3, Section XIII.15, Proposition 3]) is based on the comparison of the spectrum of the operator and the operator with added Neumann boundary condition. This proof is based on adding Neumann boundary condition at the point x, where the ground state eigenfunction of the system satisfies $\psi'(x) = 0$. To employ this approach we need additional conditions on the signs of the derivatives of the ground state function from left and right at point interactions sites, i.e. $\psi_0'(y+) < 0$ and $\psi_0'(y-) > 0$. This is needed to ensure that there is a point between the two point interaction where ψ' vanished; it follows from the assumptions on

the signs of derivatives and the convexity of the ground state. Convexity of the ground state follows from the positivity of the ground state and the eigenvector equation $-\Delta\psi = -E\psi$, $E > 0$. It can be seen that the original operator $-\Delta_{\alpha,Y}$ and the operator $-\Delta^N_{\alpha,Y}$ with the added Neumann condition have the same ground state. The Neumann condition splits the operator to two operators on halflines, i.e. $-\Delta^N_{\alpha,Y} = -\Delta^{N,(-\infty,x)}_{\alpha,Y} \oplus -\Delta^{N,(x,\infty)}_{\alpha,Y}$. Next we define the operator $-\Delta^{N,2}_{\alpha,Y} = -\Delta^{N,(-\infty,x)}_{\alpha,Y} \oplus -\Delta^N_{(0,a)} \oplus -\Delta^{N,(x,\infty)}_{\alpha,Y}$, where $-\Delta^N_{(0,a)}$ denotes Neumann Laplacian on the interval $(0,a)$ (for the definition see [3, Section XIII.15]). Adding Neumann Laplacian does not change negative point spectrum. Then we remove Neumann boundary conditions what completes the proof. This approach is discussed in [5].

There is another way how to prove our theorem. It is based on viewing the line as an unbranched graph with vertices at the point interactions sites and employ the scaling of the ground state eigenfunction at the inner part of the edges of the graph. This proof will be discussed later on in this chapter.

In this section we present the proof of our theorem based on the singularity of the resolvent of our operator $-\Delta_{\alpha,Y}$ given by Theorem 2.25.

Theorem 3.1. *Let $-\Delta_{\alpha,Y_1}$, $-\Delta_{\alpha,Y_2}$ be the point interaction Hamiltonians defined above. Suppose that* $\operatorname{card} Y_1 = \operatorname{card} Y_2$, *$\alpha_k < 0$ for all k and that $|y_{1,i} - y_{1,j}| \le |y_{2,i} - y_{2,j}|$ holds for all i, j and $|y_{1,i} - y_{1,j}| < |y_{2,i} - y_{2,j}|$ for at least one pair of i, j. Then the ground states of the operators $-\Delta_{\alpha,Y_1}$, $-\Delta_{\alpha,Y_2}$ satisfy*

$$\min \sigma_p(-\Delta_{\alpha,Y_1}) < \min \sigma_p(-\Delta_{\alpha,Y_2}). \tag{3.1}$$

Proof. The behavior of the ground state energy with respect to the distance between point interactions sites is encoded in the matrix $\Gamma_{\alpha,Y}(\kappa)$, where $-\kappa^2 = E$ is the ground state energy. The lowest eigenvalue of the operator $-\Delta_{\alpha,Y}$is related to the lowest eigenvalue of the matrix $\Gamma_{\alpha,Y}(\kappa)$. This is the simple result of the monotonicity of the elements of the matrix $\Gamma_{\alpha,Y}(\kappa)$ with the respect to κ. In view of the secular equation $\det \Gamma_{\alpha,Y}(\kappa) = 0$, the lowest eigenvalue λ_0 is given by

$$\lambda_0(\alpha, Y; \kappa) = \min_{|C|=1} (C, \Gamma_{\alpha,Y}(\kappa) C), \tag{3.2}$$

where $C \in \mathbb{C}^n$ with $|C| = 1$. According to Theorem 2.8 we know that

$$\Gamma_{\alpha,Y}(\kappa)_{ij} = -\frac{\delta_{ij}}{\alpha_i} - \frac{1}{2\kappa} e^{-\kappa L_{ij}}, \tag{3.3}$$

where $L_{ij} = |y_i - y_j|$. Now we write down λ_0 explicitly as

$$\begin{aligned} \lambda_0(\kappa) &= \min_{|C|=1} (C, \Gamma_{\alpha,Y}(\kappa) C) \\ &= \sum_{i=1}^{N} |c_i|^2 \left(-\frac{1}{\alpha_i} - \frac{1}{2\kappa} \right) - 2 \sum_{i=1}^{N} \sum_{j=1}^{i-1} Re \left(\overline{c_i} c_j \frac{e^{-\kappa L_{ij}}}{2\kappa} \right). \end{aligned} \tag{3.4}$$

The semigroup $\left\{ e^{-t\Gamma_{\alpha,Y(\kappa)}} \right\}$ is positivity improving and as a result of this fact according to [3, Section XIII.12] and [3, Problem XIII.97] we can choose C for which the minimum is achieved as strictly positive, i.e. $c_i > 0$ for all $i = 1, \ldots, n$. Now we can rewrite the previous expression as

$$\lambda_0(\alpha, Y; \kappa) = \min_{|C|=1, C>0} (C, \Gamma_{\alpha,Y}(\kappa) C). \tag{3.5}$$

We introduce two configurations of point interactions (α, Y) and $(\alpha, \tilde{Y})$, which satisfy $L_{ij} \leq \tilde{L_{ij}}$ for all (i, j) and $L_{ij} < \tilde{L_{ij}}$ for at least one pair of (i, j). Now we know that for any fixed $C > 0$ we have

$$(C, \Gamma_{\alpha,Y}(\kappa) C) < (C, \Gamma_{\alpha,\tilde{Y}}(\kappa) C) \tag{3.6}$$

which comes from monotonicity of $(C, \Gamma_{\alpha,Y}(\kappa) C)$ with respect to $|y_i - y_j|$. The inequality holds for every C from which we have

$$\lambda_0(\alpha, Y; \kappa) < \lambda_0(\alpha, \tilde{Y}; \kappa). \tag{3.7}$$

Sharpness of the inequality is a result of the existence of C for which the minimum is achieved. This inequality completes the proof. □

3.2 Ground state on the graph

The situation on the quantum graph is more complex than the situation of point interactions in $\mathbb{R}$. The situation simplifies to the property of the case on the line as long as there is no branching on the graph or alternatively the strengths of interactions on the vertices are chosen correctly, e.g. for the

case of the star graph when the interaction strength at the central vertex is $\alpha < 0$ and conditions at the endpoints of the edges are equal to Neumann conditions, i.e. $\alpha_i = 0$. Later in this chapter we show on an example how changing the point interaction strength can change the behavior of the ground state for the case of a branched graph. If there is branching on the graph there is the possibility that an increase in the distance between point interactions sites, in the case of the graph these are vertices, results in an decrease of the ground state energy. If we want to decide whether the increase in the distance of a certain edge results in an increase or a decrease of the ground state energy we have to look on the form of the ground state function on that edge. We are able to solve the eigenvector equation

$$-\Delta\psi_j = -E\psi_j, \tag{3.8}$$

where $E > 0$ and ψ_j is the eigenfunction on the j-th edge. The solution is given in the following way:

$$\psi_j = A\exp(-\kappa x) + B\exp(\kappa x), \tag{3.9}$$

where $A, B \in \mathbb{C}$ and $\kappa^2 = E$. Such a solution can be rewritten as

$$\begin{aligned} \psi_j^0 &= a\cosh(\kappa(x+d)), \\ \psi_j^0 &= b\exp(\pm\kappa x), \\ \psi_j^0 &= c\sinh(\kappa(\pm x+e)), \end{aligned} \tag{3.10}$$

where a, b, c, d, e are constants. We know that the ground state eigenfunction is according to Theorem 2.10 strictly positive. This means that we have restrictions on the constants a, b, c and e.

For the purpose of the proof we introduce the edge index. We denote the edge index σ_j according to the type of the ground state function on the j-th edge in the following way:

$$\begin{aligned} &\sigma_j = 1 \text{ for } \psi_j^0 = a\cosh(\kappa(x+d)), \\ &\sigma_j = 0 \text{ for } \psi_j^0 = b\exp(\pm\kappa x), \\ &\sigma_j = -1 \text{ for } \psi_j^0 = c\sinh(\kappa(\pm x+e)). \end{aligned} \tag{3.11}$$

This labeling is unambiguous. This is the result of the general form of the solution of the spectral equation $-\Delta\psi = -E\psi$, where $E > 0$ and the strict

positivity of the ground state. For a more complete discussion of this problem see [6].
Before stating the main theorem of this section we introduce the ground state class for the graphs. We assume that Γ and $\tilde{\Gamma}$ have the same topology differing possibly by inner edge lengths. We consider the family of interpolating graphs having the j-th edge length in the interval $[l_j, \tilde{l}_j]$ assuming that $l_j < \tilde{l}_j$. The graphs belong to the same ground state class if the edge indices do not change for the ground state function for the whole interpolating family. Now we are ready to summarize the relation between the length of the edges and the ground state energy in the following theorem.

Theorem 3.2. *Consider two graphs $\mathbb{G}$ and $\tilde{\mathbb{G}}$ which belong to the same ground state class. Let $-\Delta_{\mathbb{G},\alpha,L}$ and $-\Delta_{\tilde{\mathbb{G}},\alpha,\tilde{L}}$ be corresponding Hamiltonians with the same non-positive boundary conditions at respective vertices. λ_0 and $\tilde{\lambda}_0$ are the corresponding ground state eigenvalues. Suppose that*

$$\forall j \in q \; ((|\sigma_j| = 1 \Rightarrow \sigma_j \tilde{l_j} \leq \sigma_j l_j) \wedge (\sigma_j = 0 \Rightarrow \tilde{l_j} = l_j)) \Rightarrow \tilde{\lambda}_0 \leq \lambda_0. \quad (3.12)$$

The inequality is sharp if $\sigma_j \tilde{l_j} < \sigma_j l_j$ holds for at least one $j \in q$.

Proof. It can be seen that the theorem can be proven if we prove it for two graphs which differ by the length of one inner i-th edge for which $|\sigma_i| = 1$. We introduce quadratic forms d and $\tilde{d}$ for respective graphs $\mathbb{G}$ and $\tilde{\mathbb{G}}$. We choose the inner part of the i-th edge $J = (a, b)$. We will choose it in such a way that we can write $\mathbb{G} = \mathbb{G}_J \cup J$ and $\tilde{\mathbb{G}} = \mathbb{G}_J \cup \tilde{J}$, where $\mathbb{G}_J = \mathbb{G} \setminus J$ and $\tilde{J}$ can be obtained from J by rescaling. We note that this can be achieved if we choose J fulfilling the following inequality $b - a > l_i - \tilde{l}_i$ for $\sigma_i = 1$ and $b - a > \tilde{l}_i - l_i$ for $\sigma_i = -1$. We denote the scaling factor $\xi = \frac{|\tilde{J}|}{|J|}$. The factor ξ is larger than the one in the case we are stretching J and smaller than one in case of shrinking J. We will prove our theorem by showing that the Rayleigh quotient for the second graph satisfies:

$$\frac{\tilde{d}(\tilde{\psi})}{\|\tilde{\psi}\|} < \lambda_0, \quad (3.13)$$

where $\tilde{\psi}$ is appropriately chosen function and λ_0 is the ground state eigenvalue of our operator on original graph. We choose function $\tilde{\psi}$ equal to the ground state eigenfunction ψ on the original graph $\mathbb{G}$ and as "rescaled" ψ_i on the rescaled interval $\tilde{J}$ i.e.:

$$\tilde{\psi}_k(x) = \begin{cases} \psi_k(x) & \forall x \in \mathbb{G}_J \\ \psi_k(a + \xi(x - a)) & \forall x \in J. \end{cases} \quad (3.14)$$

Now if we want to prove the statement for $\sigma_i = 1$ we choose $\xi < 1$. We rewrite the Rayleigh quotient in following way

$$r(\xi) = \frac{\tilde{d}(\tilde{\psi})}{\|\tilde{\psi}\|} = \frac{\alpha + \beta\xi^{-1}}{\gamma + \delta\xi}, \tag{3.15}$$

where $\alpha := d_{\mathbb{G}_J}(\psi)$, $\beta := \int_J |\psi'(x)|^2 dx$, $\gamma := \|\psi\|^2_{\mathbb{G}\setminus J}$ and $\delta := \|\psi\|^2_J$. To prove our statement it is enough to check the derivative of r at $\xi = 1$, i.e.

$$\sigma_i r(1) = \frac{-\sigma_i(\beta\gamma + 2\beta\delta + \gamma\delta)}{(\gamma + \delta)}. \tag{3.16}$$

We know that $\alpha + \beta = \lambda_0$ and we can choose the ground state eigenfunction to be normalized from which we have $\gamma + \delta = 1$. From this we have

$$\sigma_i r(1) = -\sigma_i(\lambda_0\delta + \beta). \tag{3.17}$$

To prove the theorem we need to show that $\sigma_i r(1) > 0$. We show this for the case $\sigma_i = 1$ and $\lambda_0 = -\kappa^2$. The property to check is written explicitly

$$\sigma_i r(1) = -\sigma_i(-\kappa^2\|\psi_i\|^2_J + \|\psi_i'\|^2_J). \tag{3.18}$$

We can rewrite $\|\psi_i'\|^2_J$ as

$$\begin{aligned}\int_J |\psi_i'(x)|^2 dx = |c_i|^2 \int_J |\cosh'(\kappa x)|^2 dx = |c_i|^2\kappa^2 \int_J |\sinh(\kappa x)|^2 dx \\ < |c_i|^2\kappa^2 \int_J |\cosh(\kappa x)|^2 dx = -\lambda_0 \int_J |\psi_i(x)|^2 dx.\end{aligned} \tag{3.19}$$

The case $\sigma_i = -1$ is analogous to the $\sigma_i = 1$ with roles of hyperbolic sine and cosine interchanged. □

Remark 4. *We would like to note that the situation for the index $\sigma_j = 0$ is more complex. In the following section we show that there is the possibility that the increase in lengths of some edges does not result in a change of the ground state energy.*

3.3 Construction of the ground state on the graph

In this section we would like to present several examples of quantum graphs with attractive δ coupling. We will mention these configurations: a line, a

n-edged star graph and a circle. At the end of this chapter we present a lemma for the number of functions of a certain edge type, which are allowed on the edges around one vertex. For those examples we will show that their ground states are unique. Also as a result we will show that the graph without any branching has the property that a decrease in the distance between two point interactions results in a decrease of the energy of the ground state. This is a consequence of the absence of a different solutions than $\cosh(\kappa x)$.

First, for purpose of this section, we introduce the notation of the ground state eigenfunctions as follows:

$$\begin{aligned} c(\kappa, x, d_1) &= \frac{\cosh(\kappa(x+d_1))}{\cosh(\kappa d_1)}, \\ e_+(\kappa, x) &= \exp(\kappa x), \\ e_-(\kappa, x) &= \exp(-\kappa x), \\ s_+(\kappa, x, d_4) &= \frac{\sinh(\kappa(x+d_4))}{\sinh(\kappa d_4)}, \\ s_-(\kappa, x, d_5) &= \frac{\sinh(\kappa(-x+d_5))}{\sinh(\kappa d_5)}. \end{aligned} \tag{3.20}$$

These functions are normalized in such a way that for $x = 0$ they equal 1. We know that only the function e_- can be on infinite edges. This is a consequence of the ground state eigenfunction square integrability. From the condition on the positivity of the ground state eigenfunctions we have the following $d_4 > 0$ and $d_5 > l$, where l is length of the edge.

We are interested in attractive δ couplings at the vertices which means imposing the conditions on the functions on the graph in the form (2.52) and $\alpha_j \leq 0$. We note that for the vertices connecting exactly two edges we can restrict ourselves to the point interaction strengths $\alpha_j < 0$ instead of $\alpha_j \leq 0$. This is a result of the fact that vertex conditions $\alpha_j = 0$ for the two edged vertex leads to the smooth function, i.e. we can connect these two edges to one and omit the vertex. Now we are ready to show the examples of the construction of the ground state.

3.3.1 Line with n point interactions

In this subsection we introduce an alternative approach how to prove the properties of the point interactions on the line we presented at the beginning

of this chapter. We construct the line with n point interactions. We can look upon a line with n point interactions as at $n-1$ line segments of finite length and 2 half-lines.

Lemma 3.1. *The ground state eigenfunction on the quantum graph representing the line with the n attractive point interactions has the following edge indices* $\sigma = (0, 1, \ldots, 1, 0)$.

Proof. We are interested in the ground state eigenfunction $\Psi = \{\psi_i(x) \mid i \in \widehat{n+1}\}$. We know that at the semi-infinite edges there are function of the form e_-, i.e.: $c_1\psi_1 = c_{n+1}\psi_{n+1} = e_-(\kappa, x)$, where $c_1, c_{n+1} \in (0, \infty)$ are positive constants. We will show that only possible solution at the finite edges is in the form of c. We will solve conditions for each vertex separately. We rescale the functions and parameterize the vertices in such a way that at i-th vertex the variables are $x_i = 0$ and $x_{i+1} = 0$ and the function on the i-th and $(i+1)$-th edges are in the form of 3.20. The condition at i-th vertex can be then written as

$$\begin{aligned} \psi_i(0) &= \psi_{i+1}(0), \\ \alpha_i\psi_i(0) &= \psi_i'(0+) + \psi_{i+1}'(0+), \end{aligned} \tag{3.21}$$

where $\alpha < 0$. We will rewrite these conditions for the first vertex. In our parametrization condition of continuity at the vertex is automatically satisfied. We obtain the second condition in the form

$$\alpha_1 = \frac{\psi_1'(0+) + \psi_2'(0+)}{\psi_1(0)} = -\kappa + \psi_2'(0+). \tag{3.22}$$

We need the expression at the right hand side to be negative. We write down the contributions $\psi_2'(0+)$ for different functions in the form (3.20).

$$\begin{aligned} \psi_c'(0+) &= \kappa \tanh(\kappa d_1), \\ \psi_{e_+}'(0+)(\kappa, x) &= \kappa, \\ \psi_{e_-}'(0+)(\kappa, x) &= -\kappa, \\ \psi_{s_+}'(0+)(\kappa, x, d_4) &= \kappa \coth(\kappa d_4), \\ \psi_{s_-}'(0+)(\kappa, x, d_5) &= -\kappa \coth(\kappa d_5)). \end{aligned} \tag{3.23}$$

We immediately obtain the following inequalities

$$\begin{aligned} -1 < \frac{\psi_c'(0+)}{\kappa} < 1, \\ \frac{\psi_{e_+}'(0+)}{\kappa} = 1, \\ \frac{\psi_{e_-}'(0+)}{\kappa} = -1, \\ \frac{\psi_{s_+}'(0+)}{\kappa} > 1, \\ \frac{\psi_{s_-}'(0+)}{\kappa} < -1. \end{aligned} \tag{3.24}$$

From those conditions we obtain that ψ_2 can not be in the form of e_+ and s_+. This follows from the fact $-\kappa + e_+'(0+) = -\kappa + \kappa = 0$ and $-\kappa + s_+'(0+) = -\kappa(1 + \coth(\kappa d)) > 0$. Similarly we find all possible pairs of the function types connected by an inner vertex. These pairs have to fulfill the relation

$$\psi_i'(0+) + \psi_{i+1}'(0+) < 0. \tag{3.25}$$

This relation cannot be satisfied by these combinations:
(s_+, s_+), (s_+, e_+), (s_+, e_-), (s_+, c), (e_+, c), (e_+, e_+), (e_+, e_-).
We know that on the edge connected to the infinite one we can have theoretically these functions c, e_- and s_-. We note that when we inverse the parametrization, i.e. $x \longmapsto l - x$ on an finite edge of length l we have to transform types of the functions in the following way: $e_- \longmapsto e_+$, $s_+ \longmapsto s_-$ and vice versa. We will show that the only functions allowed at the inner edges are of the type c in three steps:
1) s_-: At this point we will show that we cannot connect an s_- edge to the infinite one. This can be shown by contradiction. We assume for the moment that we can connect a s_- edge. Then at the next vertex according to our reparametrization $s_- \longmapsto s_+$ we get s_+ on the second vertex and we can connect to s_+ only s_- edge. We repeat this procedure $n-2$ times and we come to the vertex with the second semi-infinite edge. At this vertex edge the functions s_+ and e_- meet which is not an allowed pair of functions.
2) e_-: Similarly we can show that we cannot use the function e_-. At the third vertex we obtain e_+ according to reparametrization $e_- \longmapsto e_+$. The only functions which we can connect there would be s_- and e_-. Now when we repeat the procedure and come to the $(n+1)$-th vertex we would have

either the combination e_+, e_- or s_+, e_- and they do not satisfy the condition (3.25).
3) c: We are now left with only one option and that is c. At the third vertex we can connect the edge with function of the type c, s_-, e_-. If we would connect s_-, e_- we would end up with either option 1) or 2) and they are not allowed. From this we have that only the c function is allowed on the inner edges of the graph representing the line, because when we come to the $(n+1)$-th vertex we obtain pair of functions in the form (c, e_-) which is allowed pair. □

Now a combination of Theorem 3.2 and Lemma 3.1 completes the alternative proof of Theorem 3.1.

3.3.2 n-edged star graph

In this subsection we construct the ground state function on the n-edged star graph with j edges of finite length. We show that the ground state function has edge indices given uniquely by boundary conditions.

We introduce a parametrization of the edges as in the figure 3.1. We need to satisfy the conditions in the following way

$$\begin{aligned} \alpha_i \psi_i(l_i) &= -\psi_i'(l_i-) \ \forall i \in \hat{j}, \\ \alpha \psi_i(0) &= \sum_{k \in \hat{n}} \psi_k'(0+) \ \forall i \in \hat{n}. \end{aligned} \tag{3.26}$$

We start by restricting the functions at the vertices with respect to the endpoints. We rewrite the conditions at the endpoint of vertices as

$$-\frac{\psi_i'(l_i-)}{\psi_i(l_i)} \leq 0 \ \forall i \in \hat{j}. \tag{3.27}$$

These conditions restrict possible functions at the edges to those c, s_+ and e_+. It is result of the fact that

$$\begin{aligned} -\frac{s_-'(l_i-)}{s_-(l_i)} &= \kappa \coth(\kappa(-l_i + d_i)) > 0, \\ -\frac{e_-'(l_i-)}{e_-(l_i)} &= \kappa > 0, \end{aligned} \tag{3.28}$$

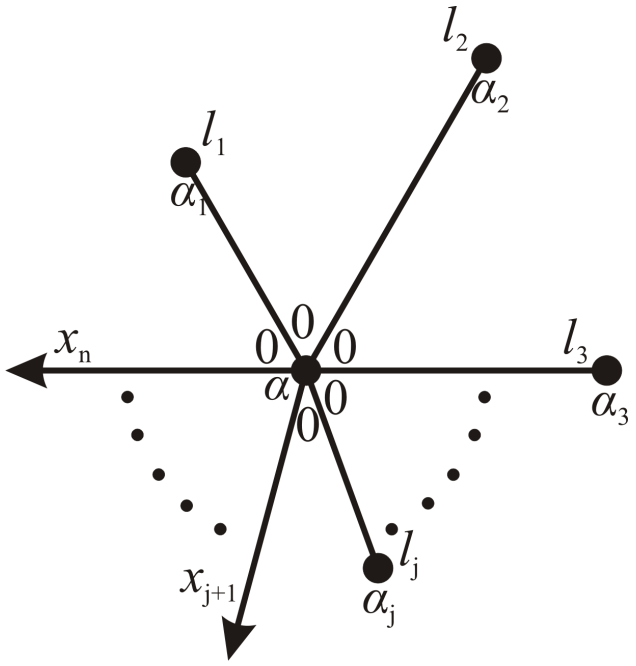

Figure 3.1: Finite n edged star graph

where $-l_i + d_i > 0$ from the condition on the positivity of the eigenfunction. Furthermore we have to restrict the parameter d_i for the function c in the following way.

$$-\frac{c'(l_i-)}{c(l_i)} = -\kappa(\tanh(\kappa(l_i + d_i))). \tag{3.29}$$

This expression is negative for $l_i + d_i > 0$. Now we solve the central vertex. We prove the theorem concerning the number of allowed edge types.

Theorem 3.3. *Let the function Ψ be the ground state eigenfunction of the operator $-\Delta_{\mathbb{G},\alpha,L}$ on the star graph with the negative point interaction strengths. Then for the number of edge types we can write*

$$n_c + n_{e_-} \geq n_{e_+} + n_{s_+} + 1, \tag{3.30}$$

where n_c is the number of edges with c function, n_{e_-} is number of infinite edges, n_{e_+} is the number of edges with e_+ function and n_{s_+} is the number of edges with s_+ function.

Proof. We write down the central point interaction α by means of contributions from the functions on the edges for a general graph with n_c edges of the c type, n_{e_+} edges of the e_+ type etc. We obtain the following

$$\alpha = \kappa \left(\sum_{i=1}^{n_c} \tanh(\kappa d_i) + \sum_{j=1}^{n_{s_+}} \coth(\kappa d_j) + \sum_{j=1}^{n_{e_+}} 1 + \sum_{j=1}^{n_{e_-}} -1 \right). \tag{3.31}$$

We approximate the expressions $\tanh(\kappa d_i)$ and $\coth(\kappa d_j)$ by $-1 + \epsilon_i = \tanh(\kappa d_i)$ and $1 + \epsilon_i = \coth(\kappa d_j)$, where $\epsilon_i > 0$. We obtain

$$\begin{aligned} \alpha &= \kappa \left(\sum_{i=1}^{n_c} (-1 + \epsilon_i) + \sum_{j=1}^{n_{s_+}} (1 + \epsilon_i) + \sum_{j=1}^{n_{e_+}} 1 + \sum_{j=1}^{n_{e_-}} (-1) \right) \\ &= \kappa \left(-n_c + n_{s_+} + n_{e_+} - n_{e_-} + \sum_{i=1}^{n_c} \epsilon_i + \sum_{j=1}^{n_{s_+}} \epsilon_i \right). \end{aligned} \tag{3.32}$$

For certain set of parameters d_i and sufficiently large l_i we obtain $\sum_{i=1}^{n_c} \epsilon + \sum_{j=1}^{n_{s_+}} \epsilon = \Upsilon < 1$. Now we substitute this expression along with the inequality $\alpha < 0$ to the equation 3.32 and we get

$$-n_c + n_{s_+} + n_{e_+} - n_{e_-} + \Upsilon < 0. \tag{3.33}$$

We rewrite this into

$$n_c + n_{e_+} > n_{s_+} + n_{e_+} + \Upsilon. \tag{3.34}$$

Because the numbers $n_c, n_{e_+}, n_{s_+}, n_{e_+} \in \mathbb{N}$ are integers we can enlarge Υ to 1 and change the sharp inequality to inequality which completes the proof. □

Now we present an alternative way of proving one part of Theorem 2.10 concerning the ground state. We show that our operator $-\Delta_{\mathbb{G},\alpha,L}$ has exactly one strictly positive eigenfunction belonging to the negative eigenvalues. This will be content the of the following theorem.

Theorem 3.4. *Let $-\Delta_{\mathbb{G},\alpha,L}$ be the operator on the star graph with the negative point interaction strengths. Then there is only one strictly positive eigenfunction with the negative eigenvalue.*

Proof. According to Theorem 2.10 the operator $-\Delta_{\mathbb{G},\alpha,L}$ with negative interaction strengths have strictly positive eigenfunction for the ground state.

Now we show that the ground state is only one strictly positive eigenfunction. It can be seen that the two function of the same type generate the same point interactions only when they are the same. Next we have to show that the two functions of different types cannot generate the same boundary conditions.
We have two function Ψ_1, Ψ_2 with their types in the form T_1 and T_2. We prove the statement for the function types c and s_+. Function Ψ_1, Ψ_2 cannot generate the same point interactions. We show it for the functions of the following types.

$$T_1 = \begin{pmatrix} c \\ \vdots \\ c \\ c \\ s_+ \\ s_+ \\ \vdots \\ s_+ \end{pmatrix}, \quad T_2 = \begin{pmatrix} c \\ \vdots \\ c \\ s_+ \\ c \\ s_+ \\ \vdots \\ s_+ \end{pmatrix}. \tag{3.35}$$

If those types would generate the same boundary conditions the following relations have to be fulfilled:

$$\begin{aligned} \kappa_1 \tanh(\kappa_1(l_i + d_i)) = \alpha_i = \kappa_2 \coth(\kappa_2(l_i + d_i')), \\ \kappa_1 \coth(\kappa_1(l_{i+1} + d_{i+1})) = \alpha_{i+1} = \kappa_2 \tanh(\kappa_2(l_{i+1} + d_{i+1}')). \end{aligned} \tag{3.36}$$

Hyperbolic tangent and cotangent have the following property: $\coth x > \tanh y$. From this and the first condition we can conclude $\kappa_1 > \kappa_2$ and from the second condition $\kappa_1 < \kappa_2$. These conditions cannot be fulfilled at the same time. Combinations of the types c and s_+ remaining to be checked are the following:

$$T_1 = \begin{pmatrix} c \\ \vdots \text{ j times type } c \vdots \\ c \\ s_+ \\ \vdots \text{n-j times type } s_+ \vdots \\ s_+ \end{pmatrix}, \quad T_2 = \begin{pmatrix} c \\ \vdots \text{ k times type } c \vdots \\ c \\ s_+ \\ \vdots \text{n-k times type } s_+ \vdots \\ s_+ \end{pmatrix}, \tag{3.37}$$

where $j > k$. For at least one index i we have the condition for the point

interactions strength as

$$\kappa_1 \tanh(\kappa_1(l_i + d_i)) = \alpha_i = \kappa_2 \coth(\kappa_2(l_i + d_i')). \tag{3.38}$$

From this condition we obtain $\kappa_1 > \kappa_2$. The conditions on the vertices with the same type are as follows

$$\begin{aligned} \kappa_1 \tanh(\kappa_1(l_i + d_i)) = \alpha_i = \kappa_2 \tanh(\kappa_2(l_i + d_i')), \\ \kappa_1 \coth(\kappa_1(l_i + d_i)) = \alpha_i = \kappa_2 \coth(\kappa_2(l_i + d_i')). \end{aligned} \tag{3.39}$$

From those conditions, $\kappa_1 > \kappa_2$ and from the monotonicity of tanh and coth we have

$$\begin{aligned} &\tanh(\kappa_1(d_i)) < \tanh(\kappa_2(d_i')) \quad i \in \hat{k}, \\ &\tanh(\kappa_1(d_j)) < \coth(\kappa_2(d_j')) \quad j \in \hat{j} \setminus \hat{k}, \\ &\coth(\kappa_1(d_k)) < \coth(\kappa_2(d_k')) \quad k \in \hat{n} \setminus \hat{j}. \end{aligned} \tag{3.40}$$

From those we obtain the condition $\alpha^{(1)} < \alpha^{(2)}$, where $\alpha^{(1)}$ is the point interaction strength on the central vertex for the function of the type T_1 and $\alpha^{(2)}$ for the second type T_2 which completes the proof. For the other combinations of the types the proof is analogous to this so we omit the details. □

3.3.3 Circle with n point interactions

As we pointed out earlier point interactions with the negative point interaction strengths have on the circle the property that a decrease of the diameter of the circle results in a decrease of the ground state energy. This is the straightforward result of the fact that only the functions $\cosh_\pm$ are allowed on the circle. This follows from the argument we will point out.

Lemma 3.2. *Let graph $\mathbb{G}$ be the circle with the boundary conditions imposed at each vertex in form of attractive δ coupling. Then only the functions in the form $C\cosh(\kappa(x + D))$ are allowed on the edges for the ground state eigenfunction, where $C \in (0, \infty)$ and $D \in \mathbb{R}$.*

Proof. We start with the circle with one point interaction. It can be seen that only the function c from 3.20 can be present on such graph. This is the result of the fact that only the function in the form of c can fulfill the

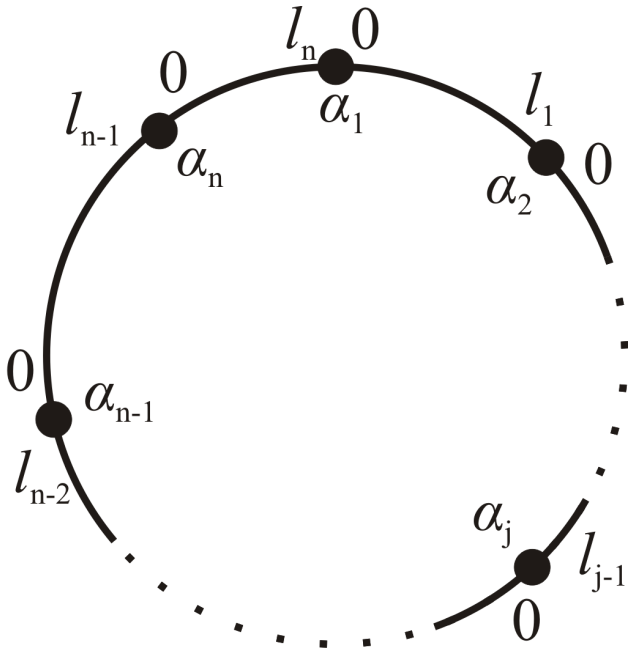

Figure 3.2: Circle with n point interactions

condition on the continuity in the form $\psi(0) = \psi(l)$.
Now we prove the statement for the circle with at least two edges. We can start at any vertex. There can be these combinations:
(c, c), (c, e_-), (c, s_-), (e_-, e_-), (s_-, s_-), (s_-, s_+), (s_-, e_-), (s_-, e_+).
We show that there can not be the function s_-. If these is the function on the edge s_-, after reparametrization mentioned earlier we obtain s_+ for solving boundary conditions on the next vertex. At another edge we can put only the function s_-. In this fashion we go around the circle and we come to the vertex which we started from. On this vertex we obtain the functions of the form s_- and s_+. This is possible from the point of view of the condition on the negativity of the point interaction strength. However the function which we have constructed can not satisfy the boundary condition on the continuity of the function. It is the result of the fact that the function of the type s_- is decreasing from which we have in parametrization showed on the figure 3.2 the following: $\psi_1(0) > \psi_1(l_1) = \psi_2(0) > \psi_2(l_2) = \ldots > \psi_n(l_n)$. In the same fashion we are able to show that there can not be the functions s_+, e_- and e_+ which completes the proof. □

3.3.4 Unbranched graph

In this subsection we prove an important property of quantum graphs with negative δ coupling. The property we will show is that for the graph with no branching there can not be the edge with the function of the type $s_\pm$ and edges of finite length with the function types $e_\pm$.

Theorem 3.5. *Let the graph $\mathbb{G}$ be without any branching, i.e. no degree of any vertex exceeds two, with the boundary conditions imposed at each vertex in the form of attractive δ coupling. Then the ground state eigenfunction can contain only the functions in the form $C\cosh(\kappa(\pm x + D))$ for finite edges and $C\exp(-\kappa x)$ for the semi-infinite ones, where $C \in (0, \infty)$ and $D \in \mathbb{R}$.*

Proof. The graph with no branching is a chain of edges either open or closed. The closed case is the circle with n attractive point interactions. We have already proved this statement for this case in the previous subsection. The case we have to deal with is the open chain. We have already proved the statement for the case of a chain ended with semi-infinite edges. The remaining cases are the chains with edges of finite length and at most one semi-infinite edge. We start with the case of one semi-infinite edge. At the semi-infinite edge there has to be function in the form e_-. It can be seen that we can connect these function c, s_- or e_- to the semi-infinite edge. If we choose s_- at the following vertex after reparametrization we would get s_+. The only function we could connect to s_+ is s_-. When we would repeat this procedure we would come to the vertex at the end of the chain and there would be connected only the edge with s_+ which results in repulsive δ coupling. Analogously we can show the case with e_- with the difference that we can connect to e_+ only the s_- which leads to the previous case. The remaining case of c can be dealt in the same way. We can connect to the edge with function of c type functions of those types s_-, e_- or c. Types s_- and e_- leads to previous cases. When we come to the last vertex function of the type c is allowed. Now we have to deal with the finite graph. We can employ same procedure as before with the difference that on the first edge we can place function of the types: c, e_- and s_- which completes the proof. □

3.4 Examples

In this section we show the properties of the ground state of two examples. The first example will show the properties on two edges connected by one

vertex. The second one will show how the behavior of the ground state changes on the three edged star graph when we change the point interaction strength on the central vertex.

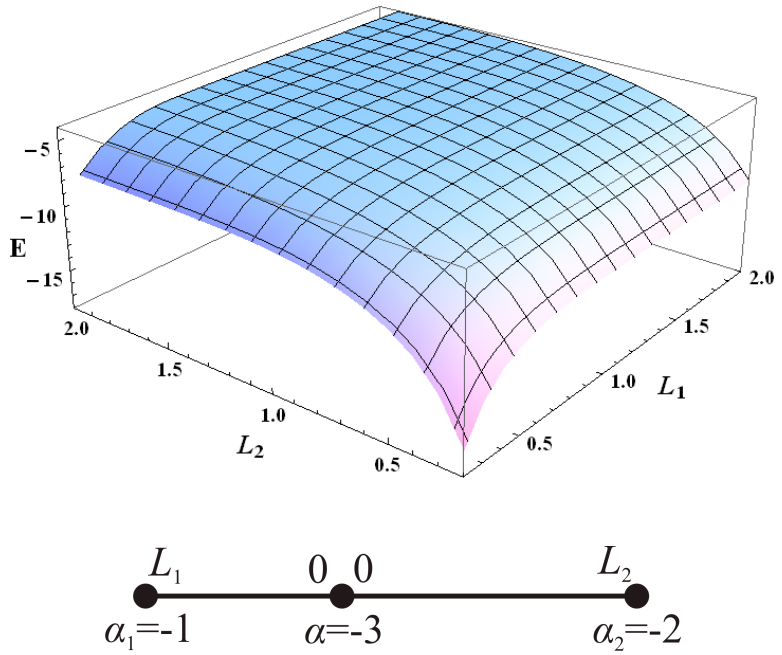

Figure 3.3: The ground state energy of two edges connected by one vertex with respect to the lengths of the edges

We start by the open chain constructed from two edges. This situation is shown on the figure 3.4. On this figure we have the ground state energy of the system with respect to the lengths of the edges. We can see that for the unbranched graph the increase of the length of the edges results in an increase of the ground state energy.

Another example will show that a change of the point interaction strength can result in a change of the edge index resulting in a change of the behavior of the ground state energy. This can be seen on a simple star graph sketched on figure 3.3. This star graph has minor symmetry. On the graph we see the ground state energy with respect to the point interaction strength at the

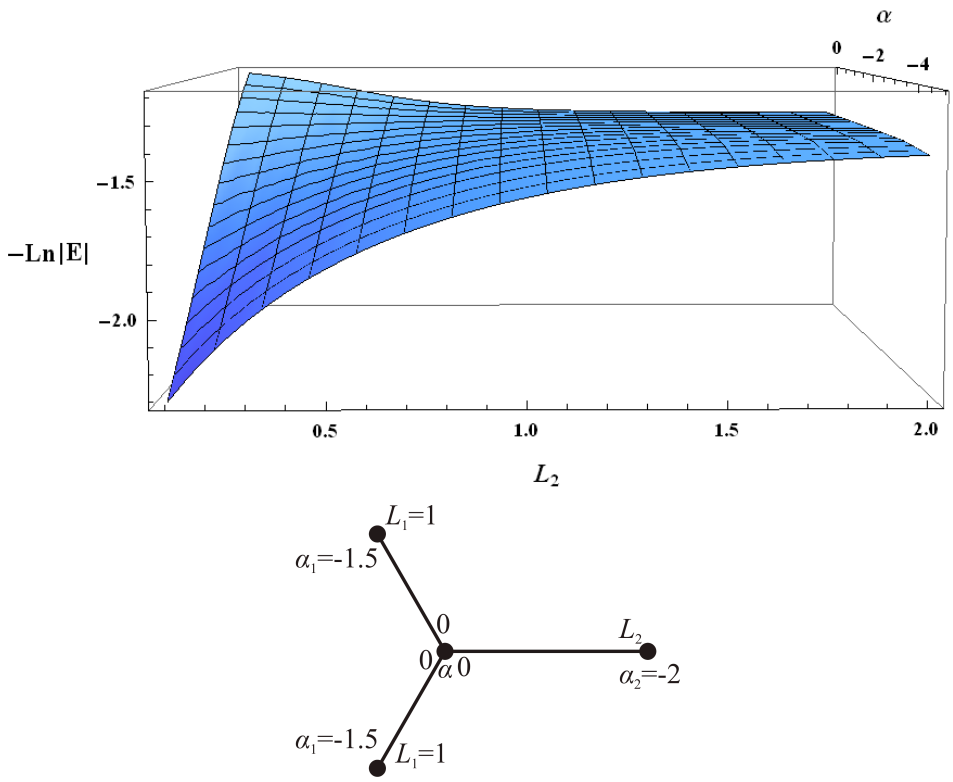

Figure 3.4: The ground state energy of 3-edged star graph with respect to the length of one edge and point interaction strength on the central vertex

central vertex and the length of one edge. On the z axis of the graph we used logarithmic scale to make the effect more visible. We are able to see two regimes which are separated by a critical value of the point interaction strength on the central vertex $\alpha_{crit} \approx -1.09088$. There is one regime for the weak attractive coupling $\alpha > \alpha_{crit}$ at the central vertex, for which an increase in length of the edge L_2 results in a decrease in the ground state energy. Another regime is for the point interaction strength large enough $\alpha < \alpha_{crit}$ with the property that a decrease in the length of the edge results in a decrease in the ground state energy. We note that for the $\alpha = \alpha_{crit}$ the ground state energy is independent of the length of the edge L_2 which is the consequence of the fact that the function on this edge is purely exponential. The symmetry allows us to write the spectral condition at the central ver-

tex in the following way: $2\psi_1'(0+) + \psi_2'(0+) = \alpha\psi_1(0)$. We note that it is not difficult to find examples of graphs with similar behavior without any symmetry.

Chapter 4

Properties of the ground state for the two and three dimensional case

We are interested in the relation between the ground state energy and the distance of the point interactions. We will work with point interactions in $\mathbb{R}^d$, $d = 2, 3$. Similarly as in the case of point interactions on the line, we will prove that an increase in the distance between the point interactions results in an increase in the ground state energy. We will show this using a variational argument in combination with properties of the resolvent. For the special case when the system has a form of reflection symmetry we are able to show a similar property with the help of the Neumann bracketing method mentioned earlier.

4.1 A variational approach

We start by addressing our problem using a variational method employing properties of the resolvent. This approach is based on the fact that the eigenvalue $k^2 = -\kappa^2 < 0$ fulfills the condition $\det \Gamma_{\alpha,Y}(k) = 0$ and the property that lowest eigenvalue of our operator $-\Delta_{\alpha,Y}$ corresponds to the lowest eigenvalue of $\Gamma_{\alpha,Y}$.

Theorem 4.1. *Let $-\Delta_{\alpha,Y}$ and $-\Delta_{\alpha,\tilde{Y}}$ be the point interaction Hamiltonians defined above for the dimension $d = 2, 3$. Suppose that* $\operatorname{card} Y = \operatorname{card} \tilde{Y}$ *and in addition, for $d = 3$ assume that the both operators have an isolated*

eigenvalue at the bottom of the spectrum. Then the ground states of the operators $-\Delta_{\alpha,Y}$ *and* $-\Delta_{\alpha,\tilde{Y}}$ *satisfy*

$$\begin{aligned} |y_j - y_{j'}| \leq |\tilde{y}_j - \tilde{y}_{j'}| \ \forall j, j' \in \hat{N} \Rightarrow \\ \min \sigma(-\Delta_{\alpha,Y}) \leq \min \sigma(-\Delta_{\alpha,\tilde{Y}}). \end{aligned} \tag{4.1}$$

If at least one inequality for the distances of the point interactions is sharp then the second inequality is also sharp.

Proof. We start with the proof of two dimensional case. Proof for the dimension three is analogical with a few differences we will point out.

Two dimensional case

The behavior of the ground state of the operator $-\Delta_{\alpha,Y}$ is governed by the secular equation $\det \Gamma_{\alpha,Y}(i\kappa) = 0$. According to (2.16) we can write $\Gamma_{\alpha,Y}$ as

$$[\Gamma_{\alpha,Y}]_{j,j'=1}^{N} = \left\{ \frac{1}{2\pi} \left[2\pi\alpha_j - \Psi(1) + \ln\left(\frac{k}{2i}\right) \right] \delta_{jj'} - \tilde{G}_k(y_j - y_{j'}) \right\}_{j,j'=1}^{N}, \tag{4.2}$$

where $\tilde{G}_k(y_j - y_{j'})$ can be written as

$$\tilde{G}_k(x) = \begin{cases} 0 & x = 0 \\ \frac{2}{\pi} K_0^{(1)}(\kappa|x|) & x \neq 0. \end{cases} \tag{4.3}$$

We have to investigate the lowest eigenvalue λ_0 of $\Gamma_{\alpha,Y}(i\kappa)$. This follows from the proof of the existence of the ground state for the point interaction in the dimension two. According to [1, Chapter II.4] we have N eigenvalues $\gamma_j(\kappa)$ of $\Gamma_{\alpha,Y}(i\kappa)$ all strictly increasing with respect to κ. The expression λ_0 is given by

$$\lambda_0(\alpha, Y; \kappa) = \min_{|C|=1} (C, \Gamma_{\alpha,Y}(i\kappa)C), \tag{4.4}$$

where $C = (c_1, \ldots, c_n) \in \mathbb{C}^n$. The energy of the ground state $-\kappa^2$ corresponds to the value of κ which fulfills $\lambda_0(\alpha, Y; \kappa) = 0$. Next we notice that the semigroup $\left\{ e^{-t\Gamma_{\alpha,Y}(\kappa)} \right\}$ is positivity improving according to [3, Section XIII.12], [3, Problem XIII.97] and therefore C for which the minimum is achieved can be chosen strictly positive, i.e. $c_i > 0$ for all $i = 1, \ldots, n$. Put together with (4.4) we obtain

$$\lambda_0(\alpha, Y; \kappa) = \min_{|C|=1, C>0} (C, \Gamma_{\alpha,Y}(i\kappa)C). \tag{4.5}$$

The explicit form of the expression on the right-hand side of the last relation is

$$(C, \Gamma_{\alpha,Y}(i\kappa)C) = \sum_{j=1}^{N} \frac{1}{2\pi} \left[2\pi\alpha_j - \Psi(1) + \ln\left(\frac{\kappa}{2}\right) \right] |c_j|^2 - \sum_{j<j'} \frac{2}{\pi} K_0^{(1)}(\kappa|y_j - y_{j'}|)(\bar{c_j} c_{j'} + \bar{c_{j'}} c_j). \tag{4.6}$$

We are interested in the relation between κ and $|y_j - y_{j'}|$. We observe that the expression $(C, \Gamma_{\alpha,Y}(i\kappa)C)$ is monotonous with respect to $|y_j - y_{j'}|$ for fixed κ, hence an increase in $|y_j - y_{j'}|$ results in an increase of the value of $(C, \Gamma_{\alpha,Y}(i\kappa)C)$. Because this is valid for all strictly positive C it is also valid for C for which the minimum of $(C, \Gamma_{\alpha,Y}(i\kappa)C)$. This means that λ_0 is monotonously increasing with respect to $|y_j - y_{j'}|$ which along with the monotonicity of λ_0 with respect to κ completes the proof.

Three dimensional case
In this case the existence of the ground state eigenvalue is not guaranteed and must be assumed - cf. Theorem 2.22. Otherwise the proof is analogous to the two-dimensional case with the above $\Gamma_{\alpha,Y}(i\kappa)$ replaced by the three-dimensional case given in Section 2.2.7 as

$$[\Gamma_{\alpha,Y}]_{j,j'=1}^{N} = \left(\alpha_j + \frac{\kappa}{4\pi}\right) \delta_{jj'} - \tilde{G}_k(y_j - y_{j'}), \tag{4.7}$$

where $\tilde{G}_k(y_j - y_{j'})$ can be written as

$$\tilde{G}_k(x) = \begin{cases} 0 & x = 0 \\ \frac{\exp(ik|x|)}{4\pi|x|} & x \neq 0. \end{cases} \tag{4.8}$$

Since for $k = i\kappa$, $\kappa > 0$, this function is again strictly monotonous with respect to $|x|$ the proof proceeds as in the two-dimensional case. □

4.2 Neumann bracketing

An alternative way how to address our problem is to use the so-called Neumann bracketing. This approach can be used only in particular situations but on the other hand, it gives results also in situations which are not covered by the results of the previous section. Specifically, we will be able to

demonstrate monotonicity with respect to the distance between two clusters of point interactions provided the system has a mirror symmetry. In the same way we will demonstrate monotonicity also in some cases when some distances increase and some decrease. First we will state an important lemma for the proof of the following theorem.

Lemma 4.1 (Neumann bracketing)**.** *Let* Ω_1,Ω_2 *be disjoint subsets such that* $\overline{\Omega_1 \cup \Omega_2}^{int} = \Omega$*, and* $\Omega \backslash \Omega_1 \cup \Omega_2$ *has Lebesgue measure zero. Then*

$$0 \leq -\Delta_N^{\Omega_1 \cup \Omega_2} \leq -\Delta_N^{\Omega}. \tag{4.9}$$

Proof: Can be found in [3, Section XIII.15]

For the proof of the following theorem a manifold of codimension one is needed on which the ground state eigenfunction Ψ has vanishing normal derivative

$$\partial_{\vec{n}_x} \Psi(x) = 0, \tag{4.10}$$

where $\partial_{\vec{n}_x}$ is the normal derivative to the manifold at the point x; it is clear that the orientation we choose for it is not important. This condition can be equivalently rewritten as

$$\vec{n}_x \cdot \nabla \Psi(x) = 0, \tag{4.11}$$

where $\cdot$ represents the scalar product. In general it may not be easy to establish the existence of such manifolds. It is straightforward, however, when the system has a mirror symmetry and the said manifolds have a simple form being lines in $\mathbb{R}^2$ and planes in $\mathbb{R}^3$ dividing the space into regions containing at least one point interaction.

Lemma 4.2. *Let* Ψ *be the ground state eigenfunction of the operator* $-\Delta_{\alpha,Y}$ *with even number of point interactions defined above for the dimension two. Suppose that the operator* $-\Delta_{\alpha,Y}$ *has reflection symmetry with respect to the line* l *and* $Y \cap l = \emptyset$*, i.e.* $\overrightarrow{y_i\, y_{n/2+i}} \perp l$*,* $\mathrm{dist}(y_i, l) = \mathrm{dist}(y_{n/2+i}, l) \neq 0$ *and* $\alpha_i = \alpha_{n/2+i}$ *for* $i \in \{1, \ldots n/2\}$*,* $n/2 \in \mathbb{N}$*. Then for the points* $x \in l$ *the ground state function satisfies*

$$\partial_{\overrightarrow{n}} \Psi(x) = 0, \tag{4.12}$$

where $\overrightarrow{n}$ *is normal vector of the line* l*.*

Proof. It can be seen that the ground state of the operator with certain symmetry will possess the same symmetry. This follows from the fact that the eigenfunction for the operator with the reflection symmetry can be either symmetric or antisymmetric with respect to this reflection symmetry. The ground state function of the operator $-\Delta_{\alpha,Y}$ is according to Theorem 2.16 strictly positive from which the ground state eigenfunction has to be symmetric. Without loss of generality we can translate and rotate our system in such a way that the line l can be written as $l = \{(z,0) \mid z \in \mathbb{R}\}$. Now we can write symmetry of the ground state function as

$$\Psi((x,y)) = \Psi((x,-y)). \tag{4.13}$$

This implies that $\nabla\Psi((x,0)) = (c,0)$, $c \in \mathbb{R}$ which completes the proof. □

Now we are ready to prove the theorem concerning our problem in two dimensions.

Theorem 4.2. *Let $-\Delta_{\alpha,Y_1}$, $-\Delta_{\alpha,Y_2}$ be the point interaction Hamiltonians defined above for the dimension $d = 2$, where $Y_i = \{y_{1,i}, \ldots, y_{N,i}\}$. Suppose that* $\operatorname{card} Y_1 = \operatorname{card} Y_2$. *Suppose further that the operator $-\Delta_{\alpha,Y_1}$ satisfies conditions of Lemma 4.2. Furthermore let Y_2 be obtainable from Y_1 by shifting the points $\{y_{n/2+1,1}, \ldots, y_{n,1}\}$ in the direction of the vector $\overrightarrow{X}$, i.e.:*

$$\begin{aligned} y_{i,1} &= y_{i,2} \quad \text{for} \quad i \in \{1, \ldots, \tfrac{n}{2}\}, \\ y_{i,1} &= y_{i,2} + \overrightarrow{X} \quad \text{for} \quad i \in \{\tfrac{n}{2}+1, \ldots, n\}. \end{aligned} \tag{4.14}$$

The vector $\overrightarrow{X}$ fulfills $\overrightarrow{y_{i,1}\, y_{n/2+i,1}} \cdot \overrightarrow{X} \geq 0$. Then the ground states of the operators $-\Delta_{\alpha,Y_1}$, $-\Delta_{\alpha,Y_2}$ satisfies

$$\min \sigma_p(-\Delta_{\alpha,Y_1}) \leq \min \sigma_p(-\Delta_{\alpha,Y_2}). \tag{4.15}$$

Proof. We prove this theorem in two steps. First we will show its validity for the case $\overrightarrow{y_{i,1}\, y_{n/2+i,1}} \cdot \overrightarrow{X} > 0$. In the second part of the proof we will work with the case $\overrightarrow{y_{i,1}\, y_{n/2+i,1}} \cdot \overrightarrow{X} = 0$, i.e. shifting mirror image of the point interactions along the direction of the line l.

We consider the operator $-\Delta_{\alpha,Y_1}$ discussed above. We add the Neumann condition at $x \in l$. According to Lemma 4.3 this line satisfies $\vec{n}_x \cdot \nabla\Psi(x) = 0$, where $\Psi(x)$ is the ground state function of the operator $-\Delta_{\alpha,Y_1}$. We denote

the operator with the Neumann condition as $-\Delta^{(1)}_{\alpha,Y_1}$ on the line l. The domain of $-\Delta^{(1)}_{\alpha,Y_1}$ is

$$\mathscr{D}(-\Delta^{(1)}_{\alpha,Y_1}) = \{g \in \mathscr{D}(-\Delta_{\alpha,Y_1}) \mid \overrightarrow{n_l} \cdot \nabla g(x) = 0 \ \forall x \in l\}. \tag{4.16}$$

The ground state eigenfunctions for $-\Delta_{\alpha,Y_1}$ and $-\Delta^{(1)}_{\alpha,Y_1}$ are the same, because we chose l in such a way that the function of the ground state Ψ fulfills Neumann condition at points of l. We note that the line l decomposes $\mathbb{R}^2$ into two separate regions. Next we write $-\Delta^{(1)}_{\alpha,Y_1}$ as a direct sum of 2 self-adjoint operators

$$-\Delta^{(1)}_{\alpha,Y_1} = -\Delta_{\tilde{\alpha}_1,\tilde{Y}_1,l} \oplus -\Delta_{\tilde{\alpha}_2,\tilde{Y}_2,l}, \tag{4.17}$$

where $\tilde{\alpha}_1 = \{\alpha_1, \ldots, \alpha_{n/2}\}$, $\tilde{\alpha}_2 = \{\alpha_{n/2+1}, \ldots, \alpha_n\}$, $\tilde{Y}_1 = \{y_{1,1}, \ldots y_{n/2,1}\}$ and $\tilde{Y}_2 = \{y_{n/2+1,1}, \ldots y_{n,1}\}$. The operators $-\Delta_{\tilde{\alpha}_i,\tilde{Y}_i,l}$ are defined on a half-plane with Neumann boundary condition. Now we define the operator $-\Delta^{(2)}_{\alpha,Y_1}$ as

$$-\Delta^{(2)}_{\alpha,Y_1} = -\Delta_{\tilde{\alpha}_1,\tilde{Y}_1,l} \oplus -\Delta^{\hat{l}}_N \oplus -\Delta_{\tilde{\alpha}_2,\tilde{Y}_2,l}, \tag{4.18}$$

where $-\Delta^{\hat{l}}_N$ is Neumann Laplacian at the region of space $\hat{l}$ which is obtained as $\hat{l} = \{l + cX \mid c \in [0,1]\}$ (for the definition of the Neumann Laplacian see [3, Section XIII.15]). The region $\hat{l}$ is nonempty because we assume that $\overrightarrow{y_{i,1}\, y_{n/2+i,1}} \cdot \overrightarrow{X} > 0$. Neumann Laplacian is a positive operator, in particular, all its eigenvalues are positive. We are interested in the ground state of $-\Delta^{(2)}_{\alpha,Y_1}$. The discrete spectrum of $-\Delta^{(2)}_{\alpha,Y_1}$ is the union of discrete spectra of the orthogonal sum components, i.e.

$$\sigma_p(-\Delta^{(2)}_{\alpha,Y_1}) = \bigcup_{i \in \hat{2}} \sigma_p(-\Delta_{\tilde{\alpha}_i,\tilde{Y}_i,l}) \cup \sigma_p(-\Delta^{\hat{l}}_N). \tag{4.19}$$

The ground state of $-\Delta^{(2)}_{\alpha,Y_1}$ is negative (Theorem 2.16) which implies that the ground state is not affected by $-\Delta^{\hat{l}}_N$ because $-\Delta^{\hat{l}}_N \geq 0$. Next we define the operator $-\Delta^{(3)}_{\alpha,Y_1}$ which is obtained from the operator $-\Delta^{(2)}_{\alpha,Y_1}$ by removing the Neumann conditions at the boundary of $\hat{l}$. It can be easily seen that $-\Delta^{(3)}_{\alpha,Y_1}$ is equal to $-\Delta_{\alpha,Y_2}$. According to Lemma 4.1 we have $-\Delta^{(2)}_{\alpha,Y_1} \leq -\Delta^{(3)}_{\alpha,Y_1}$. Also as we pointed out earlier $-\Delta_{\alpha,Y_1}$ is unitarily equivalent to $-\Delta^{(1)}_{\alpha,Y_1}$ and $-\Delta^{(3)}_{\alpha,Y_1}$ to Δ_{α,Y_2}. In combination with minmax principle [3, Section XIII.1]

we arrive at the inequality:

$$\inf\sigma(-\Delta_{\alpha,Y_1}) = \inf\sigma(-\Delta^{(1)}_{\alpha,Y_1}) \leq \inf\sigma(-\Delta^{(2)}_{\alpha,Y_1}) \leq \inf\sigma(-\Delta^{(3)}_{\alpha,Y_1} \equiv -\Delta_{\alpha,Y_2}). \tag{4.20}$$

From this we have $\inf\sigma(-\Delta_{\alpha,Y_1}) \leq \inf\sigma(-\Delta_{\alpha,Y_2})$ which completes the proof for the case $\overrightarrow{y_{i,1}\, y_{n/2+i,1}} \cdot \overrightarrow{X} > 0$.

The case $\overrightarrow{y_{i,1}\, y_{n/2+i,1}} \cdot \overrightarrow{X} = 0$ can be proven similarly as the previous case $\overrightarrow{y_{i,1}\, y_{n/2+i,1}} \cdot \overrightarrow{X} > 0$ with the difference that we do not insert $-\Delta^{\hat{l}}_N$ into the operator

$$-\Delta^{(1)}_{\alpha,Y_1} = -\Delta_{\tilde{\alpha}_1,\tilde{Y}_1,l} \oplus -\Delta_{\tilde{\alpha}_2,\tilde{Y}_2,l}, \tag{4.21}$$

but we shift points $\tilde{Y}_2$ in the direction of the $\overrightarrow{X}$, apply Lemma 4.1 and minmax principle [3, Section XIII.1] which completes the proof. □

A claim analogous to Theorem 4.2 can be given for the operators in the dimension three. We mention a counterpart of Lemma 4.2 in dimension three.

Lemma 4.3. *Let Ψ be the ground state eigenfunction of the operator $-\Delta_{\alpha,Y}$ with even number of point interactions defined above for the dimension 3. Suppose that the operator $-\Delta_{\alpha,Y}$ has reflection symmetry with respect to the plane p and $Y_1 \cap l = \emptyset$, i.e. $\overrightarrow{y_i\, y_{n/2+i}} \perp p$, $\mathrm{dist}(y_{i,1}, p) = \mathrm{dist}(y_{n/2+i}, p) \neq 0$ and $\alpha_i = \alpha_{n/2+i}$ for $i \in \{1, \dots n/2\}$, $n/2 \in \mathbb{N}$. Then for the points $x \in p$ the ground state function satisfies*

$$\partial_{\overrightarrow{n}}\Psi(x) = 0, \tag{4.22}$$

where $\overrightarrow{n}$ is normal vector of the plane p.

Proof. Proof of the lemma is analogous to the proof of Lemma 4.2 for the dimension 2 so we omit the details. □

Now we are ready to write down the statement for dimension three.

Theorem 4.3. *Let $-\Delta_{\alpha,Y_1}$, $-\Delta_{\alpha,Y_2}$ be the point interaction Hamiltonians defined above for the dimension $d = 3$, where $Y_i = \{y_{i,1}, \dots, y_{i,N}\}$ and $\mathrm{card}\, Y_1 = \mathrm{card}\, Y_2$. Furthermore assume that the ground state for the both operators $-\Delta_{\alpha,Y_1}$ and $-\Delta_{\alpha,Y_2}$ exists. Suppose that the operator $-\Delta_{\alpha,Y_1}$ has reflection symmetry with respect to the plane p and $Y_1 \cap l = \emptyset$, i.e. $\overrightarrow{y_{i,1}\, y_{n/2+i,1}} \perp p$, $\mathrm{dist}(y_{i,1}, p) = \mathrm{dist}(y_{n/2+i,1}, p) \neq 0$ and $\alpha_i = \alpha_{n/2+i}$ for $i \in \{1, \dots n/2\}$,*

$n/2 \in \mathbb{N}$. *Furthermore let* Y_2 *be obtainable from* Y_1 *by shifting the points* $\{y_{n/2+1,1}, \ldots, y_{n,1}\}$ *in the direction of the vector* $\overrightarrow{X}$*, i.e.:*

$$\begin{aligned} y_{i,1} &= y_{i,2} \qquad \text{for} \qquad i \in \{1, \ldots, \tfrac{n}{2}\}, \\ y_{i,1} &= y_{i,2} + \overrightarrow{X} \quad \text{for} \quad i \in \{\tfrac{n}{2}+1, \ldots, n\}, \end{aligned} \tag{4.23}$$

where vector $\overrightarrow{X}$ *fulfills* $\overrightarrow{y_{i,1}\, y_{n/2+i,1}} \cdot \overrightarrow{X} \geq 0$*. Then the ground states of the operators* $-\Delta_{\alpha,Y_1}$*,* $-\Delta_{\alpha,Y_2}$ *satisfies*

$$\min \sigma_p(-\Delta_{\alpha,Y_1}) \leq \min \sigma_p(-\Delta_{\alpha,Y_2}). \tag{4.24}$$

Proof. Proof of the theorem can be made step by step as the proof of Theorem 4.2 so we omit the details. □

It is worth noting that for the system with more than just one line or plane of reflection symmetry we could generalize Theorems 4.2 or 4.3, e.g. for the case of two lines or planes of symmetry we could shift four parts of the space instead of two. Using such an approach we are able to treat situations not covered by Theorems 4.2 or 4.3. We skip details because the formulation and the proofs will be similar to the case of single reflection symmetry.

Remark 5. *By means of Neumann bracketing, we can prove statement similar to the Theorem 4.1 also for other operators* $-\Delta_{\alpha,Y}$*. For the systems with rotational symmetry, i.e. all point interactions strengths are the same and point interactions are placed on circle in such a way that the distance between neighboring point interactions are the same. This system has a discrete rotational symmetry around the center of the circle. For such systems we can find the Neumann condition for the ground state eigenfunction to be satisfied on the n-edged star. Such n-edged star separates the plane to n sectors each one containing one point interactions. Moving these sectors apart from each other cause increase of the ground state energy. We can use the similar proof as the proof presented earlier for Theorem 4.2.*

Remark 6. *Another possible application of the Neumann bracketing would be to compare operators described in the previous remark not with respect to the distance between the point interactions but with respect to the number of the point interactions. We consider operator* $-\Delta_{\alpha,n,Y}$ *with n point interactions and* $-\Delta_{\alpha,m,Y}$ *with m point interactions. We can show that the ground state of these operators satisfy*

$$\min \sigma_p(-\Delta_{\alpha,n,Y}) \leq \min \sigma_p(-\Delta_{\alpha,m,Y}) \tag{4.25}$$

for $n \leq m$. This can be proven by means of Neumann bracketing as sketched on the figure 4.1.

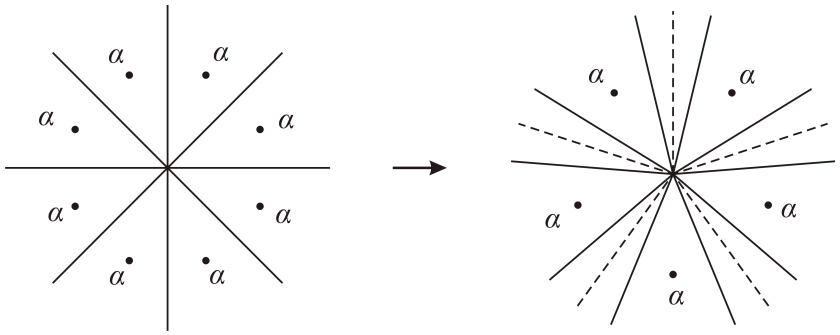

Figure 4.1: Alternative use of Neumann bracketing

Chapter 5

Singular interactions with compact support of codimension one

In this chapter we focus our attention to properties of Hamiltonians which can be written formally in the following form

$$H_{\mu,\Gamma} = -\Delta - \mu(x)\delta(x - \Gamma), \tag{5.1}$$

where $-\Delta$ is the kinetic energy operator on the appropriate Hilbert space $L^2(\mathbb{R}^d)$ where $d = 2, 3$, $-\mu(x)$ is the bounded negative function with the compact support Γ and Γ is a manifold in $\mathbb{R}^d$ with the codimension 1.

At this point it is worth mentioning that for the case $d = 1$ the resolvent written as in Lemma 2.1 gives the same result as the one which we obtained by Krein's formula for the point interactions on the line. This is the reason why we will be interested only in the dimension 2 and 3. The proof which we will give later in this chapter can be easily generalized to any dimension, which is the result of the fact that only properties which we need are strict positivity of the ground state and monotonicity of the integral kernel $G_{i\kappa}(x, y)$ of the free particle Hamiltonian H_0 with respect to κ and to $|x-y|$.

We will be interested in the relation between the geometry of the singular interaction support Γ and the ground state energy. We will show that an increase in distance between points of the Γ results in an increase of the

ground state energy. We will show this using a variational argument analogous to the one we used for point interactions in the previous chapter. For the case that the system possesses reflection symmetry with respect to the line or plane for the dimension 2 or 3, respectively, we are able to show the property with help of Neumann bracketing.

In dimension 2 we will work with manifolds of the codimension one which can be represented by graphs embedded in $\mathbb{R}^2$. These graphs have to satisfy the conditions at the end of Section 2.3. For the purposes of this chapter we introduce classes of equivalence on graphs Γ. We say that Γ_1 and Γ_2 are from the same class of equivalence if they are related by shifting and rotating in $\mathbb{R}^2$. By this approach we also make the same curves with different parametrization equivalent.

We introduce the natural parametrization by length of the curve and we denote the curve in this parametrization as $(\gamma_i)_j \in C^1$ for j-th part of the graph Γ_i. We say that the classes Γ_1 and Γ_2 equipped by the bounded Borel measurable functions $\mu_1 : \Gamma_1 \to \mathbb{R}$ and $\mu_2 : \Gamma_2 \to \mathbb{R}$ are related if:
a) Γ_1 is constructed from the same number of curves as Γ_2,
b) $\int_{\mathbb{R}^2} (\gamma_1)_i vol_1(dx) = \int_{\mathbb{R}^2} (\gamma_2)_i vol_1(dx)$ for all i,
c) $\mu_1((\gamma_1)_j(x)) = \mu_2((\gamma_2)_j(x))$,
d) $\mathrm{card}\{(\gamma_1)_i(x) \cap (\gamma_1)_j(y) \mid \forall x \neq y, i \neq j\} = \mathrm{card}\{(\gamma_2)_i(x) \cap (\gamma_2)_j(y) \mid \forall x \neq y, i \neq j\}$.

For surfaces Γ in the $\mathbb{R}^3$ we introduce analogous classes of equivalence and relations as for the curves in $\mathbb{R}^2$.

5.1 A variational approach

In this section we derive one theorem and two corollaries concerning the ground state energy. The first option is as follows: the compact set Γ of codimension 1 is a union of disjoint subsets, i.e. $\Gamma_i \cap \Gamma_j = \emptyset$ for all $i \neq j$. Shifting and rotating the parts of Γ in such a way that distances between respective points of each pair of Γ_i and Γ_j increases results in increase of the ground state energy. Second theorem will state that if we "squeeze" Γ reducing distances between its points, it will result in decrease of the ground state energy.

Theorem 5.1. *Let H_{μ_1,Γ_1} and H_{μ_2,Γ_2} be operators defined above for the dimension 2 or 3. Let μ_1, Γ_1 and μ_2, Γ_2 be related and for all i, j, x, y the following relation is satisfied*

$$|(\gamma_1)_i(x) - (\gamma_1)_j(y)| \leq |(\gamma_2)_i(x) - (\gamma_2)_j(y)|. \tag{5.2}$$

Then the ground states of H_{μ_1,Γ_1} and H_{μ_2,Γ_2} satisfy

$$\min \sigma_p(H_{\mu_1,\Gamma_1}) \leq \min \sigma_p(H_{\mu_2,\Gamma_2}). \tag{5.3}$$

Proof. Proof of this theorem will be analogous to one with Krein's formula with some small yet significant differences. The secular equation of the operator $H_{\mu,\Gamma}$ is given in Lemma 2.1. To show properties of the ground state we will use Birman Schwinger principle which states that $-\kappa^2 \in \sigma(H_{\mu,\Gamma})$ is equal to the fact that the operator $[I - \mu R_{\Gamma,\Gamma}(i\kappa)]$ is not invertible which means that $1 \in \sigma(\mu R_{\Gamma,\Gamma}(i\kappa))$, where

$$R_{\Gamma,\Gamma}(i\kappa)h = G_{i\kappa} * h\delta(x - \Gamma) \quad \delta(x - \Gamma)dx - a.e., \tag{5.4}$$

where $G_{i\kappa}$ represents the resolvent kernel of the free particle. The integral kernel of $G_{i\kappa}(x, x')$ can be written, depending on the dimension of the space, as

$$\begin{aligned} G_{i\kappa}(x, x') &= \frac{2}{\pi} K_0(\kappa|x - x'|), \quad d = 2, \\ G_{i\kappa}(x, x') &= \frac{\exp(-\kappa|x - x'|)}{4\pi \mid x - x' \mid}, \quad d = 3. \end{aligned} \tag{5.5}$$

We are interested in the highest eigenvalue of $\mu R_{\Gamma,\Gamma}(i\kappa)$. This is a simple result of the fact that the function $\mu R_{\Gamma,\Gamma}(i\kappa)$ is decreasing with respect to κ which implies that the eigenvalues are also decreasing with respect to κ. Because we are interested in the largest value of κ we need to look also at the highest eigenvalue of $\mu R_{\Gamma,\Gamma}(i\kappa)$. The highest eigenvalue $\lambda_0(\kappa)$ of $\mu R_{\Gamma,\Gamma}(i\kappa)$ can be written as follows

$$\lambda_0(\kappa) = \max_{\|\psi\|=1} (\psi, \mu R_{\Gamma,\Gamma}(i\kappa)\psi). \tag{5.6}$$

The energy of the ground state $-\kappa^2$ fulfills $\lambda_0(\kappa) = 1$. Now we will show that $\mu R_{\Gamma,\Gamma}(i\kappa)$ has strictly positive eigenfunction belonging to the eigenvalue

1. Our operator $\mu R_{\Gamma,\Gamma}(i\kappa)$ is strictly positive and according to [3, Section XIII.12] a bounded positivity preserving operator $A \in L^2(M, d\sigma)$ with the eigenvalue $\|A\|$ which is ergodic has $\|A\|$ as a simple eigenvalue with strictly positive eigenvector. The integral operator with strictly positive integral kernel is ergodic. Now we can rewrite λ_0 as

$$\lambda_0(\kappa) = \max_{\|\psi\|=1, \psi>0} (\psi, \mu R_{\Gamma,\Gamma}(i\kappa)\psi). \tag{5.7}$$

We can easily establish, using the Green function monotonicity, that an increase in κ results in an increase of the value $(\psi, \mu R_{\Gamma,\Gamma}(i\kappa)\psi)$ as long as ψ is positive. Furthermore the expression $(\psi, \mu R_{\Gamma,\Gamma}(i\kappa)\psi)$ is monotonously increasing with respect to $|x_i - x_j|$, where $x_i, x_j \in \Gamma$, $x_i \neq x_j$ and ψ positive. In other words the function $\lambda_0(\kappa)$ is monotonous with respect to both κ and distances between points belonging to the manifold Γ of singular interactions for the ground state eigenfunction which completes the proof. □

As a consequence of the previous theorem we can derive the following two corollaries. The first one describes the ground state energy for the case that parts of Γ are moved with respect to each other. This case is similar to the point interactions in the way that increase in distance between parts of Γ results in increase of the ground state energy.

Corollary 5.1. *Let H_{μ_1,Γ_1} and H_{μ_2,Γ_2} be operators defined above. μ_1, Γ_1 and μ_2, Γ_2 are related in the following way:*

$$\begin{gathered} |(\gamma_1)_i(x) - (\gamma_1)_j(y)| \leq |(\gamma_2)_i(x) - (\gamma_2)_j(y)| \text{ where } i \neq j, \\ |(\gamma_1)_i(x) - (\gamma_1)_i(y)| = |(\gamma_2)_i(x) - (\gamma_2)_i(y)| \text{ for all } i. \end{gathered} \tag{5.8}$$

Then the ground state of H_{μ_1,Γ_1} and H_{μ_2,Γ_2} satisfies

$$\min \sigma_p(H_{\mu_1,\Gamma_1}) \leq \min \sigma_p(H_{\mu_2,\Gamma_2}). \tag{5.9}$$

Proof. This is the direct consequence of the theorem 5.1. □

For the second special case of Theorem 5.1 we will assume that Γ is composed of one curve. We show that the crumpling up Γ results in the decrease of the ground state energy, e.g. bending of the line segment results in the decrease of the ground state energy. Analogous mechanism gives rise to existence of the ground state for the case of bending a line as demonstrated in [16].

Corollary 5.2. *Let H_{μ_1,Γ_1} and H_{μ_2,Γ_2} be operators defined above. Let μ_1, Γ_1 and μ_2, Γ_2 be related as*

$$|\gamma_1(x) - \gamma_1(y)| \leq |\gamma_2(x) - \gamma_2(y)| \tag{5.10}$$

for all x, y. Then the ground states of H_{μ_1,Γ_1} and H_{μ_2,Γ_2} satisfy

$$\min \sigma_p(H_{\mu_1,\Gamma_1}) \leq \min \sigma_p(H_{\mu_2,\Gamma_2}). \tag{5.11}$$

Proof. This is the direct consequence of the theorem 5.1. □

As an example of application of the previous corollary we can take in the two dimensional space the following configurations: circle and a closed curve obtained from the circle by reflecting smaller sector of the circle with respect to the secant.

5.2 Neumann bracketing

In this section we will prove statements based on Neumann bracketing. This approach will be quite similar to the one for the point interactions in the dimension 2 and 3. Similarly as for point interactions we will require additional conditions on the system. We require the reflection symmetry with respect to line or plane in the dimension 2 or 3 respectively. The main difference between the results using singularity of the resolvent and Neumann bracketing are the assumptions of the theorems. When we want to employ the singularity of the resolvent we have to increase or at least maintain distances between all the points of the support of the singular interactions. For the case of the Neumann bracketing we need symmetry of the system but as a trade off we do not have to increase distance between all the points of the support of the singular interactions but for certain cases some distances can be even decreased.

First we write down two lemmas we will need later for the proofs of the following theorems. These lemmas will be analogous to Lemmas 4.2 and 4.3 for the Neumann bracketing for the point interactions in dimension two and three.

Lemma 5.1. *Let Ψ be the ground state eigenfunction of the operator $H_{\mu,\Gamma}$ defined above for the dimension two. Suppose that the manifold Γ and function μ has reflection symmetry with respect to the line l and $\Gamma \cap l = \emptyset$. Then the ground state function of the operator $H_{\mu,\Gamma}$ satisfies for $x \in l$*

$$\overrightarrow{n} \cdot \nabla\Psi(x) = 0, \tag{5.12}$$

where $\overrightarrow{n}$ is normal vector of the line l and $\cdot$ represents the scalar product.

Proof. Proof of this lemma is based on the fact that the ground state possesses same kind of symmetry as the Hamiltonian. This follows from the strict positivity of the ground state and the fact that the eigenfunction of the operator with the reflection symmetry can be either symmetric or antisymmetric with respect to the line of this symmetry. We transform the Hamiltonian in such a way that the line l will coincide with the x axis of the plane. From the symmetry of the ground state we obtain the following

$$\Psi((x, y)) = \Psi((x, -y)), \tag{5.13}$$

where Ψ is the ground state eigenfunction. This implies that $\nabla\Psi((x, 0))$ is in the form $(c, 0)$, $c \in \mathbb{R}$ which completes the proof. □

The following lemma will be the analogy of the previous one for three dimensions.

Lemma 5.2. *Let Ψ be the ground state eigenfunction of the operator $H_{\mu,\Gamma}$ defined above for the dimension three. Suppose that the operator $H_{\mu,\Gamma}$ has reflection symmetry with respect to the plane p and $\Gamma \cap p = \emptyset$. Then the ground state function satisfies for $x \in p$*

$$\overrightarrow{n} \cdot \nabla\Psi(x) = 0, \tag{5.14}$$

where $\overrightarrow{n}$ is normal vector of the plane p and $\cdot$ represents the scalar product.

Proof. Proof of this lemma is analogous to the proof of Lemma 5.1 so we omit details. □

Now we are ready to state the main result of this section. We will write it down as two theorems, each corresponding to different dimension. We start with the case for the dimension two.

Theorem 5.2. *Let H_{μ_1,Γ_1} be the Hamiltonian defined above for the dimension 2 satisfying the assumptions of Lemma 5.1. Suppose that $\Gamma_1 = \Gamma_1^1 \cup \Gamma_1^2$, where Γ_1^2 is the reflection image of the Γ_1^1 with respect to the line l from Lemma 5.1. Let Γ_2 be the manifold of the codimension one satisfying the following $\Gamma_2 = \Gamma_1^1 \cup \{x + \overrightarrow{T} \mid x \in \Gamma_1^2\}$ where $\overrightarrow{T} \in \mathbb{R}^2$ is the vector fulfilling for all $x \in \Gamma_1^1, y \in \Gamma_1^2$: $\overrightarrow{xy} \cdot \overrightarrow{T} \geq 0$ where y is reflection image of x with respect to l. Furthermore assume that Γ_1 equipped with $\mu_1(x)$ and Γ_2 equipped with $\mu_2(x)$ are related as mentioned at the beginning of this chapter. Then the ground state energy of the operators H_{μ_1,Γ_1} and H_{μ_2,Γ_2} satisfy*

$$\min \sigma_p(H_{\mu_1,\Gamma_1}) \leq \min \sigma_p(H_{\mu_2,\Gamma_2}). \tag{5.15}$$

Proof. Proof of this theorem is analogous to the proof of Theorem 4.2 so we omit details. □

Now we write down, in analogy of the previous, the theorem for the dimension three.

Theorem 5.3. *Let Γ_1 be the manifold of codimension one in dimension three satisfying reflection symmetry with respect to the plane p. Suppose that $\mu_1(x)$ satisfy same reflection symmetry as Γ_1. Furthermore Γ_1 can be written as $\Gamma_1 = \Gamma_1^1 \cup \Gamma_1^2$, where Γ_1^2 is reflection image of the Γ_1^1 with respect to the plane p. Suppose that μ_1, Γ_1 and μ_2, Γ_2 be related in the following way: $\Gamma_2 = \Gamma_1^1 \cup \{x + \overrightarrow{T} \mid x \in \Gamma_1^2\}$ where $\overrightarrow{T} \in \mathbb{R}^3$ is the vector fulfilling for all $x \in \Gamma_1^1, y \in \Gamma_1^2$: $\overrightarrow{xy} \cdot \overrightarrow{T} \geq 0$ where y is reflection image of x with respect to the plane p. Then the ground state energy of the operators H_{μ_1,Γ_1} and H_{μ_2,Γ_2} satisfy*

$$\min \sigma_p(H_{\mu_1,\Gamma_1}) \leq \min \sigma_p(H_{\mu_2,\Gamma_2}). \tag{5.16}$$

Proof. Proof of this theorem is analogous to the proof of Theorem 4.2 so we omit the details. □

Chapter 6

One point interaction and the regular potential

In this chapter we will work with Hamiltonians which can be formally written in the following form:

$$H = -\Delta + V(x) + \alpha\delta(y), \tag{6.1}$$

where $-\Delta$ act as second derivative on $L^2(\mathbb{R})$, $V(x)$ is a regular potential, $y \in \mathbb{R}$ and α is the point interaction strength. For several cases of different potentials V we will optimize the position of the point interaction with respect to the potential. We will minimize the energy of the ground state with respect to the position of the point interaction site. We will work with the following types of potential: a rectangular potential well, a piecewise linear potential, a monotonous potential and a mirror-symmetric confining potential. One might expect that the minimum of energy will be obtained by placing point interaction into the minimum of the potential. We will show that this is true for a class of symmetric potentials and attractive point interaction. On the other hand for asymmetric potentials this statement may not hold as we shall demonstrate on the example of a piecewise linear potential.

6.1 Rectangular potential well

In this section we will work with the Hamiltonian which can be written as

$$H_{\alpha,y} = -\Delta - V\chi_{(-a,a)}(x), \tag{6.2}$$

where $V \in \mathbb{R}^+$ and $\chi_{(-a,a)}$ is characteristic function of the interval $(-a, a)$. The domain of our operator is $\mathscr{D}(H_{\alpha,y}) = \{\psi \in H^{2,2}(\mathbb{R} \setminus \{y\}) \cap H^{2,1}(\mathbb{R}) \mid \alpha\psi(y) = \psi'(y+) - \psi'(y-)\}$.

We want to obtain the spectral condition. First we construct the ground state eigenfunction. We will find solutions in four separate regions, namely $(-\infty, -a)$, $(-a, y)$, (y, a) and (a, ∞). We employ the following notation:

$$\begin{aligned} \psi(x) &= \psi_1(x) \text{ for } x \in (-\infty, -a), \\ \psi(x) &= \psi_2(x) \text{ for } x \in (-a, y), \\ \psi(x) &= \psi_3(x) \text{ for } x \in (y, a), \\ \psi(x) &= \psi_4(x) \text{ for } x \in (a, \infty). \end{aligned} \tag{6.3}$$

We want our function to be from the domain of our operator. This means that we have to employ boundary conditions at the points $-a, a$ and y. The conditions at the points $-a, a$ require continuity of the function and its first derivative. Condition at the point y will correspond to the point interaction on the line, i.e. continuity of the function and finite jump in the derivative of the function. These conditions can be written as follows:

$$\begin{aligned} \psi_1(-a) = \psi_2(-a), \quad \psi_1'(-a) = \psi_2'(-a), \\ \alpha\psi_2(y) = \psi_3'(y+) - \psi_2'(y-) = \alpha\psi_3(y), \\ \psi_3(a) = \psi_4(a), \quad \psi_3'(a) = \psi_4'(a). \end{aligned} \tag{6.4}$$

Eigenvector equation $H_{\alpha,y}\psi_i = E\psi_i$ on the indicated intervals can be solved exactly. We obtain:

$$\begin{aligned} \psi_1(x) &= a\exp(\kappa x), \\ \psi_2(x) &= b\exp(-kx) + c\exp(kx), \\ \psi_3(x) &= d\exp(-kx) + e\exp(kx), \\ \psi_4(x) &= f\exp(-\kappa x), \end{aligned} \tag{6.5}$$

where $\kappa^2 = -E$ and $k^2 = -E - V$. Without loss of generality we can fix the length of the rectangular potential well, because the result for another a can be obtained by a rescaling with a simultaneous change of the values of V and α. We choose a to be equal to 1, because it simplifies explicit form of the conditions. Now using the conditions (6.4) we obtain spectral conditions for the rectangular potential well, where $a = 1$ in the following form

$$\alpha = k\frac{B\exp(ky) - A\exp(-ky) - F(A\exp(ky) + B\exp(-ky))}{A\exp(-ky) - B\exp(ky)}, \tag{6.6}$$

where $A = \frac{k+\kappa}{2k}\exp(-\kappa+k)$, $B = \frac{k-\kappa}{2k}\exp(-\kappa-k)$ and $F = \frac{A\exp(-ky)+B\exp(ky)}{A\exp(ky)+B\exp(-ky)}$. We can simplify the previous expression to the following form

$$\alpha = k\frac{B^2 - A^2}{A^2 + B^2 + 2AB\cosh(2ky)}. \tag{6.7}$$

Now we plot the ground state energy with respect to the point interaction strength α and position of the point interaction obtained by solution of the spectral condition written above. The graph for the potential $V(x) = -5\chi_{(-1,1)}(x)$ can be seen on the figure 6.1. On this graph we can notice several things. We see that the behavior of the ground state with respect to the position of the point interaction changes for the value of the point interaction strength $\alpha = 0$, which corresponds to absence of the point interaction. For attractive point interaction, $\alpha < 0$, the optimal position is at the center of the rectangular potential well and moving point interaction towards the center results in a decrease of the ground state energy. For repulsive point interaction, $\alpha > 0$, the behavior is different. The ground state energy decreases when the repulsive point interaction is shifted towards the boundary of the rectangular potential well and then away from the rectangular potential well. From this we can conclude that minimal energy for the repulsive point interaction is obtained when the point interaction site goes to $\pm\infty$. On the graph we can also notice that for the higher states the previous statements are no longer valid, e.g. the roles of attractive and repulsive point interactions are interchanged for the behavior of the first excited state energy. The energy of the system without the point interaction, $\alpha = 0$, equals $E \approx -3.8525$.

In figure 6.2 we can see the behavior of the ground state energy when we move point interaction outside of the rectangular potential well. For the point interaction strength $\alpha < -3.9256$ the ground state energy goes to the value $E = -\alpha^2/4$, when point interaction moves far away from potential well. This value corresponds to the ground state energy of the point interaction without rectangular potential well. For the point interaction strength $\alpha \geq -3.9256$ the energy goes in the limit to the ground state energy of the potential rectangular well without point interaction. Similar behavior can be seen for the first excited state with lower limit value of the ground state energy of the rectangular potential well and higher limit value of first excited state of the rectangular potential well.

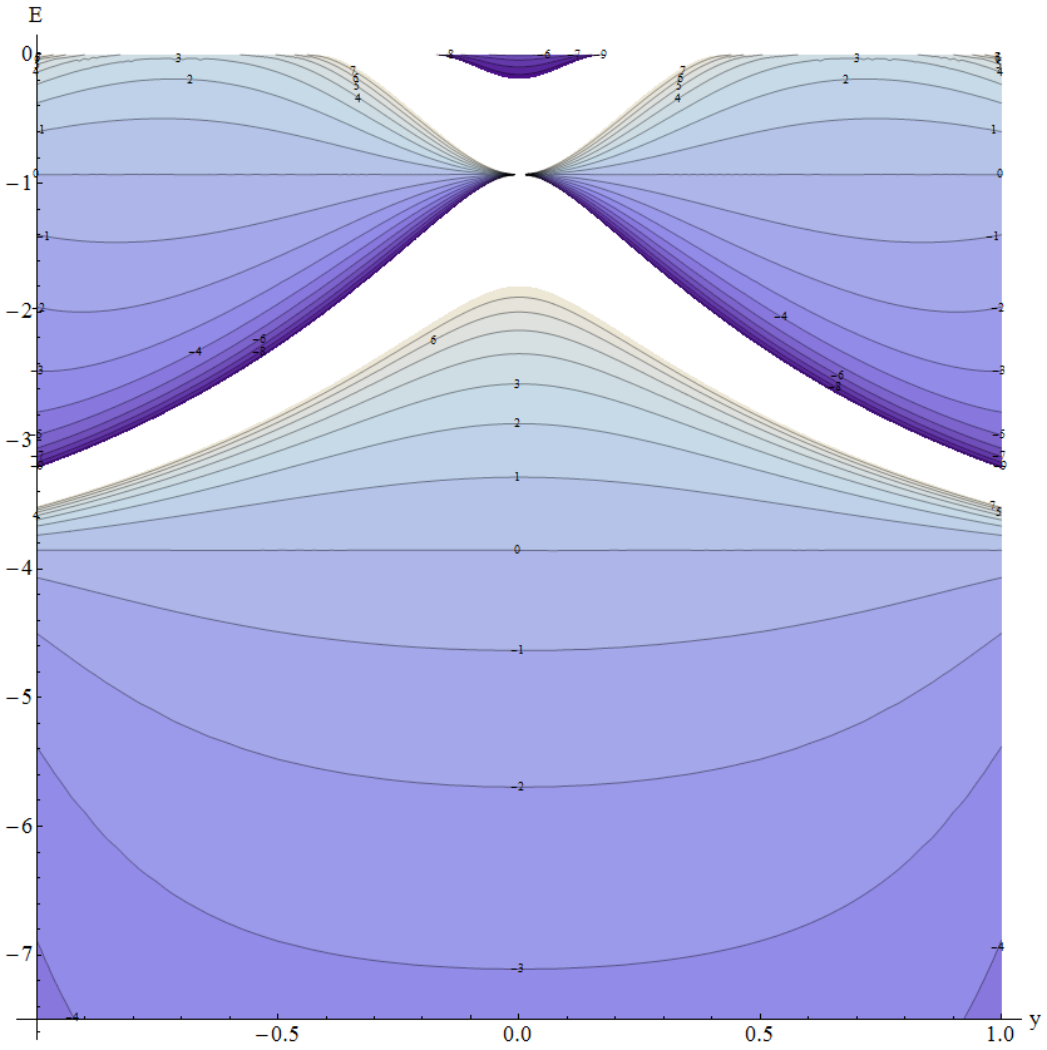

Figure 6.1: The ground state energy with respect to the point interaction strength and point interaction position in the rectangular potential well $V(x) = -5\chi_{(-1,1)}(x)$

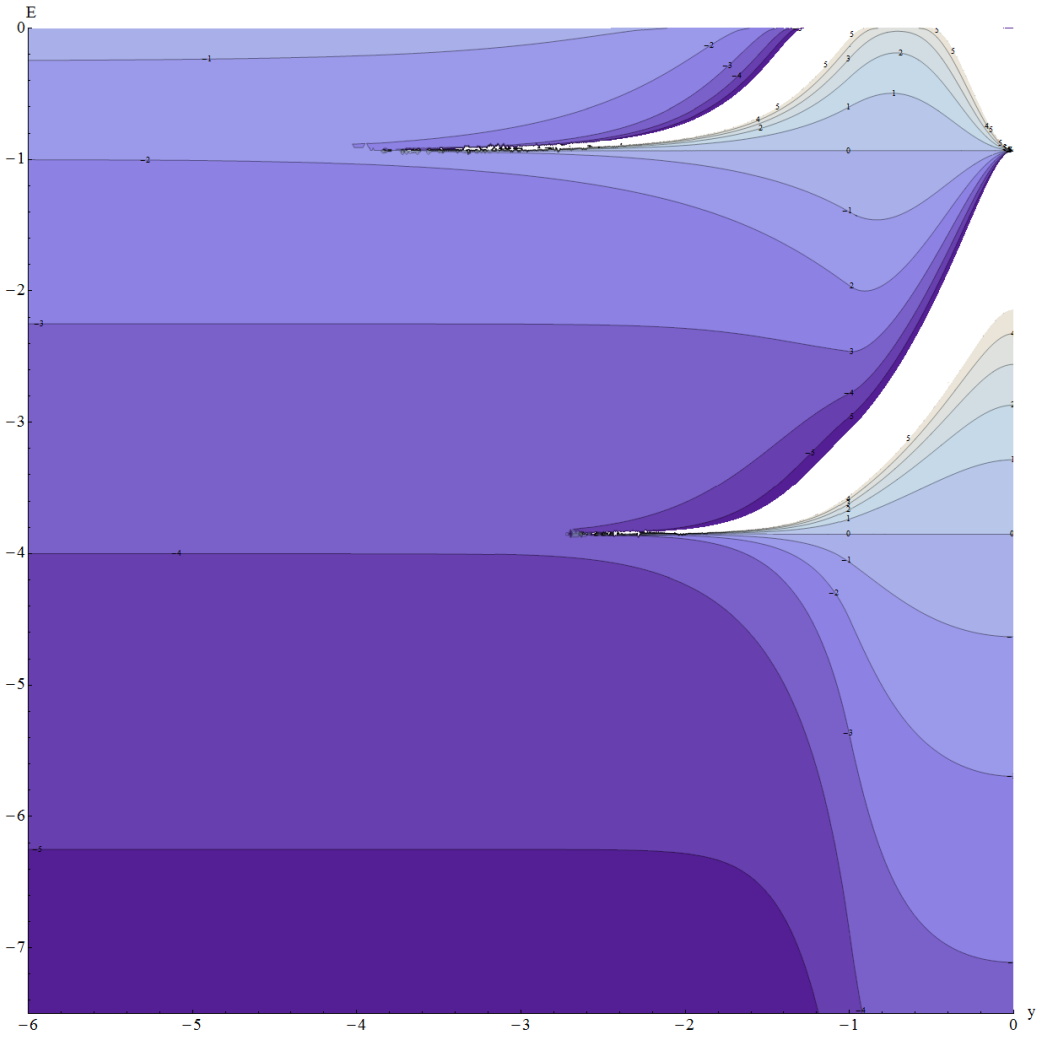

Figure 6.2: The ground state energy with respect to the point interaction strength and point interaction position in the rectangular potential well $V(x) = -5\chi_{(-1,1)}(x)$

6.2 Piecewise linear potential well

In this section we work with piecewise linear potential which can be written in the following way

$$V(x) = \begin{cases} kx & x \geq 0 \\ lx & x < 0, \end{cases} \tag{6.8}$$

where k is a positive number and l a negative one. We are interested in the ground state of the operator

$$\begin{gathered} H_{\alpha,y} = -\Delta + V(x), \\ \mathscr{D}(H_{\alpha,y}) = \{\psi \in H^{2,2}(\mathbb{R} \setminus \{y\}) \cap H^{2,1}(\mathbb{R}) \mid \alpha\psi(y) = \psi'(y+) - \psi'(y-)\}. \end{gathered} \tag{6.9}$$

We will show that for the symmetric potential, i.e. $|k| = |l|$ the optimal position of the attractive point interaction is at the point $y = 0$. For the asymmetric case this is no longer true. The optimal position for this case is shifted in the direction away from the potential with steeper slope. Similarly as for the rectangular potential well we will solve the eigenfunction problem separately at three intervals $(-\infty, y)$, $(y, 0)$ and $(0, \infty)$ and then we will connect these solutions by suitable boundary conditions at the points y and 0.

We will use the notation

$$\begin{aligned} &\psi(x) = \psi_1(x) \text{ for } x \in (-\infty, y), \\ &\psi(x) = \psi_2(x) \text{ for } x \in (y, 0), \\ &\psi(x) = \psi_3(x) \text{ for } x \in (0, \infty). \end{aligned} \tag{6.10}$$

The conditions which have to be satisfied at the points $y, 0$ are the following

$$\begin{aligned} \alpha\psi_1(y) = \psi_2'(y+) - \psi_1'(y-) = \alpha\psi_2(y), \\ \psi_2(0) = \psi_3(0), \quad \psi_2'(0) = \psi_3'(0). \end{aligned} \tag{6.11}$$

We are able to solve the eigenvector equation $H_{\alpha,y}\psi = E\psi$ on the intervals $(-\infty, y)$, $(y, 0)$ and $(0, \infty)$ exactly:

$$\begin{aligned} \psi_1(x) &= a\mathrm{Ai}\left(\tfrac{-E+lx}{|l|^{2/3}}\right), \\ \psi_2(x) &= b\mathrm{Ai}\left(\tfrac{-E+lx}{|l|^{2/3}}\right) + c\mathrm{Bi}\left(\tfrac{-E+lx}{|l|^{2/3}}\right), \\ \psi_3(x) &= \mathrm{Ai}\left(\tfrac{-E+kx}{|k|^{2/3}}\right), \end{aligned} \tag{6.12}$$

where the symbols Ai and Bi denotes Airy functions which are two linearly independent solutions of the equation $y'' - xy = 0$, for more information about them see [10]. With the help of the conditions (6.11) we can obtain explicit forms of the constants a, b and c and the spectral condition. We will work with the spectral condition given in (6.11) as the condition at the point interaction site, i.e.

$$\alpha = \frac{\psi_2'(y+) - \psi_1'(y-)}{\psi_1(y)}. \tag{6.13}$$

Similarly as for the case of the rectangular potential well we plot the ground state energy with respect to α and position of the point interaction. On figure 6.3 we see the case $k = -l = 10$. This situation is symmetric and as we mentioned before, the optimal position for the attractive point interaction is at the center at the minimum of potential energy. When we move the attractive point interaction towards the center the ground state energy decreases. On figure 6.4 we have an asymmetric case $k = 10$, $l = -1$ for which is no longer true that minimal energy is obtained by placing the attractive point interaction at the minimum of the potential.

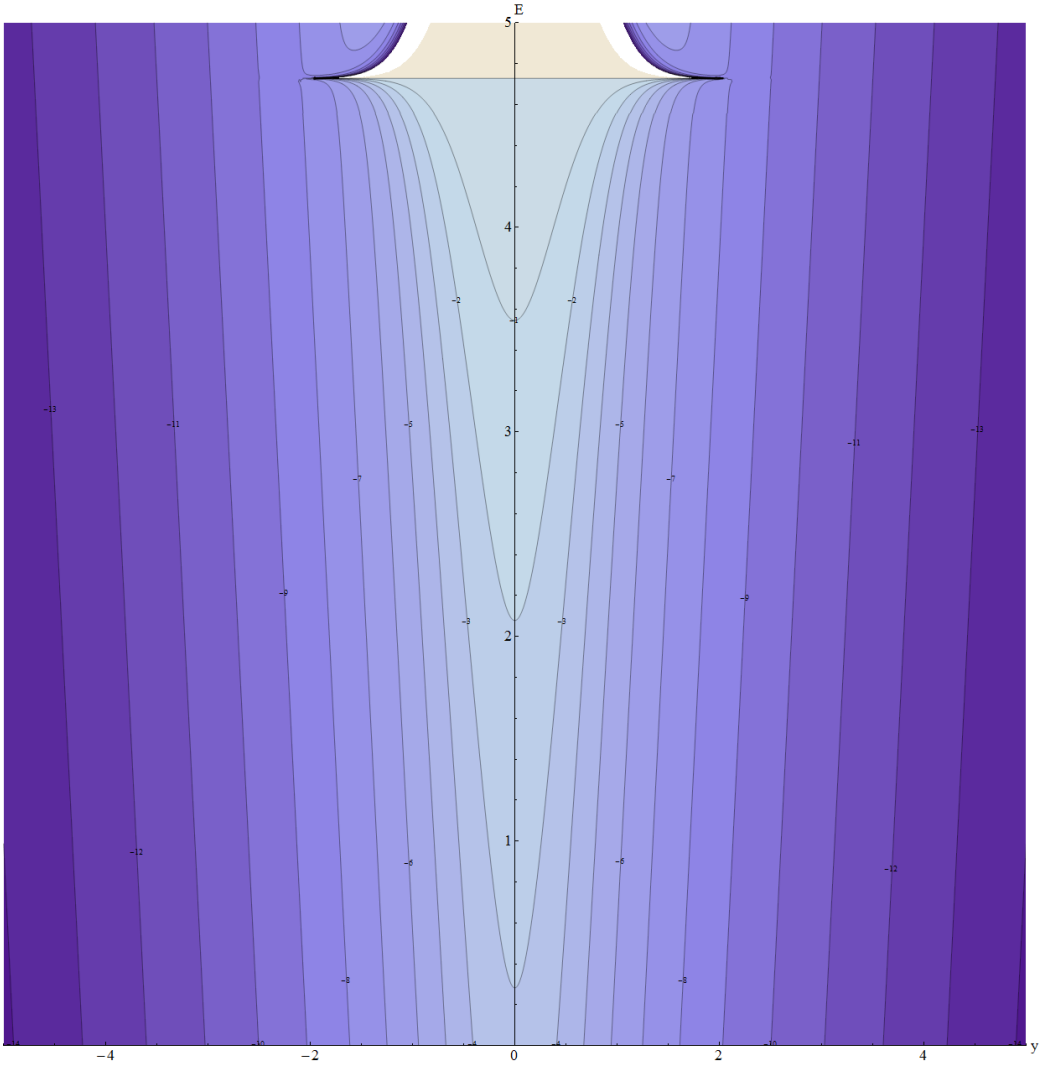

Figure 6.3: Ground state energy with respect to the point interaction strength and point interaction position for the piecewise linear potential $k = -l = 10$

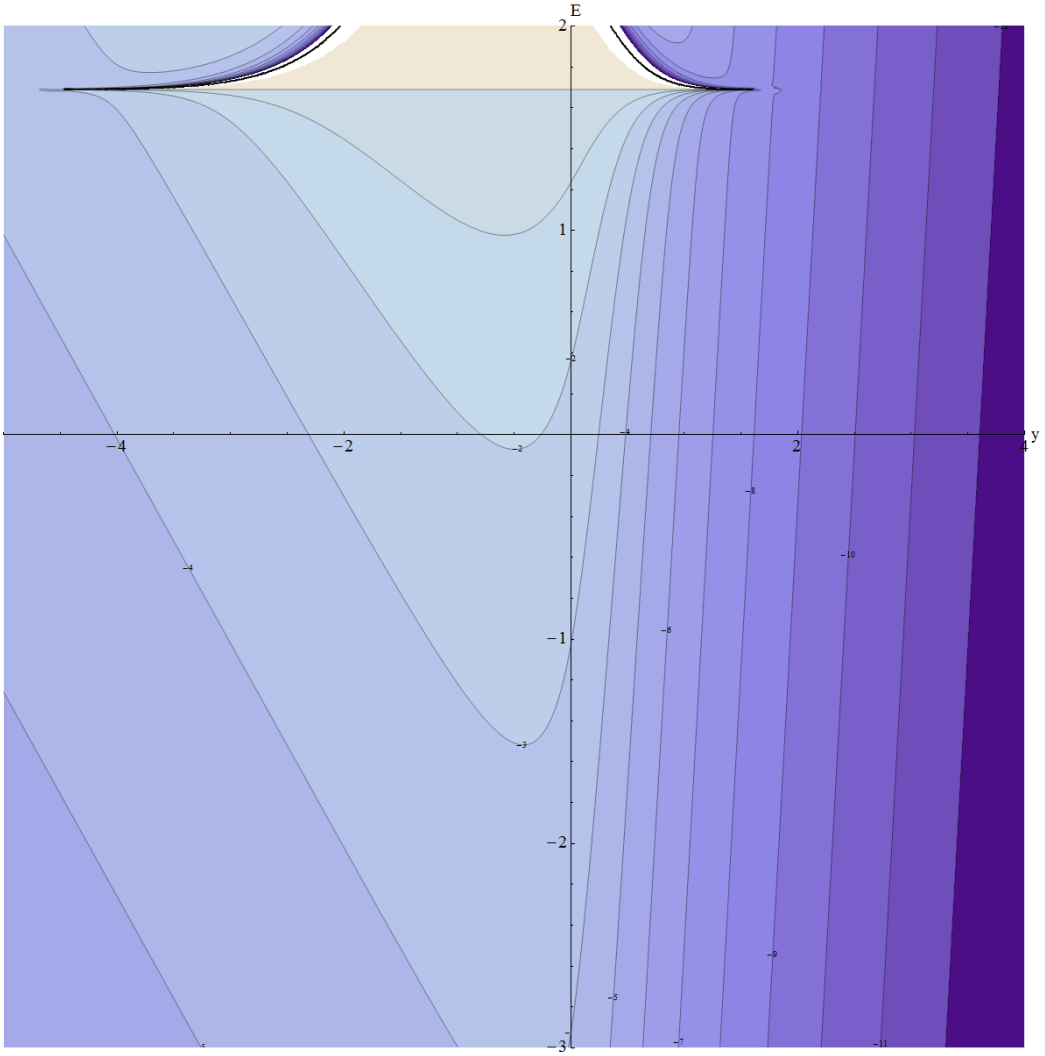

Figure 6.4: Ground state energy with respect to the point interaction strength and point interaction position for the piecewise linear potential $k = 10$ and $l = -1$

6.3 Monotonous Potential

As a warm-up for the next section with symmetric potential we start with a monotonous potential and we show that the ground state energy goes down when we move the attractive point interaction in the direction of the potential decrease. We will work with the operator which can be written as follows

$$\begin{gathered} H_{\alpha,y} = -\Delta + V(x), \\ \mathscr{D}(H_{\alpha,y}) = \{\psi \in H^{2,2}(\mathbb{R} \setminus \{y\}) \cap H^{2,1}(\mathbb{R}) \mid \alpha\psi(y) = \psi'(y+) - \psi'(y-)\}, \end{gathered} \tag{6.14}$$

where the potential V is differentiable and satisfies $\frac{dV}{dx}(x) \leq 0$ for all $x \in \mathbb{R}$.

The potential $V(x)$ is quantum-mechanically complete which means that the operator $-\Delta+V(x)$ is essentially self-adjoint on $C_0^\infty(0,\infty)$. The condition when the real valued continuous function $V(x)$ is complete according to [4, Theorem X.8] is the following:

$$V(x) \geq -M(x), \tag{6.15}$$

where $M(x)$ is positive differentiable function satisfying

$$\begin{gathered} \int_1^\infty \frac{1}{\sqrt{M(x)}} dx = \infty, \\ \frac{M'(x)}{M(x)^{3/2}} \text{ is bounded near } \infty. \end{gathered} \tag{6.16}$$

These conditions are for example satisfied for the potential which behaves as $c(-x)^{-\beta}$ for $x \to -\infty$, where c is constant and $\beta \leq 2$.

For the proof of the following theorem we will need the Hellman-Feynman theorem. This theorem states how the eigenvalues changes with respect to the changes of the Hamiltonian depending on a parameter. For the non-degenerate ground state energy it can be written as follows

$$\frac{dE(\lambda)}{d\lambda} = \left(\psi(\lambda), \frac{dH(\lambda)}{d\lambda}\psi(\lambda)\right), \tag{6.17}$$

where $\psi(\lambda)$ is the ground state eigenfunction of the operator $H(\lambda)$. Now we will state theorem which relates position of the point interaction and the ground state energy.

Theorem 6.1. *Let H_{α,y_1} and H_{α,y_2} be the operators defined above with $\alpha < 0$. Then the ground state energy of the operators H_{α,y_1} and H_{α,y_2} satisfy*

$$\min \sigma_p(H_{\alpha,y_1}) \leq \min \sigma_p(H_{\alpha,y_2}), \tag{6.18}$$

where $y_1 > y_2$. The inequality is sharp for the case that the expression $\frac{dV}{dx}(x)$ is not equal to zero for all x.

Proof. We prove this theorem by means of the Hellman-Feynman theorem. It is sufficient to prove this for the operator $H_{\alpha,y+\lambda}$ with general point $y \in \mathbb{R}$ and infinitesimally small λ, i.e. we need to show that

$$\left(\psi, \frac{dH_{\alpha,y+\lambda}}{d\lambda}\psi\right) = \left(\psi, \frac{dV(\lambda)}{d\lambda}\psi\right) < 0, \tag{6.19}$$

where ψ is the ground state of the operator $H_{\alpha,y}$. If we write explicitly the right hand side of previous relations we obtain

$$\left(\psi, \frac{dV(\lambda)}{d\lambda}\psi\right) = \int_{\mathbb{R}} \frac{dV(x)}{dx}|\psi(x)|^2 dx, \tag{6.20}$$

where we put $\lambda = 0$. The expression on the right hand side is obviously negative because it is integral from the product of positive function $|\psi(x)|^2$ and negative one $\frac{dV(x)}{dx}$ which completes the proof. □

We note that we can show analogous theorem for the dimension 2 and 3, where moving the point interaction in the direction of the decrease of the potential would result in decrease of the ground state energy.

6.4 Mirror-symmetric confining potential

In this section we work with Hamiltonians which can be written as follows

$$\begin{gathered} H_{\alpha,y} = -\Delta + V(x), \\ \mathscr{D}(H_{\alpha,y}) = \{\psi \in H^{2,2}(\mathbb{R} \setminus \{y\}) \cap H^{2,1}(\mathbb{R}) \mid \alpha\psi(y) = \psi'(y+) - \psi'(y-)\}, \end{gathered} \tag{6.21}$$

where $V(x)$ is a positive differentiable function with mirror symmetry with respect to zero, i.e. $V(x) = V(-x)$, fulfilling that $V(x)$ is increasing for the $x \in [0, \infty)$. Without loss of generality we will assume that $V(0) = 0$. We will show that for this situation the optimal position of the attractive point

interaction is at the minimum of the potential. We will need additional condition concerning the value of the ground state energy E. It can be written as $E < 0$. This condition can be satisfied if we choose the point interaction strength $|\alpha|$ large enough.

The property mentioned above concerning the ground state energy can be shown in a similar way as for the monotonous potential. First we will state certain properties of the ground state we will need later.

Lemma 6.1. *Let $H_{\alpha,y}$ be the operator defined above with $\alpha < 0$. Furthermore assume that $E < 0$, where E is the ground state energy. Then the ground state function of the operator is strictly positive, convex with exactly one maximum at the point interaction site y.*

Proof. We will split the proof of this lemma into three parts. We will start by proving the strict positivity of the ground state eigenfunction. Then we show the convexity and then existence of one maximum.

Positivity of the ground state

We will show that the ground state function ψ does not possess any nodal points, i.e. there is no point in $x \in \mathbb{R}$ for which is the eigenfunction equal to zero, i.e. $\psi(x) = 0$. We construct the ground state by connecting solutions ψ_1 on the interval $(-\infty, y)$ and ψ_2 on the interval (y, ∞) by point interaction boundary condition at y. These functions satisfy the equation $(-\Delta + V(x))\psi_i(x) = H_i\psi_i(x) = E\psi_i(x)$. We will show that these solutions do not fulfill $\psi_i(z) = 0$ for any $z \in \mathbb{R}$ with the help of Neumann bracketing. For the moment we assume that there exist such a point where $\psi_1(z)$ is equal to zero. We introduce the operator $H^{D,z}_{\alpha,y}$ which acts on functions on the interval $(-\infty, y)$ as operator $-\Delta + V(x)$ and has at the point z Dirichlet boundary condition. Because we chose the point z in such a way that the eigenfunction ψ_1 fulfills the Dirichlet condition at z. The operators H_1 and $H^{D,z}_{\alpha,y}$ have the same eigenvalue belonging to function ψ_1. Now according to [3, Section XIII.15] taking the Dirichlet boundary condition away from the operator $H^{D,z}_{\alpha,y}$ results in decrease of the energy. From this we have that the operator without Dirichlet condition which act as H_1 has a lower or at least the same eigenvalue with eigenvector without nodal point at point z. By this approach we can show that the functions ψ_1 and ψ_2 has no nodal points $\psi_i(x) = 0$. From the continuity condition at the point interaction site we have that both ground state function ψ_1 and ψ_2 have the same sign. Furthermore both these function do not change sign because they are not equal

to zero anywhere on $\mathbb{R}$ from which we have that the function ψ can be either strictly positive or negative which completes the proof.

Convexity of the ground state
The convexity of the ground state follows from the eigenvalue equation given as $(-\Delta + V(x))\psi(x) = E\psi(x)$. This equation can be rewritten as

$$\psi''(x) = (V(x) - E)\psi(x) > 0. \tag{6.22}$$

The inequality follows from the strict positivity of the ground state and assumption $E < 0$.

One maximum property
The property of the ground state having one maximum follows from the convexity and square integrability of the ground state. The convex smooth functions have a maximum at the endpoint of its domain. Our ground state eigenfunction is smooth and convex on two intervals $(-\infty, y)$ and (y, ∞). At the point y these functions are connected by the conditions describing point interaction, i.e. continuity of the function and finite jump in the first derivative depending on the value of the function at this point. The ground state eigenfunction is square integrable which implies that $\lim_{x\to\pm\infty} \psi(x) = 0$. This and the positivity of the ground state eigenfunction implies that the functions on the intervals $(-\infty, y)$ and (y, ∞) has at the point y maximum which completes the proof. □

We will show that the ground state function ψ of the operator $H_{\alpha,y}$ satisfying $E < 0$ and $y < 0$ fulfills: $\psi(-x) > \psi(x)$ where $x > 0$.

Lemma 6.2. *Let $H_{\alpha,y}$ be the operator defined above with $\alpha < 0$ and $y < 0$. Furthermore assume that the ground state energy is $E < 0$. Then the ground state of the operator satisfies $\psi(-x) > \psi(x)$ for all $x \in (0, \infty)$.*

Proof. We will prove this statement in two steps for the intervals $-x \in (y, 0)$ and $-x \in (-\infty, y)$, where $x \in \mathbb{R}^+$.

We start with the interval $-x \in (y, 0)$. In the previous lemma we have established that the ground state eigenfunction $\psi(x)$ has only one maximum. From the square integrability we have $\lim_{x\to\pm\infty} \psi(x) = 0$. This along with convexity implies that $\psi(y) > \psi(y + c)$ where $c \in \mathbb{R}^+$ and completes the

proof for the interval $x \in (0, -y)$.

The property for the interval $-x \in (-\infty, y)$ can be proven in the following way. The ground state eigenfunction $\psi_1(-x)$ at the interval $-x \in (-\infty, y)$ satisfies $(-\Delta + V(-x) - E)\psi_1(-x) = 0$ and ground state function $\psi_2(x)$ on the interval $x \in (-y, \infty)$ fulfills $(-\Delta + V(x) - E)\psi_2(x) = 0$. From the mirror symmetry of the potential $V(x) = V(-x)$ and strict positivity of the ground state we have that $\psi_1(x) = c\psi_2(-x)$, where $c \in \mathbb{R}^+$. We have already established that $\psi(y) > \psi(-y)$ which implies that $c > 1$. □

Now we are ready to prove the main theorem of this section concerning optimization of the position of the point interaction with respect to the ground state energy.

Theorem 6.2. *Let H_{α,y_1} and H_{α,y_2} be the operators defined above with $\alpha < 0$. Assume that the ground state energy of both operators fulfill $E < 0$. Then the ground state energy of the operators H_{α,y_1} and H_{α,y_2} satisfy*

$$\min \sigma_p(H_{\alpha,y_1}) < \min \sigma_p(H_{\alpha,y_2}), \tag{6.23}$$

where $|y_1| < |y_2|$.

Proof. We will employ Hellman-Feynman theorem presented in the previous section. We will show that moving the point interaction towards the center of the potential results in decrease of the energy. It can be seen that it is sufficient to prove the theorem for $y < 0$. It is a result of the fact that the symmetry of the problem implies $\sigma_p(H_{\alpha,y}) = \sigma_p(H_{\alpha,-y})$. We will work with the class of the operators $H_{\alpha,y+\lambda}$ depending on the real parameter $\lambda \in (-\infty, -y)$. We write down explicit form of the ground state energy dependence on λ as

$$\frac{dE(\lambda)}{d\lambda} = \left(\psi, \frac{dV(\lambda)}{d\lambda}\psi\right), \tag{6.24}$$

where ψ is the ground state eigenfunction of the operator $H_{\alpha,y+\lambda}$. It is sufficient to show the inequality $\frac{dE(\lambda)}{d\lambda} < 0$ for $\lambda = 0$ and general point $y \in (-\infty, 0)$. We rewrite relation $\frac{dE(\lambda)}{d\lambda}$ as

$$\left(\psi, \frac{dV(\lambda)}{d\lambda}\psi\right) = \int_{\mathbb{R}} \frac{dV(x)}{dx}|\psi(x)|^2 dx = \int_{\mathbb{R}^+} \frac{dV(x)}{dx}(|\psi(x)|^2 - |\psi(-x)|^2)dx. \tag{6.25}$$

We know that $\frac{dV(x)}{dx} > 0$ and according to Lemma 6.2 we have $\psi(x) < \psi(-x)$ for $x \in \mathbb{R}^+$ which implies $|\psi(x)|^2 - |\psi(-x)|^2 < 0$ and this completes the proof. $\square$

Chapter 7

Conclusion

We have studied the relation between the ground state energy and geometry of the point interactions sites for several systems. We have analyzed a generalization of this problem to singular interactions supported by the manifold of codimension one. We have studied one, two and three dimensional systems. We have shown that an increase in distance between the attractive point interaction sites results in an increase in the ground state energy in $\mathbb{R}^d$, $d = 1, 2, 3$. For systems with more complex topology such as graphs the situation can be more complicated. On graphs the property of the ground state with respect to length of the edge depends on the type of the ground state function on the edge. There is the possibility that an increase in length of an edge can result in an decrease of the ground state energy or even to remain unchanged. The situation on graphs degenerate to the previous case in cases of graphs without any branching. For several cases of one dimensional systems with the potential and one point interaction we have minimized the ground state energy with respect to the position of the point interaction.

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