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Geometrically induced properties of the ground state of quantum graphs Hamiltonians

Geometricky podmíněné vlastnosti základního stavu kvantových grafů

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Chapter 1

Introduction

In this work we will discuss the properties of the ground state of the free quantum particle moving on the graph. We will be working with the operator, which acts on the edges of the graph as

$$\hat{H} = -\frac{\partial^2}{\partial x^2} \tag{1.1}$$

We need our operator to be self-adjoint which can be accomplished by imposing certain boundary conditions on each vertex of the graph. We will be working with the so-called delta coupling which is analogous to delta interaction on the line. It can be expressed as

$$\psi_i(0) = \psi_j(0) = \alpha \sum_{k=1}^{n} \psi_k'(0+) \tag{1.2}$$

for each vertex. We are especially interested in the ground state of the graph where all the interaction strengths α are negative.
We are interested in the ground state, because the ground state as the state with the lowest energy has its natural importance. The particle in the isolated system remains in its given eigenstate, however in reality the physical system interacts with the surroundings which usually acts as the heat bath. This results in exchange of the energy typically in the form of electromagnetic field and that results in the dissipation of the energy. Such energy dissipation results in the lowering the energy of the system to the energy of the ground state.
In this work we focus on the relation between the length of the edges and the

energy of the ground state. We will show that the situation is more complex than the similar situation on the line which we have studied in a previous work [9]. On the line we have the property that the increase in the distance between two point interactions with negative constant results in the increase of the energy of the ground state. The situation on the graph is more interesting because there are two possible options of the behavior of the ground state. First is similar to the situation on the line i.e. the increase of the length of the edge results in increase of the energy of the ground state and the other one is exactly opposite i.e. the increase of the length of the edge results in the decrease of the energy of the ground state. In this work we show necessary and sufficient conditions of the ground state function on the edges of the graph which have to be met for the ground state to have the properties mentioned above.

Chapter 2

Setting of the problem

We are interested in the ground state of the quantum particle on the graph $\mathbb{G}$. We consider our graph $\mathbb{G}$ to be finite and to be constructed from p vertices and q edges, where $p, q \in \mathbb{N}$. Our edges can be either of finite length or semi-finite length. We represent the lengths of the edges by the vector $L = (l_i \mid i \in \hat{q})^T$, where $l_i \in \mathbb{R}^+ \cup \{+\infty\}$. We can define in the natural way the Lebegue measure dx on the graph. We construct the space $L^2(\mathbb{G})$ on the graph $\mathbb{G}$ from all measurable square integrable functions on each edge i.e.

$$\parallel f \parallel^2_{L^2(\mathbb{G})} = \sum_{i=1}^{q} \parallel f \parallel^2_{L^2(0,l_i)} < \infty \tag{2.1}$$

in other words we construct our space as orthogonal direct sum of $L^2(0, l_i)$ i.e.

$$L^2(\mathbb{G}) = \bigoplus_{i=1}^{q} L^2(0, l_i) \tag{2.2}$$

From this we can write functions from our Hilbert space $L^2(\mathbb{G})$ as $\psi = (f_i \mid f_i \in L^2(0, l_i), i \in \hat{q})^T$. Our Hamiltonian which we will be working with acts as

$$H\psi_i = -\psi_i'' \tag{2.3}$$

We need our operator to be self-adjoint. This can be accomplished by introducing certain boundary conditions at each vertex. General conditions can be written in the matrix form according to [6] as

$$A\Psi + B\Psi' = 0 \tag{2.4}$$

where $A, B \in \mathbb{C}^{n\times n}$ fulfill

$$\begin{aligned} \mathrm{rank}(A \mid B) &= n \\ AB^{+} &\text{ is self adjoint} \end{aligned} \tag{2.5}$$

It is obvious that the matrices A and B are not unique. For example the boundary condition given by the set of matrices (A, B) and (CA, CB), where C is regular matrices are same. A suitable choice for the matrices A and B which would be unique is

$$\begin{aligned} A &= U - I \\ B &= i(U + I) \end{aligned} \tag{2.6}$$

where I is identity matrix and $U =$ is unitary matrix.
We will be working with the conditions in the form

$$\begin{aligned} f_{j_g}(0) = f_{j_h}(0) = f_{k_m}(l_{k_m}) &= f_{k_n}(l_{k_n})\,\forall g,h \in \hat{m}_y\,\forall m,n \in \hat{n}_y \\ \sum_{i=1}^{m_y} f'_{j_i}(0+) - \sum_{i=1}^{n_y} f'_{k_i}(l_{k_i}-) &= \alpha_y f_{j_1}(0) \end{aligned} \tag{2.7}$$

for all y where m_y and n_y are number of edges entering the y-th vertex or leaving respectively. Among the conditions (2.4), these conditions (2.7) are the only ones having wave function continuous at the vertices. Put together we have Hamiltonian with domain $H^{2,2}(\mathbb{G})$ fulfilling condition (2.7). It is worth mentioning that for the vertex with one edge this condition is the same as the Robin condition when $\alpha \neq 0$ and Neumann condition when $\alpha = 0$. Our condition can be rewritten in the matrix form as

$$\begin{aligned} A_i f + B_i f' &= 0 \\ A_i &= \begin{pmatrix} 1 & -1 & 0 & \ddots & 0 \\ 0 & 1 & -1 & \ddots & 0 \\ 0 & \ddots & \ddots & \ddots & 0 \\ 0 & \ddots & 0 & 1 & -1 \\ \alpha_i & 0 & \cdots & 0 & 0 \end{pmatrix} \\ B_i &= \begin{pmatrix} 0 & 0 & \cdots & 0 \\ 0 & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & 0 \\ 1 & \cdots & 1 & 1 \end{pmatrix} \end{aligned} \tag{2.8}$$

where $i \in \hat{p}$, $A_i \in \mathbb{R}^{m_i+n_i X m_i+n_i}$ and $B_i \in \mathbb{R}^{m_i+n_i X m_i+n_i}$. Another suitable choice for the matrices A_i and B_i is

$$\begin{aligned} A_i &= U_i - I \\ B_i &= i(U_i + I) \end{aligned} \tag{2.9}$$

where I is identity matrix and $U_i = \frac{2}{n+i\alpha_i} J - I$ where n is number of edges entering and leaving the vertex and J is matrix having all entries equal to 1. It is not necessary to work with set of conditions for each vertex separately. We can restate the problem to different graph $\mathbb{G}_0$ with one vertex where all the conditions and the topology of the original graph is encoded as the boundary condition for one vertex as it is described in [7]. The space of the new graph $\mathbb{G}_0$ is isomorphic with $\mathbb{G}$ which can be easily seen from the fact that we leave the length of all edges the same. We also do not change the action of our operator. Our condition (2.7) can be transferred to a new graph as

$$Af + Bf' = 0 \tag{2.10}$$

where A, B are block diagonal matrices fulfilling

$$\begin{gathered} \operatorname{rank}(A \mid B) = \sum_{y=1}^{p} m_y + n_y \\ A_v B_v^* \text{ is self-adjoint} \end{gathered} \tag{2.11}$$

We construct the matrix A as direct sum of A_i $i \in \hat{p}$ i.e.

$$A = \bigoplus_{i=1}^{q} U_i = \begin{pmatrix} A_1 & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & A_p \end{pmatrix} \tag{2.12}$$

and matrix B as direct sum of Bi $i \in \hat{p}$ i.e.

$$B = \bigoplus_{i=1}^{q} B_i = \begin{pmatrix} B_1 & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & B_p \end{pmatrix} \tag{2.13}$$

Now we are ready to describe the operator, which we will be working with for now on. Our operator acts as

$$(-\Delta_{\mathbb{G},\alpha,L}\psi)_i = -(\psi'')_i \tag{2.14}$$

with the domain $\mathrm{D}(-\Delta_{\mathbb{G},\alpha,L}) = \{\psi \in \bigoplus_{j=1}^{q} H^{2,2}(l_i) \mid A\psi + B\psi' = 0\}$ where $\alpha = (\alpha_1, \ldots, \alpha_p)$. We can associate the quadratic form with our operator $-\Delta_{\mathbb{G},\alpha,L}$. The the quadratic form associated with our operator $-\Delta_{\mathbb{G},\alpha,L}$ can be expressed as

$$d[\Psi] = (\Psi, -\Delta_{\mathbb{G},\alpha,L}\Psi) = \sum_{i=1}^{q} \int_0^{l_i} \mid (\psi')_i(x) \mid^2 dx + \sum_{i=1}^{p} \alpha_i \mid \psi_i(0) \mid^2 \tag{2.15}$$

where $\psi_i(0)$ is the value of function at the i-th vertex. The domain of the form consists of $\Psi \in L^2(\mathbb{G})$ which are $H^{1,2}(\mathbb{G})$ on the edges and continuous on the vertices of the graph.

Chapter 3

Properties of the ground state

First we state some basic properties of the ground state of our operator $-\Delta_{\mathbb{G},\alpha,L}$.

Theorem 3.1. $\inf(\sigma(-\Delta_{\mathbb{G},\alpha,L})) < 0$ *if* $\alpha_i \leq 0$ *holds for all* $i \in \hat{q}$ *and* $\sum_{i=1}^{q} \alpha_i < 0$.

Proof. We will find the test function for which will be the value of the quadratic form associated with our operator negative. From the conditions of the theorem we have that at least one $\alpha_{j_0} < 0$. We divide the proof to the two parts. First part is special case when all the edges are finite i.e. $l_i < \infty$ for all $i \in q$. Second part of the proof is for the general case of a graph with finite number of edges.
1) We take constant test function $\Psi = (c, \ldots, c)^T$. This function belong to the form domain because we have finite length of all edges and from that we have

$$\| \Psi \|_{L^2(\mathbb{G})}^2 = \sum_{i=1}^{q} \| \psi_i \|_{L^2(0,l_i)}^2 = c^2 \sum_{i=1}^{q} l_i^2 < \infty \tag{3.1}$$

When we apply the quadratic form associated with our operator $-\Delta_{\mathbb{G},\alpha,L}$ on the test function we acquire

$$d[\Psi] \leq \alpha_{j_0} \mid c \mid^2 \tag{3.2}$$

2) When we allow the semi-infinite edges we construct the test function in the following way. The test function is $\psi_i = c$ for all edges of finite length and $\psi_i = c \exp(-\kappa x)$ for the semi-infinite edges. From this we get

$$d[\Psi] \leq (\alpha_{j_0} + \frac{1}{2}\kappa m) \mid c \mid^2 \tag{3.3}$$

where m is number of semi-infinite edges. This expression on the right side can be made negative for κ small enough which completes the proof. $\square$

Theorem 3.2. *Let the graph $\mathbb{G}$ be connected, then the bottom of the spectrum $\lambda_0 = \inf \sigma(-\Delta_{\mathbb{G},\alpha,L})$ is simple isolated eigenvalue. The corresponding eigenfunction Ψ^0 can be chosen strictly positive on $\mathbb{G}$ being convex on each edge.*

Proof. We consider the graph $\mathbb{G}'$ which differs from the graph $\mathbb{G}$ by boundary condition at each vertex, which are changed to Dirichlet boundary condition. This results in disjoint graph. Such graph can be solved exactly and we know that such graph has positive spectrum, which is discrete, when all the edges have finite length or the spectrum is equal to $\mathbb{R}^+$ for the graph with some infinite edges. Krein's formula([5, Proposition 2.3.]) couples the original operator with the disjoined one by finite rank operator in the resolvent. From this and Weyl's theorem we have the fact that the essential spectra are the same and discrete spectrum is created with finite number of eigenvalues with finite multiplicity. According to previous statement discrete spectrum is nonempty and the ground-state exists.
Ground state positivity follows from modified Courant theorem [8]. Convexity of the ground state comes from the positivity of the ground state and the fact that eigenfunction is twice differentiable at the edged away from vertices. Put together we have

$$-(\psi_j^0)'' = -\lambda_0 \psi_j^0 < 0 \tag{3.4}$$

from which we have the convexity. $\square$

3.1 Construction of the eigenfunction

We are interested in the ground state which we know from the previous theorem to be strictly positive. All possible eigenfunctions, which can be a part of the ground state function at the edges are those, which fulfill these conditions

$$\begin{aligned} -\psi_i''(x) &= -\kappa^2 \psi_i(x) \\ \psi(x) &> 0 \end{aligned} \tag{3.5}$$

for all $x \in (0, l_i)$, where $-\kappa^2$ is the ground state energy. From this we can deduce that only possible forms of the ground state eigenfunctions are

$$\begin{aligned} \psi_{1,+}(\kappa, x, d_1) &= c_1 \cosh(\kappa(x + d_1)) \\ \psi_{1,-}(\kappa, x, d_2) &= c_2 \cosh(\kappa(-x + d_2)) \\ \psi_{0,+}(\kappa, x) &= c_3 \exp(\kappa(x)) \\ \psi_{0,-}(\kappa, x) &= c_4 \exp(\kappa(-x)) \\ \psi_{-1,+}(\kappa, x, d_5) &= c_5 \sinh(\kappa(x + d_5)) \\ \psi_{-1,-}(\kappa, x, d_6) &= c_6 \sinh(\kappa(-x + d_6)) \end{aligned} \tag{3.6}$$

where c_i are positive constants. The functions $\psi_{1,+}$ and $\psi_{1,-}$ are the same because hyperbolic cosine is even function and for this reason we define

$$\psi_1(\kappa, x, d_1) = \psi_{1,+}(\kappa, x, d_1) \tag{3.7}$$

the other two pairs of functions are odd and we need either both of them or we need to define the orientation of the edges. There is a valid question, if these are all possible positive eigenfunctions of the operator $-\frac{\partial^2}{\partial x^2}$. General solution with the eigenvalue $-\kappa^2$ is expressed as linear combination of the functions $\exp(-\kappa x)$ and $\exp(\kappa x)$. This can be expressed as

$$a \exp(\kappa(x)) + b \exp(\kappa(-x) \tag{3.8}$$

where $a, b \in \mathbb{R}$. When either one of the constants a, b are equal to 0 we get the solution in the form of $\psi_{0,\pm}$. We will show that for $a, b \in \mathbb{R} \setminus \{0\}$ we can write the solution as either $\psi_{1,\pm}$ or $\psi_{-1,\pm}$. It can be easily seen that

$$\forall a, b \in \mathbb{R}, ab \in \mathbb{R}^+ \exists c, d \in \mathbb{R} : a = c \exp(d) \wedge b = c \exp(-d) \tag{3.9}$$

When we introduce this substitution into the solution 3.8 we acquire

$$c \exp(\kappa(x + d)) \pm c \exp(\kappa(-x - d)) = \frac{c}{2}\left(\frac{\exp(\kappa(x + d)) \pm \exp(\kappa(-x - d))}{2}\right) \tag{3.10}$$

where $c \in \mathbb{R}^+$ and $d \in \mathbb{R}$. The expression on the right side can be written as either $\psi_{-1,\pm}$ for the minus sign or $\psi_{1,\pm}$ for the plus sign.
Now we denote the edge index σ_j which will be important in the following theorem. The edge index has value according to the type of the function on

the j-th edge.

$$\begin{aligned}\sigma_j &= 1 \text{ for } \psi_j^0 = \psi_1 \\ \sigma_j &= 0 \text{ for } \psi_j^0 = \psi_{0,\pm} \\ \sigma_j &= -1 \text{ for } \psi_j^0 = \psi_{-1,\pm}\end{aligned} \tag{3.11}$$

We are interested in properties of the ground state, for which we have the conditions (3.5). From this we have to state the conditions for the parameters of the functions $\psi_{i,\pm}$ where $i \in \{-1, 0, 1\}$. We know that $\kappa \in \mathbb{R}^+$ and $x \in \langle 0, l\rangle$ where $l \in \mathbb{R}^+$ for finite edges and $x \in \mathbb{R}^+$ for the infinite edges. Because we are constructing strictly positive ground state we have to restrict parameter d_i. For the parameter d_i $i \in \widehat{2}$, we have no restrictions and $d_i \in \mathbb{R}$ because $\cosh x$ is always positive. The situations is different for d_5 and d_6 because $\sinh x$ is positive only for the $x > 0$ from which we have $d_5 \in (0, \infty)$ and $d_6 \in (l, \infty)$.

Chapter 4

Dependence of the ground state eigenvalue on the length of edges

In this section we will state the theorem concerning the relation between the energy of the ground state and the length of the edges. Without loss of generality we will be working only with connected graph, because otherwise we would dealt with each connected component separately.

Theorem 4.1. *Consider two graph* $\mathbb{G}$ *and* $\tilde{\mathbb{G}}$ *with the same topology differing only by the edge lengths. 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 all vertices.* λ_0 *and* $\tilde{\lambda}_0$ *are corresponding ground state eigenvalues. Suppose*

$$\forall j \in q \; \sigma_j \tilde{l}_j \leq \sigma_j l_j \Rightarrow \tilde{\lambda}_0 \leq \lambda_0 \tag{4.1}$$

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 it is sufficient to compare the graphs which differ only in the length of one fixed finite edge with the index $j \in q$. We choose finite length segment $J = (a, b)$ inside the j-th edge. We write the $\mathbb{G}$ as union of J and $\mathbb{G}_J := \mathbb{G} \setminus J$. Without loss of generality we can choose $b - a > | l_j - \tilde{l}_j |$, then $\tilde{\mathbb{G}}$ can be written as $\tilde{\mathbb{G}} = (\mathbb{G} \setminus J) \cup \tilde{J}$, where $\tilde{J}$ is acquired by scaling of J with the parameter $\xi := \frac{|\tilde{J}|}{|J|}$. Parameter ξ is larger then one in case of enlarging and less then one in case of shrinking. To prove our statement we need to find the the function of $\Psi \in L^2(\tilde{\mathbb{G}})$ which satisfies

$$\frac{\tilde{d}[\Psi]}{\| \Psi \|^2} < \lambda_0 \tag{4.2}$$

for $\xi > 1$ if $\sigma_j = -1$ and $\xi < 1$ if $\sigma_j = 1$. We construct the trial function $\tilde{\Psi}^0$ as:

$$\begin{aligned} \tilde{\Psi}^0(x) &= \Psi^0(x) \text{ for } x \in \mathbb{G}_J \\ \tilde{\Psi}^0_j(\tilde{a} + \xi y) &= \Psi^0_j(a + y) \text{ for } x \in \langle 0, | J | \rangle \end{aligned} \tag{4.3}$$

Put together with the expression (4.2) we get

$$\frac{\tilde{d}[\tilde{\Psi}^0]}{\| \tilde{\Psi}^0 \|^2} = \frac{a + b\xi^{-1}}{c + d\xi} =: f(\xi) \tag{4.4}$$

where

$$a := d_{\mathbb{G}_J}[\Psi^0] \quad b := \int_J | (\Psi^0_j)'(x) |^2 \, dx \quad c :=\| \Psi^0 \|^2_{\mathbb{G}_J} \quad d :=\| \Psi^0 \|^2_J$$

We know that

$$\frac{\partial f(\xi)}{\partial \xi} = \frac{\frac{a + b\frac{1}{\xi}}{c + d\xi}}{\partial \xi} = \frac{-bc - 2bd\xi - ad\xi^2}{(\xi(c + d\xi))^2} \tag{4.5}$$

We can notice that for the proof of our statement it is sufficient to prove

$$\sigma_j \frac{\partial f(\xi)}{\partial \xi} > 0 \text{ for } \xi = 1 \tag{4.6}$$

Without loss of generality we can normalize Ψ^0 so we have $a + b = \lambda_0$ and $c + d = 1$ from which we have property to check in the form

$$-\sigma_j(\lambda_0 d + b) > 0 \tag{4.7}$$

which explicitly is equal to

$$-\sigma_j(\lambda_0 \| \Psi^0 \|^2_J + \int_J | (\Psi^0_j)'(x) |^2 \, dx) > 0 \tag{4.8}$$

We have for $\sigma_j = 1$ using $\lambda_0 = -\kappa^2$

$$\begin{aligned}\int_J \mid (\Psi_j^0)'(x) \mid^2 dx = c_j^2\kappa^2 \int_J (\sinh \kappa x)^2 dx < c_j^2\kappa^2 \int_J (\cosh \kappa x)^2 dx = \\ -\lambda_0 \int_J \mid (\Psi_j^0)(x) \mid^2 dx\end{aligned} \tag{4.9}$$

and for $\sigma_j = -1$

$$\begin{aligned}-\lambda_0 \int_J \mid (\Psi_j^0)(x) \mid^2 dx = c_j^2\kappa^2 \int_J (\cosh \kappa x)^2 dx > c_j^2\kappa^2 \int_J (\sinh \kappa x)^2 dx = \\ \int_J \mid (\Psi_j^0)'(x) \mid^2 dx\end{aligned} \tag{4.10}$$

which completes the proof. □

Chapter 5

Examples of the ground state construction

We will construct the ground state function of some simple graphs and we will show when there is possible situation that the energy of the ground state increases with decreasing length of the edge of the graph. From the theorem 4.1 we know that the edges on which we have the eigenfunction in the form $c\sinh(\kappa(x+d))$ have the property that their increase in length results in decrease of the energy of the ground state. Also from the same theorem we have that the increase of the length of the edges on which the eigenfunction is in the form $c\cosh(\kappa(x+d))$ results in the increase of the energy of the ground state. We will show that the eigenfunction of the form $c\sinh(\kappa(x+d))$ can be present only on the branched graphs. For the each graph we construct the eigenfunction and show the restrictions on the parameters as a result of boundary conditions.
Now we are ready to write eigenfunction on the graph and then calculate the strength of the point interaction on each vertex. Boundary conditions constructed in this way have to fulfill

$$\forall i : \alpha_i \leq 0 \wedge \exists j : \alpha_j < 0 \tag{5.1}$$

These conditions are necessary and sufficient for existence of the eigenvalue $E < 0$. By this approach we are able to create eigenfunction with necessary properties for the theorem 4.1 in the rprevious chapter. The question remains if we construct the ground state by this approach. It is worth mentioning that only possible eigenfunction for the infinite edge is the function $\psi_{0,-}$. Now we take a closer look on the ground state function on the simple graphs.

5.1 Star graph

The best class of graphs on which we can show construction of the ground state are the star graphs. First we will be talking about graphs created from the two edges finite or infinite. In this section we will use the notation

$$\begin{aligned} c(\kappa, x, d_1) &= \frac{\cosh(\kappa(x + d_1))}{\cosh(\kappa d_1)} \\ e_+(\kappa, x) &= \exp(\kappa x) \\ e_-(\kappa, x) &= \exp(-\kappa x) \\ s_+(\kappa, x, d_4) &= \frac{\sinh(\kappa(x + d_4))}{\sinh(\kappa d_4)} \\ s_-(\kappa, x, d_5) &= \frac{\sinh(\kappa(-x + d_5))}{\sinh(\kappa d_5)} \end{aligned} \tag{5.2}$$

where $d_1 \in \mathbb{R}$, $d_4 \in \mathbb{R}^+$ and $d_5 \in (l_5, +\infty\rangle$. We choose these functions to be 1 for $x = 0$. This is useful because we choose the variables on the edges to be 0 at the central vertex which results in automatic fulfilment of the continuity condition.

5.1.1 Finite two edged star graph

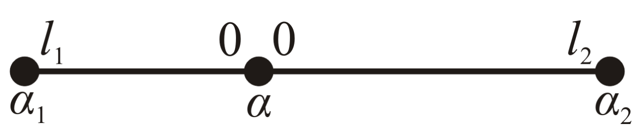

Figure 5.1: General finite two edged star graph

We will start with the finite two edged star graph, which we can see on figure (5.1). We choose direction of variables $x_1 \in \langle 0, l_1\rangle$, $x_2 \in \langle 0, l_2\rangle$ as shown on the figure. The strength of the point interactions are chosen as α, α_1 and α_2. As mentioned above we are only interested in the graphs with non-positive point interactions, i.e.

$$\begin{aligned} \alpha &\leq 0 \\ \alpha_1 &\leq 0 \\ \alpha_2 &\leq 0 \end{aligned} \tag{5.3}$$

We have the boundary conditions in the form of

$$\begin{aligned} \alpha &= \frac{\psi_1'(0)+\psi_2'(0)}{\psi_1(0)} \\ \alpha_1 &= -\frac{\psi_1'(l_1-)}{\psi_1(l_1)} \\ \alpha_2 &= -\frac{\psi_2'(l_2-)}{\psi_2(l_2)} \end{aligned} \tag{5.4}$$

This automatically limit the possible form of the ground state because we cannot use the functions e_- and s_-. This is the result of

$$\begin{aligned} -\frac{s_-'(l_i-)}{s_-(l_i)} &= \kappa(\coth(\kappa(-l_i+d_i^s))) > 0 \\ -\frac{e_-'(l_i-)}{e_-(l_i)} &= \kappa > 0 \end{aligned} \tag{5.5}$$

where $-l_i+d_i^s > 0$ from the condition mentioned above. The other functions leads to the point interaction strength in the form

$$\begin{aligned} -\frac{s_+'(l_i-)}{s_+(l_i)} &= -\kappa(\coth(\kappa(l_i+d_i^s))) < 0 \\ -\frac{e_+'(l_i-)}{e_+(l_i)} &= -\kappa < 0 \\ -\frac{c'(l_i-)}{c(l_i)} &= -\kappa(\tanh(\kappa(l_i+d_i^c))) < 0 \text{ for } l_i+d_i^c > 0 \end{aligned} \tag{5.6}$$

Condition on the non-positivity of α_1 and α_2 limits possible eigenfunctions to those:
a) $(c,c)^T$
b) $(c,s_+)^T$, $(s_+,c)^T$
c) $(c,e_+)^T$, $(e_+,c)^T$
d) $(s_+,s_+)^T$
e) $(s_+,e_+)^T$, $(e_+,s_+)^T$
f) $(e_+,e_+)^T$
The options in b), c) and e) are same with the roles of index 1 and index 2 interchanged. We choose the first ones in these options. Our eigenfunction has to fulfill also the condition on the α. Simple calculation show that the

strength of point interaction α on the central vertex for these combinations mentioned above are as follows:

$$\begin{aligned}\alpha_a &= \kappa(\tanh(\kappa d_1) + \tanh(\kappa d_2)) \\ \alpha_b &= \kappa(\tanh(\kappa d_1) + \coth(\kappa d_2)) > 0 \\ \alpha_c &= \kappa(\tanh(\kappa d_1) + 1) > 0 \\ \alpha_d &= \kappa(\coth(\kappa d_1) + \coth(\kappa d_2)) > 0 \\ \alpha_e &= \kappa(\coth(\kappa d_1) + 1) > 0 \\ \alpha_f &= 2\kappa > 0\end{aligned} \tag{5.7}$$

These inequalities are the result of the fact that we have the conditions on the phase from $\sinh d \geq 0$ and

$$\forall x \in \mathbb{R}^+ y \in \mathbb{R} : \coth(x) > \tanh(y) \tag{5.8}$$

The inequalities 5.7 show that only the option a) can have the point interaction strength on the central vertex negative. We can see that the other options have the point interaction strength on the central vertex positive. Put all together we have that the only possible ground state eigenfunction with eigenvalue $-\kappa^2$ on the finite two edged star graph is $\Psi = (\cosh(\kappa(x + d_1)), \cosh(\kappa(x + d_2)))^T$, with the point interaction strengths

$$\begin{aligned}\alpha &= \kappa(\tanh(\kappa d_1) + \tanh(\kappa d_2)) \\ \alpha_1 &= -\kappa(\tanh(\kappa(l_1 + d_1))) \\ \alpha_2 &= -\kappa(\tanh(\kappa(l_2 + d_2)))\end{aligned} \tag{5.9}$$

where $0 \geq \tanh(\kappa d_1) + \tanh(\kappa d_2) = \frac{\sinh(\kappa(d_1+d_2))}{\cosh(\kappa(d_1))\cosh(\kappa(d_2))}$ from which we have $d_1 \geq -l_1$, $d_1 \geq -l_2$ and $d_1 + d_2 \leq 0$. We note here that for existence of the negative eigenvalue one of inequalities have to be sharp. From this we can conclude that for the finite two edged star graph with the negative point interactions on the vertices there is only possible relation between the ground state energy and the length of the edges as follows: Increase in the length of the edges results in the increase of the energy of the ground state. We note the fact that the point interaction strength $\alpha = 0$ results in transforming the problem from the two edged star graph to the line with the only possible eigenfunction of the type c with the length $l_1 + l_2$.

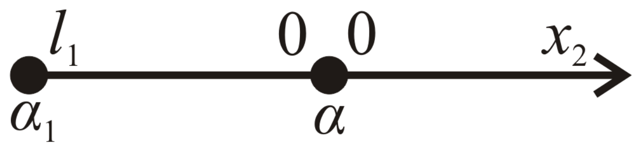

Figure 5.2: General semifinite two edged star graph

5.1.2 Semi-infinite two edged star graph

Next example is the graph consisting of one semi-infinite and one finite edge. As mentioned before only possible function on the semi-infinite edge is e_-. We can apply same approach as with the finite two edged star graph and we come to the conclusion that the only two possible eigenfunction with the eigenvalue $-\kappa^2$ are

$$\begin{aligned} \Psi_1 &= (\cosh(\kappa(x+d_1)), \exp(-\kappa x))^T \\ \Psi_2 &= (\exp(\kappa x), \exp(-\kappa x))^T \end{aligned} \tag{5.10}$$

where $d_1 \geq -l_1$. The point interaction strengths for these eigenfunctions are

$$\begin{aligned} \alpha^{(1)} &= \kappa(\tanh(\kappa d_1) - 1) \\ \alpha_1^{(1)} &= -\kappa \tanh(\kappa l_1 + d_1) \\ \alpha^{(2)} &= 0 \\ \alpha_1^{(2)} &= -\kappa \end{aligned} \tag{5.11}$$

From this we can see that the second option is not interesting because it is just the halfline with Robin condition at the end and for the first options we have the same conclusion as for the finite two edged star graph i.e.: Increase in the length of the edge results in the increase of the energy of the ground state.

5.1.3 Finite three edged star graph

More interesting situation is for the case with star graph with more than two edges because there are more possibilities of the eigenfunction. Approach of solving this graph is the same as before. After applying the restrictions on the value of the point interactions on the ends of the edges, which are the same as in the case of the two edged star graph, we come to the result that

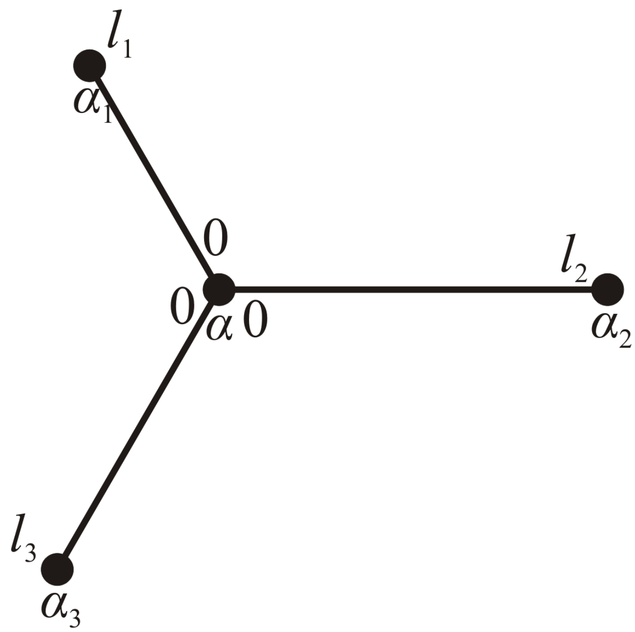

Figure 5.3: Finite three edged star graph

only admissible eigenfunctions are the combinations of functions c, $e+$ and $s+$. Now we shift our attention to the condition at the central vertex. We can calculated it as:

$$\alpha = \frac{\psi_1'(0) + \psi_2'(0) + \psi_3'(0)}{\psi_1(0)} \tag{5.12}$$

Now we write down the contributions of the possible function for $x = 0$ to the central vertex:

$$\begin{aligned} \alpha_c &= \frac{c'(\kappa, 0, d_1)}{c(\kappa, 0, d_1)} = \kappa \tanh(\kappa d_i) \\ \alpha_{e_+} &= \frac{e_+'(\kappa, 0, d_1)}{e_+(\kappa, 0, d_1)} = \kappa \\ \alpha_{s_+} &= \frac{s_+'(\kappa, 0, d_1)}{s_+(\kappa, 0, d_1)} = \kappa \coth(\kappa d_i) \end{aligned} \tag{5.13}$$

The conditions of strict positivity of the ground state and the conditions on κ and d_i imply:

$$\begin{aligned} -\kappa \leq \alpha_c &\leq \kappa \\ \alpha_{e_+} &= \kappa > 0 \\ \kappa &\leq \alpha_{s_+} \end{aligned} \tag{5.14}$$

It can be seen that applying the condition $\alpha \leq 0$ will restrict the ground state eigenfunction to one of those options:
a) $(c,c,c)^T$
b) $(s_+,c,c)^T$, $(c,s_+,c)^T$, $(c,c,s_+)^T$
c) $(e_+,c,c)^T$, $(c,e_+,c)^T$, $(c,c,e_+)^T$
Option a) is simple analogy of the two edged finite graph with the restrictions on the constants d_i in the form $d_1 \geq -l_1$, $d_2 \geq -l_2$, $d_3 \geq -l_3$ and $\tanh(\kappa d_1) + \tanh(\kappa d_2) + \tanh(\kappa d_3) \leq 0$. Also the behavior of the ground state energy is the same i.e.: Increase in the length of the edges results in the increase of the energy of the ground state. However options b) and c) are more complex.
Option b) have two edges with the behavior same as for the case a) and one edge with totally opposite property as follows: Increase in the length of the edges results in the decrease of the energy of the ground state.
Option c) has stranger behavior then it would seem on the first look. The problem is with the point interaction strength at the end of the edge with e_+. For this point interaction we have the condition $\alpha_{e_+} = -\kappa$ which immediately imply constant energy of the ground state, because we cannot change the point interaction strengths of the graph but only the lengths. From this we acquire the fact that we cannot change the lengths of two edges with the c type functions. Only one edge for which we can change its length is the one with the function of e_+ type for which we have the property: change of the length of the edge with the function of e_+ type does not change the energy of the ground state.
There is the valid question if the options b) and c) are not the higher states of the system with the ground state represented by option a). We prove that all options in the list above are the ground states of different quantum systems. We prove this on the example of the eigenfunctions $(c,c,c)^T$ and $(c,c,s_+)^T$. Other examples are either permutations of the edges of these or simple analogy. To prove this we need the point interactions strength which belong to the eigenfunctions $(c,c,c)^T$ and $(c,c,s_+)^T$. The point interactions

strengths belonging to the eigenfunction $(c, c, c)^T$ are

$$\begin{aligned}\alpha^a = \kappa_a(\tanh(\kappa_a d_1^a) + \tanh(\kappa_a d_2^a) + \tanh(\kappa_a d_3^a))\\ \alpha_1^a = -\kappa_a \tanh(\kappa_a(l_1 + d_1^a))\\ \alpha_2^a = -\kappa_a \tanh(\kappa_a(l_2 + d_2^a))\\ \alpha_3^a = -\kappa_a \tanh(\kappa_a(l_3 + d_3^a))\end{aligned} \tag{5.15}$$

where $d_1 \geq -l_1$, $d_2 \geq -l_2$, $d_3 \geq -l_3$ and $\tanh(\kappa d_1)+\tanh(\kappa d_2)+\tanh(\kappa d_3) \leq 0$. The point interactions strengths belonging to the eigenfunction $(c, c, s_+)^T$ are

$$\begin{aligned}\alpha^b = \kappa_b(\tanh(\kappa_b d_1^b) + \tanh(\kappa_b d_2^b) + \coth(\kappa_b d_3^b))\\ \alpha_1^b = -\kappa_b \tanh(\kappa_b(l_1 + d_1^b))\\ \alpha_2^b = -\kappa_b \tanh(\kappa_b(l_2 + d_2^b))\\ \alpha_3^b = -\kappa_b \coth(\kappa_b(l_3 + d_3^b))\end{aligned} \tag{5.16}$$

where $d_1 \geq -l_1$, $d_2 \geq -l_2$, $d_3 \geq 0$ and $(\tanh(\kappa_b d_1^b)+\tanh(\kappa_b d_2^b)+\coth(\kappa_b d_3^b)) \leq 0$. The question whether or not these eigenfunctions belong to the same system is analogical to existence of parameters κ_a, κ_b, d_i^a and d_i^b where $i \in \hat{3}$ for which these equalities are true:

$$\begin{aligned}\alpha^a &= \alpha^b\\ \alpha_1^a &= \alpha_1^b\\ \alpha_2^a &= \alpha_2^b\\ \alpha_3^a &= \alpha_3^b\end{aligned} \tag{5.17}$$

We will prove that such parameters do not exist. From the fourth equation (5.17) we have $\kappa_a > \kappa_b$, because $\tanh(\kappa_a(l_3+d_3^a)) < \coth(\kappa_b(l_3+d_3^b))$ for all κ_a, κ_b, d_3^a and d_3^b. If we take $\kappa_a > \kappa_b$ to consideration, we have from the second and third equation (5.17) the relation $\tanh(\kappa_a(l_2+d_2^a) < \tanh(\kappa_b(l_2+d_2^b)$ and $\tanh(\kappa_a(l_1 + d_1^a) < \tanh(\kappa_b(l_1 + d_1^b)$. Those imply $(\kappa_a(l_2 + d_2^a) < (\kappa_b(l_2 + d_2^b)$ and $(\kappa_a(l_1 + d_1^a) < (\kappa_b(l_1 + d_1^b)$. From these inequalities we have $\kappa_a d_1^a < \kappa_b d_1^b$ and $\kappa_a d_2^a < \kappa_b d_2^b$ but more importantly they imply $\alpha^a < \alpha^b$ which is in contradiction to the first equality (5.17) which completes the proof.

5.1.4 General finite star graph

Now let us consider general star graph with finite number of edges. Without loss of generality we can assume that the first j edges are of the finite length

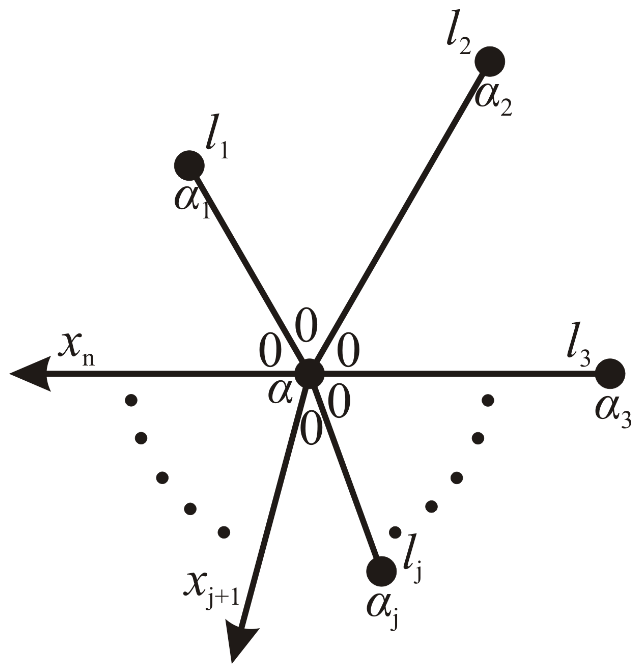

Figure 5.4: Finite n edged star graph

and the last ones are of the infinite length. We are interested in the possible ground state functions and its point interaction strength. There are the analogical restriction as for the examples before. First restriction is that we cannot generally use all the functions from (5.2) because we have to have non-negative point interaction at all vertices. This results in the fact that we can use only certain functions on the edges of the star graph. Also we have the restrictions in the form $\alpha \leq 0$. To each function from (5.2) we can write the value by which they contribute to the central point interaction, where the index corresponds to the name of the contributing eigenfunctions:

$$\begin{aligned} \alpha_c &= \kappa \tanh(\kappa d_i) \\ \alpha_{e_+} &= \kappa \\ \alpha_{e_-} &= -\kappa \\ \alpha_{s_+} &= \kappa \coth(\kappa d_i) \\ \alpha_{s_-} &= -\kappa \coth(\kappa d_i) \end{aligned} \tag{5.18}$$

Some of these contributions are from the function which can not be part of the star graph. Allowable contributions for the star graph are

$$\begin{aligned} -1 < \frac{\alpha_c}{\kappa} = \tanh(\kappa d_i) < 1 \text{ where } d_i \in \mathbb{R} \\ \frac{\alpha_{e_+}}{\kappa} = 1 \\ 1 < \frac{\alpha_{s_+}}{\kappa} = \coth(\kappa d_j) \text{ where } d_j \in \mathbb{R}^+ \\ \frac{\alpha_{e_-}}{\kappa} = -1 \end{aligned} \tag{5.19}$$

First three function c,s_+,e_+ are allowed on the finite length edges and the fourth function e_- is only one allowed on the infinite edge. Because we are interested only in graphs with negative point interactions, we obtain the relation between the number of the edge "types". We denote the edge type according to the function which is on the edge. From the inequalities we can see that there have to be always at least certain number of edges with c function. Such edges have the property: Increase in the length of the edge with c function results in the increase of the energy of the ground state. For the edge with s_+ or s_- function we have: Increase in the length of the edge with s_+ or s_- function results in the decrease of the energy of the ground state. We can state one important inequality for the number of the edge "types" based on the function which is on this edge:

Theorem 5.1. *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*

$$n_c + n_e - \geq n_{e_+} + n_{s_+} + 1 \tag{5.20}$$

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

Proof. We assume a general star graph with n_c edges of the c type, n_{e_+} edges of the e_+ type etc. We will write down the central point interaction α in means of contributions from the functions on the edges.

$$\alpha = \kappa(\sum_{i=1}^{n_c} \tanh(\kappa d_i) + \sum_{j=1}^{n_{s_+}} \coth(\kappa d_j) + \sum_{j=1}^{n_{e_+}} 1 + \sum_{j=1}^{n_{e_-}} -1) \tag{5.21}$$

We substitute the $\tanh(\kappa d_i)$ and $\coth(\kappa d_j)$ as $-1+\epsilon_i = \tanh(\kappa d_i)$ and $1+\epsilon_i = \coth(\kappa d_j)$, where $\epsilon_i > 0$. We acquire

$$\begin{aligned} \alpha &= \kappa(\sum_{i=1}^{n_c}(-1+\epsilon) + \sum_{j=1}^{n_{s_+}}(1+\epsilon) + \sum_{j=1}^{n_{e_+}} 1 + \sum_{j=1}^{n_{e_-}}(-1)) \\ \alpha &= \kappa(-n_c + n_{s_+} + n_{e_+} - n_{e_-} + \sum_{i=1}^{n_c} \epsilon_i + \sum_{j=1}^{n_{s_+}} \epsilon_i) \end{aligned} \tag{5.22}$$

It can be seen that for certain set of parameters d_i and sufficiently large l_i then we acquire $\sum_{i=1}^{n_c} \epsilon + \sum_{j=1}^{n_{s_+}} \epsilon = \Upsilon < 1$. We have the inequality $\alpha < 0$ from which we have

$$-n_c + n_{s_+} + n_{e_+} - n_{e_-} + \Upsilon < 0 \tag{5.23}$$

From which we can conclude

$$n_c + n_{e_+} > n_{s_+} + n_{e_+} + \Upsilon \tag{5.24}$$

The fact that $n_c, n_{e_+}, n_{s_+}, n_{e_+} \in \mathbb{N}$ completes the proof. $\square$

Similarly as for three edged star-graph we can ask ourselves, if all the combination of the functions on the edges fulfilling the condition (5.20) are the ground state eigenfunctions. We will show that all the possible combinations fulfilling the conditions $\alpha, \alpha_i < 0$ are the ground state eigenfunctions of different systems. This means that the two eigenfunctions with the different types cannot generate same point interaction strengths. We will prove this statement.

Theorem 5.2. *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. We have already established in the theorem 3.2 that we have strictly positive eigenfunction for the ground state. Now we prove stronger claim that only strictly positive eigenfunction is the ground state. It can be easily seen that the two function of the same type are generating the same point interactions only when they are the same. We will show that two function with different types cannot generate same point interaction strengths which completes the proof. Let assume that we have two function Ψ_1, Ψ_2 with the types T_1 and T_2. First we prove the statement for the star graph with the function types c and s_+. We show that the types which can be written as below cannot generate same point interactions.

$$T_1 = \begin{pmatrix} c \\ \vdots \\ c \\ s_+ \\ \vdots \\ s_+ \end{pmatrix} \quad T_2 = \begin{pmatrix} c \\ \vdots \\ s_+ \\ c \\ \vdots \\ s_+ \end{pmatrix} \tag{5.25}$$

From this we have the condition for the two endpoints of the star graph in the form:

$$\begin{aligned} \kappa_1 \tanh(\kappa_1(l_i + d_i)) = \alpha_i = \kappa_2 \coth(\kappa_2(l_i + d_i')) \\ \kappa_1 \coth(\kappa_1(l_{i+1} + d_{i+1})) = \alpha_{i+1} = \kappa_2 \tanh(\kappa_2(l_{i+1} + d_{i+1}')) \end{aligned} \tag{5.26}$$

We know that $\coth x > \tanh y$. From the first condition we have $\kappa_1 > \kappa_2$ and from the second $\kappa_1 < \kappa_2$, which cannot be achieved at the same time. From this we can assume that when we allow only the types c and s_+ the only possible types remaining to be checked are those:

$$T_1 = \begin{pmatrix} c \\ \vdots \text{ j times type } c \vdots \\ c \\ s_+ \\ \vdots \text{n-j times type } s_+ \vdots \\ s_+ \end{pmatrix} \quad T_2 = \begin{pmatrix} c \\ \vdots \text{ k times type } c \vdots \\ c \\ s_+ \\ \vdots \text{n-k times type } s_+ \vdots \\ s_+ \end{pmatrix} \tag{5.27}$$

where $j > k$. From this we have that there is at least one i for which we have the equality

$$\kappa_1 \tanh(\kappa_1(l_i + d_i)) = \alpha_i = \kappa_2 \coth(\kappa_2(l_i + d_i')) \tag{5.28}$$

From which we acquire $\kappa_1 > \kappa_2$. We can repeat the process described in the previous section for the finite three edged star graph. By this approach we acquire that the contributions from the edges fulfill

$$\begin{aligned} \tanh(\kappa_1(d_i)) < \tanh(\kappa_2(d_i')) \\ \tanh(\kappa_1(d_j)) < \coth(\kappa_2(d_j')) \\ \coth(\kappa_1(d_k)) < \coth(\kappa_2(d_k')) \end{aligned} \tag{5.29}$$

From which we can acquire $\alpha^{(1)} < \alpha^{(2)}$, 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 analogical to this so we omit the details. $\square$

We note that there is similar pathological situation for the general star graphs with the edges of the type e_+ as for the three edged star graph. For the graphs with the edges with e_+ type functions we have the property concerning the lengths of the edges as follows: We can change only the lengths of the edges with the function of e_+ type and the change of the lengths do not affect the ground state.

5.2 Line with finitely many point interactions

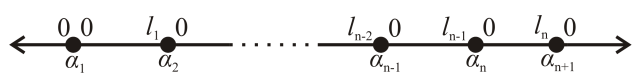

Figure 5.5: General finite star graph

Next elemental graph which we will discuss is a line divided at n sites by the vertices. The arguments which we used on the star graphs can be easily applied on this graph so we omit the details. There are two possible eigenfunctions. First possible eigenfunction is function of the type c on the finite edges and function of the type e_- on the infinite edges. This eigenfunction has the behavior as follows: Increase in the length of the edges results in the increase of the energy of the ground state, which is the same result as in [9]. The second eigenfunction is similar but on the finite edge next to the infinite one we have function of the type e_+. This option is not interesting because it leads to the line divided by $n-1$ sites. This is a simple result of continuity of the eigenfunction at each vertex. It is worth mentioning that this situation is essentially the same as for the semi-infinite two edged star graph.

5.3 Loop from finitely many edges

Another simple graph is a loop created from n edges. If we allow only the non-positive point interactions we can show that only possible positive eigen-

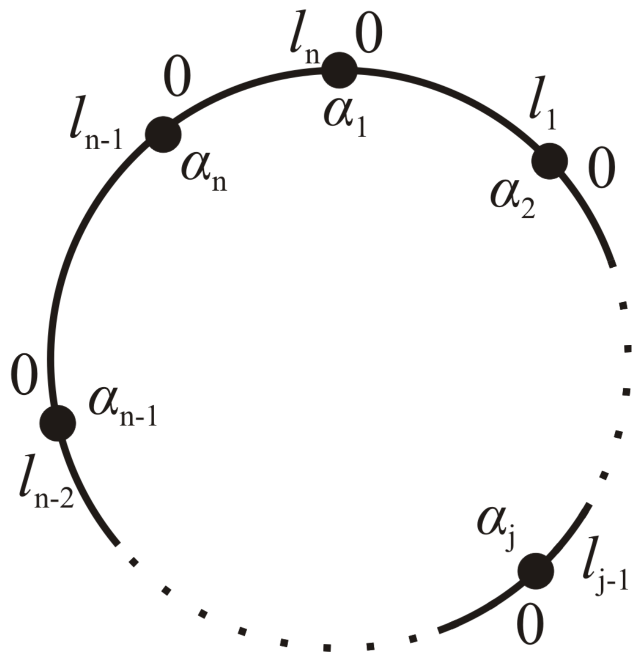

Figure 5.6: Finite three edged star graph

function at the edges are functions of the type c which implies the behavior: Increase in the length of the edges results in the increase of the energy of the ground state.

5.4 Conclusion from the examples

From the examples in this chapter we can deduce several things. Main conclusion is that for the unbranched graphs with at most two edges per vertex such as loops, lines, halflines or line segments, the ground state stabilizes with lowering the distance between non-positive point interactions. On the other hand for the graphs with more branched vertices the situation can be more complex. It is caused by the fact that when we have vertex with at least three edges it results in theoretical possibility of having the edge with the property that the increase in its length results in the decrease of the ground state energy.

Chapter 6

Numerical examples

In this chapter we show numerically evaluated examples of the properties of the ground state. We find numerically the solution of the set of equations:

$$\begin{aligned} \alpha &= \kappa(\tanh(\kappa d_1) + \tanh(\kappa d_2)) \\ \alpha_1 &= -\kappa(\tanh(\kappa(l_1 + d_1))) \\ \alpha_2 &= -\kappa(\tanh(\kappa(l_2 + d_2))) \end{aligned} \tag{6.1}$$

where we are numerically searching for κ, d_1 and d_2 for the fixed α, α_1, α_2, l_1 and l_2. On the first two graphs (6.1 and 6.2) we have finite two edged star graphs. As we have proven in the previous chapter for the two edged star graph there is only one kind of the relation between the length of the edges and the energy of the ground state i.e. Increase in the length of the edges results in the increase of the energy of the ground state.

The situation on the three edged star graph is more complex because there are two types of the graphs. First one has the ground state function in the form (c, c, c) and the other one in the form (c, c, s_+). First we will choose the eigenfunction to which we calculate the point interaction strengths. For the type (c, c, c) we have:

$$\begin{aligned} \alpha^a &= \kappa_a(\tanh(\kappa_a d_1^a) + \tanh(\kappa_a d_2^a) + \tanh(\kappa_a d_3^a)) \\ \alpha_1^a &= -\kappa_a \tanh(\kappa_a(l_1 + d_1^a)) \\ \alpha_2^a &= -\kappa_a \tanh(\kappa_a(l_2 + d_2^a)) \\ \alpha_3^a &= -\kappa_a \tanh(\kappa_a(l_3 + d_3^a)) \end{aligned} \tag{6.2}$$

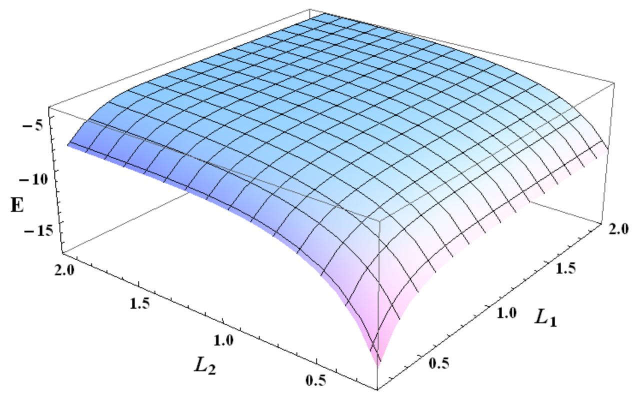

Figure 6.1: Energy of the ground state of the finite two edged star graph with the point interaction strengths $\alpha = -3$,$\alpha_1 = -1$ and $\alpha_2 = -2$

and for the type $(c, c, s+)$ we have:

$$
\begin{aligned}
\alpha^b &= \kappa_b(\tanh(\kappa_b d_1^b) + \tanh(\kappa_b d_2^b) + \coth(\kappa_b d_3^b)) \\
\alpha_1^b &= -\kappa_b \tanh(\kappa_b(l_1 + d_1^b)) \\
\alpha_2^b &= -\kappa_b \tanh(\kappa_b(l_2 + d_2^b)) \\
\alpha_3^b &= -\kappa_b \coth(\kappa_b(l_3 + d_3^b))
\end{aligned}
\tag{6.3}
$$

Now we choose the parameters d_i the lengths l_i and the energy of the ground state. After calculating the point interaction strengths we numerically solve the equations (6.2) and (6.3) in the same way as for the previous examples i.e. we numerically search for κ, d_1 d_2 and d_3 for the fixed α, α_1, α_2, α_3 and different lengths l_1, l_2 and l_3.
On the graph 6.3 we have the energy of the ground state of the type (c, c, c) as a function of the lengths of the edges. We see that for this type we have the following relation between the energy and the lengths of the edges: increase in the length of the edges results in increase of the ground state energy.

On the following graph 6.4 we have the energy of the ground state of the type (c, c, s_+) as a function of the lengths of the edges. We can see that the situation is more complex. When we shorten the first two edges it results in the stabilization of the system, but when we shorten the third edge it results in destabilization of the system. Next graph 6.5 shows dependence of the

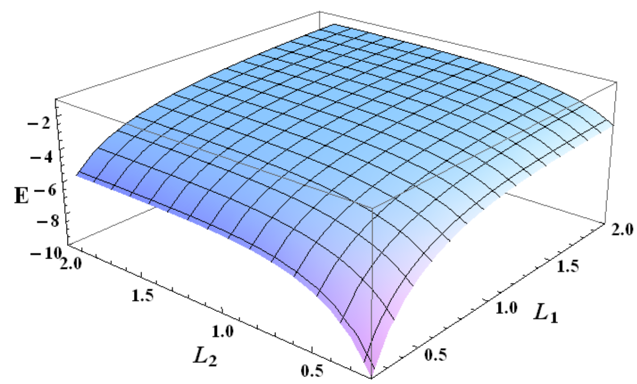

Figure 6.2: Energy of the ground state of the finite two edged star graph with the point interaction strengths $\alpha = -2$,$\alpha_1 = -1.2$ and $\alpha_2 = -0.6$

ground state energy of the ground state of the type (e_+, c, s_+). We can see that one edge has the property: increase in the length of the one edge results in increase in the ground state energy and another one: increase in the length of the one edge results in decrease in the ground state energy.

Last example is showed on the graph 6.6. On this graph there is the dependence of the ground state energy on the length of the edge of the graph of the type (e_-, e_-, c).

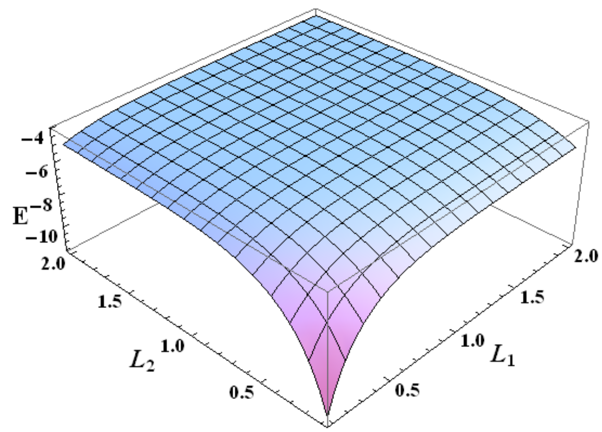

Figure 6.3: Energy of the ground state of the finite three edged star graph with the point interaction strengths $\alpha = -3$, $\alpha_1 = -1$, $\alpha_2 = -1.5$ and $\alpha_3 = -2$ and fixed length $L_3 = 1$

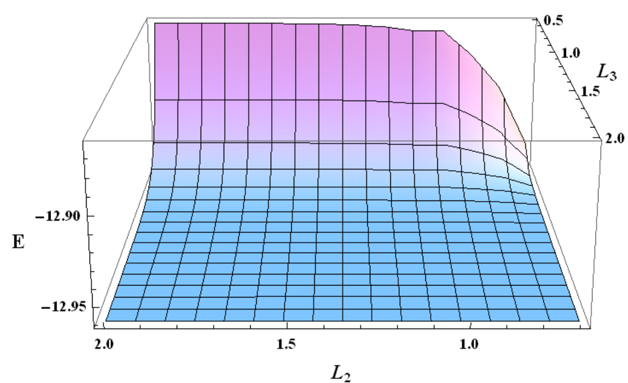

Figure 6.4: Energy of the ground state of the finite three edged star graph with the point interaction strengths $\alpha = -3$, $\alpha_1 = -3$, $\alpha_2 = -3$ and $\alpha_3 = -3.6$ and fixed length $L_1 = 1$

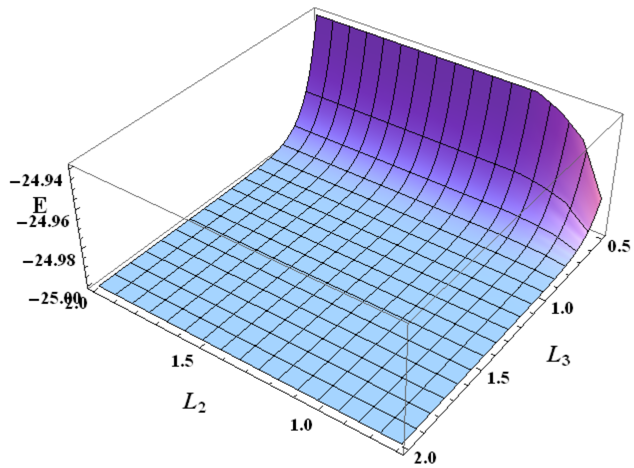

Figure 6.5: Energy of the ground state of the finite three edged star graph with one infinite edge with the point interaction strengths $\alpha = -5$, $\alpha_2 = -4$ and $\alpha_3 = -1$

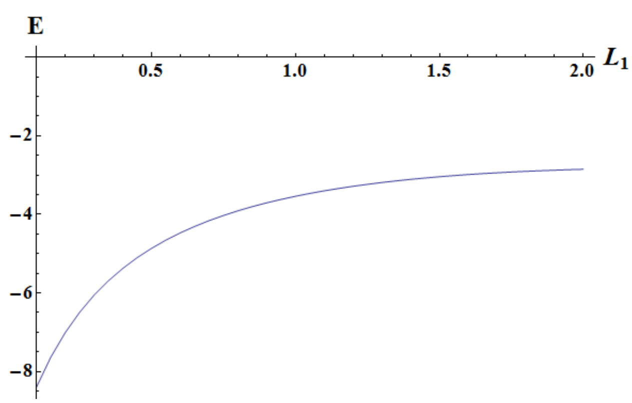

Figure 6.6: Energy of the ground state of the finite three edged star graph with two infinite edges with the point interaction strengths $\alpha = -5$, $\alpha_1 = -1.5$

Chapter 7

Another approach-Neumann bracketing

We can approach our problem from different perspective. One of the alternative approaches is to use Neumann bracketing. We will be able to prove weaker claim. First we will state useful statement for comparison of spectral properties of operators with different boundary conditions.

Lemma 7.1 (About Neumann bracketing). *Let* Ω_1,Ω_2 *be disjoined subsets such that* $\overline{\Omega_1 \cup \Omega_2}^{int} = \Omega$, *and* $\Omega \backslash \Omega_1 \cup \Omega_2$ *has Lebesgue measure zero. Then* $0 \leq -\Delta_N^{\Omega_1 \cup \Omega_2} \leq -\Delta_N^{\Omega}$.

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

Now we are ready to state the theorem based on the Neumann bracketing.

Theorem 7.1. *Let* $-\Delta_{\mathbb{G},\alpha,L_1}$, $-\Delta_{\mathbb{G},\alpha,L_2}$ *be the graph Hamiltonians defined above where* $L_i = \{l_{i,1}, \dots, l_{i,N}\}$. *Suppose that* $\operatorname{card} L_1 = \operatorname{card} L_2$, $\alpha_k \leq 0$ *for all* $k \in q$ *and for at least one* $j_0 \in q$ $\alpha_{j_0} < 0$. *Suppose that there is an* i *such that* $l_{1,i} \leq l_{2,i}$. *Suppose further the ground state of the first operator fulfills* $\psi_i'(0+) < 0$ *and* $\psi_i'(l_{1,i}-) > 0$. *If these conditions are fulfilled then the ground states of the two operators* $-\Delta_{\mathbb{G},\alpha,L_1}$, $-\Delta_{\mathbb{G},\alpha,L_2}$ *satisfy* $\min \sigma_p(-\Delta_{\Gamma,\alpha,L_1}) \leq \min \sigma_p(-\Delta_{\Gamma,\alpha,L_2})$.

Proof. We consider the operator $-\Delta_{\mathbb{G},\alpha,L}$ discussed above. According to the theorem 3.2 our operator have a strictly positive convex ground state function. By assumption we also have $\psi_i'(0+) < 0$ and $\psi_i'(l_{1,i}-) > 0$. Thanks to that we can find $x_i \in (0, l_{1,i})$ such that $\psi_i'(x_i) = 0$ Now we add Neumann condition at x_i to $-\Delta_{\mathbb{G},\alpha,L}$. We denote the operator with the Neumann condition as $-\Delta^{(1)}_{\mathbb{G},\alpha,L_1}$. The domain of $-\Delta^{(1)}_{\mathbb{G},\alpha,L_1}$ is

$$\mathrm{D}(-\Delta^{(1)}_{\mathbb{G},\alpha,L_1}) = \{\psi \in H^{2,2}(\mathbb{G}) \mid \\ (U-I)\psi + i(U+I)\psi' = 0, \psi_i(x_i) = 0\}.$$

Properties of the ground state for $-\Delta_{\mathbb{G},\alpha,L_1}$ and $-\Delta^{(1)}_{\mathbb{G},\alpha,L_1}$ are the same, because we chose x_i in such a way the ψ_i fulfills Neumann condition for the wave function of the ground state. Now we define $-\Delta^{(2)}_{\mathbb{G},\alpha,L_1}$ as a direct sum of two self-adjoint operators

$$-\Delta^{(2)}_{\mathbb{G},\alpha,L_1} = -\Delta^{(1)}_{\mathbb{G},\alpha,L_1} \oplus -\Delta^{(0,x)}_{N} \tag{7.1}$$

where $-\Delta^{x,y}_{N}$ is Neumann Laplacian at the interval (x, y) (for the definition see [3, Section XIII.15]). This operator is basically the same as $-\Delta^{(1)}_{\mathbb{G},\alpha,L_1}$ with Neumann Laplacian squeezed between Neumann condition. It is worth mentioning that $-\Delta^{(2)}_{\mathbb{G},\alpha,L_1}$ coincides with $-\Delta^{(1)}_{\mathbb{G},\alpha,L_1}$ for $x = 0$. The domain of the newly constructed operator is

$$\mathrm{D}(-\Delta^{(2)}_{\mathbb{G},\alpha,L_1}) = \mathrm{D}(-\Delta^{(1)}_{\mathbb{G},\alpha,L_1}) \oplus \mathrm{D}(-\Delta^{(0,x)}_{N}).$$

Neumann Laplacian is a positive operator, in particular, all its eigenvalues are positive. We are interested in the ground state of $-\Delta^{(2)}_{\mathbb{G},\alpha,L_1}$. The discrete spectrum of $-\Delta^{(2)}_{\mathbb{G},\alpha,L_1}$ is the union of discrete spectra of the orthogonal sum components,

$$\sigma_p(-\Delta^{(2)}_{\mathbb{G},\alpha,L_1}) = \sigma_p(-\Delta^{(1)}_{\mathbb{G},\alpha,L_1}) \cup \sigma_p(-\Delta^{(0,x)}_{N})$$

The ground state of $-\Delta^{(2)}_{\mathbb{G},\alpha,L_1}$ is negative which implies that the ground state is not affected by $-\Delta^{(0,x)}_{N}$ because $-\Delta^{(0,x)}_{N} \geq 0$. Next we define $-\Delta^{(3)}_{\mathbb{G},\alpha,L_1}$ which is obtained from the operator $-\Delta^{(3)}_{\mathbb{G},\alpha,L_1}$ by removing the Neumann conditions at the points 0 and x. It can be easily seen that $-\Delta^{(3)}_{\mathbb{G},\alpha,L_1}$ is equal to $-\Delta_{\mathbb{G},\alpha,L_2}$ for $l_{l,i}+x = l_{1=2,i}$. According to Lemma (7.1) we have $-\Delta^{(2)}_{\mathbb{G},\alpha,L_1} \leq -\Delta^{(3)}_{\mathbb{G},\alpha,L_1}$. Also as we pointed out earlier we can write $\inf\sigma(-\Delta_{\mathbb{G},\alpha,L_1}) = \inf\sigma(-\Delta^{(1)}_{\mathbb{G},\alpha,L_1})$ and $\inf\sigma(-\Delta^{(3)}_{\mathbb{G},\alpha,L_1}) = \inf\sigma(-\Delta_{\mathbb{G},\alpha,L_2})$. In combination with minmax principle [3, Section XIII.1] we arrived at the inequality:

$$\inf\sigma(-\Delta_{\mathbb{G},\alpha,L_1}) = \inf\sigma(-\Delta^{(1)}_{\mathbb{G},\alpha,L_1}) \leq \inf\sigma(-\Delta^{(2)}_{\mathbb{G},\alpha,L_1}) \leq \inf\sigma{-}\Delta^{(3)}_{\mathbb{G},\alpha,L_1} \tag{7.2}$$

and the fact $\inf \sigma(-\Delta^{(3)}_{\mathbb{G},\alpha,L_1} \equiv \inf \sigma(-\Delta_{\mathbb{G},\alpha,L_2})$ completes the proof. $\square$

As we can see theorem we have just proven is weaker than theorem (4.1) however it gives us different insight of the problem. From this theorem is obvious that only the edge with the function c can have the property that increase in length results in increase of the energy of the ground state, because c function is the only one which can have first derivative equal to 0.

Chapter 8

Conclusion

In this work we shown the relation between the shape of the ground state eigenfunction, length of the edges and the energy of the ground state of the quantum particle on the graph. We have shown that there are two options of monotonous behavior of the ground state energy on the length of the edge. We have found the rule which distinguishes between these options:
a) "Increase in the length of the edge results in the increase of the energy of the ground state." and
b) "Increase in the length of the edges results in the decrease of the energy of the ground state."
The rule is based on determination of the shape of the eigenfunction on corresponding edge. We need the eigenfunction to be in the form of $c\cosh(\kappa(x+d))$ for the option a) and $c\sinh(\kappa(x+d))$ for the option b). Also we have found different behavior for the star graphs with the edges with the $c\exp(\kappa x)$ functions. For these graphs we cannot change all the lengths of the edges but only those which they have the function $c\exp(\kappa x)$. The change of the lengths of those edges does not change the ground state energy.

Bibliography

[1] Albeverio S., Gesztesy F., Høegh-Krohn R., Holden H.: *Solvable Models in Quantum Mechanics*, 2nd edition AMS Chealsea Publishing, United States of America (2005)

[2] Blank J., Exner P., Havlíček M.: *Lineární operátory v kvantové fyzice*, Karolinum, Praha (1993).

[3] Reed M., Simon B.: *Methods of Modern Mathematical Physics IV: Analysis of operators*, Academic press, San Diego (1978).

[4] Reed M., Simon B.: *Methods of Modern Mathematical Physics II: Fourier Analysis, Self-Adjointness*, Academic press, San Diego (1975).

[5] Pankrashkin K.: *Sur lanalyse de modeles mathématiques issus de la mécanique quantique*, Habiltation thesis, University Paris-Sud (2010).

[6] Cheon T., Exner P., Turek O.: *Approximation of a general singular vertex coupling in quantum graphs*, (2009).

[7] Kuchment P.: *Quantum graphs: an introduction and a brief survey, Analysis on Graphs and its Applications*, Proc. Symp. Pure. Math., AMS (2008), pp.291314.

[8] Band R., Berkolaiko G., Raz H., Smilansky U.: *On the connection between number of nodal domains on quantum graphs and the stability of graph partitions*, arXiv: 1103.1423

[9] Jex M.: *Geometrically induced properties of the ground state of point-interaction Hamiltonians*, Bachelor thesis, Czech Technical University in Prague, (2010)