Opérateurs de Schrödinger sur des graphes métriques

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Schrödinger Operators on Metric Graphs

(Schrödingerovy operátory na metrických grafech)

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Abstract

This thesis is devoted to investigation of "quantum graphs", in other words, quantum systems in which a nonrelativistic particle is confined to a graph. One of the main questions addressed in this work concerns the physical meaning of wave function couplings in the graph vertices. We consider the standard form of boundary conditions in a vertex of degree n, namely $A\Psi(0) + B\Psi'(0) = 0$, where A and B are matrices of the sizes $n \times n$, $\Psi(0)$ and $\Psi'(0)$ signify vectors containing the values of the wave function components on all the outgoing edges and of its derivatives, $\mathrm{rank}(A|B) = n$, $AB^* = BA^*$, and we propose a new way to represent the matrices A, B. With the help of this result we solve the longstanding open problem of approximating by regular graphs all singular vertex couplings in quantum graph vertices. We present a construction in which the edges are disjunct and the pairs of the so obtained endpoints are joined by additional connecting edges of lengths $2d$. Each connecting edge carries a δ potential and a vector potential, and its endpoints are coupled to the disjunct edges by δ-couplings. It is shown that when the lengths $2d$ of the connecting edges shrink to zero and the added potentials properly depend on d, the limit can yield any requested singular vertex coupling, and moreover that the approximation converges in the norm-resolvent sense.

We discuss also a simpler approximation arrangement where the edges are not disjunct. Instead of that, a δ-coupling is imposed at the vertex, and additional δ-interactions and vector potentials are placed on the n outgoing edges. We show that this arrangement allows one to approximate a $3n$-parameter subfamily of Schrödinger operators provided the δ-coupling and the δ-interactions parameters, as well as the vector potentials strengths, are properly chosen.

This type of boundary conditions is used to examine scattering properties of singular vertices of degrees 2 and 3. We identify the δ and δ' components of the connection condition and show that the couplings between each pair of the outgoing edges are individually tunable, which could enable the design of quantum spectral junction filters.

We also study Schrödinger operators on an infinite quantum graph of a chain form which consists of identical rings connected at the touching points by the δ-couplings with the coupling constant $\alpha \in \mathbb{R}$. If the graph is straight, i.e. periodic, the Hamiltonian has a band spectrum with infinite number of gaps whenever $\alpha \neq 0$. We consider a "bending" deformation of the chain consisting in changing the position of the point of contact between two rings and we show that this deformation gives rise to eigenvalues in the spectral gaps. We analyze dependence of these eigenvalues on α and on the "bending angle" as well as resonances of the system created by this bending.

Shrnutí

Tato dizertační práce se věnuje výzkumu „kvantových grafů", neboli kvantových systémů, v nichž je nerelativistická částice vázaná na graf. Jedna z hlavních v práci zkoumaných otázek se týká fyzikálního významu vazeb vlnových funkcí ve vrcholech těchto grafů. Uvážíme standardní formu okrajových podmínek ve vrcholu stupně n, tedy $A\Psi(0) + B\Psi'(0) = 0$, kde A a B jsou matice o rozměru $n \times n$, $\Psi(0)$ a $\Psi'(0)$ označují vektory obsahující hodnoty komponent vlnové funkce na všech vycházejících hranách vyčíslené v daném vrcholu a hodnoty jejich derivací, $\mathrm{rank}(A|B) = n$, $AB^* = BA^*$, a navrhneme nový způsob, jak reprezentovat matice A, B. S pomocí tohoto výsledku vyřešíme po mnoho let otevřenou úlohu, jak regulárními grafy aproximovat všechny singulární vazby ve vrcholech kvantového grafu. Představíme konstrukci, v níž jsou hrany ve vrcholu rozpojeny a dvojice takto získaných koncových bodů spojeny přídavnými úsečkami o délce $2d$. Každá spojující úsečka nese δ-potenciál a vektorový potenciál a její koncové body jsou vázané ke koncovým bodům rozpojených hran pomocí δ-vazeb. Ukážeme, že když se d blíží k nule a přidané potenciály vhodně závisejí na d, může limita vést ke každé požadované singulární vrcholové vazbě, a navíc, že tato aproximace konverguje v norm-rezolventním smyslu.

Prozkoumáme rovněž jiné, jednodušší aproximující uspořádání, v němž nejsou hrany rozpojeny. Namísto toho je ve vrcholu předepsána δ-vazba a na n hranách, které z něj vycházejí, jsou rozmístěny δ-interakce a vektorové potenciály. Ukážeme, že toto uspořádání umožňuje aproximovat $(3n)$parametrickou podmnožinu Schrödingerových operátorů, pokud jsou parametry δ-vazby, δ-interakcí a vektorových potenciálů vhodně zvoleny.

Námi odvozenou formu okrajových podmínek dále využijeme k vyšetření rozptylových vlastností singulárních vrcholů o stupních 2 a 3. Ve vazebné podmínce identifikujeme složky odpovídající interakcím δ a δ' a ukážeme, že vazby mezi všemi dvojicemi hran vycházejících z vrcholu jsou nastavitelné individuálně, což lze využít k návrhu kvantových filtrů typu „spektrální výhybky".

Také se zabýváme Schrödingerovými operátory na nekonečném kvantovém grafu ve tvaru řetízku, který je tvořen shodnými kroužky spojenými v bodech dotyku pomocí δ-vazeb s parametrem vazby $\alpha \in \mathbb{R}$. Je-li graf přímý a tedy periodický, hamiltonián má pásové spektrum s nekonečným počtem mezer pro všechna $\alpha \neq 0$. Uvážíme „ohybovou" deformaci spočívající ve změně polohy bodu dotyku mezi dvěma kroužky a ukážeme, že tato deformace má za následek vznik vlastních hodnot ve spektrálních mezerách. Podrobně prozkoumáme závislost těchto vlastních hodnot na α a na „úhlu ohybu", stejně tak jako rezonance systému způsobené ohybem.

Résumé

Cette thèse concerne l'étude des «graphes quantiques», c'est á dire, des systèmes quantiques dans lesquels une particule non relativiste est confiné sur un graphe. Une des questions principales adressées dans ce travail concerne le choix et le sens physique des couplages des fonctions d'ondes aux sommets (vertex) de ces graphes. Nous considérons la forme standard des conditions aux limites dans un sommet de degré n, à savoir $A\Psi(0) + B\Psi'(0) = 0$, où A et B sont matrices de taille $n \times n$, $\Psi(0)$ et $\Psi'(0)$ désignent les vecteurs contenant toutes les valeurs sur chaque arête de la fonction d'onde et de sa dérivée, et $\mathrm{rang}(A|B) = n$, $AB^* = BA^*$, et nous proposons une nouvelle voie pour représenter les matrices A, B. A l'aide de ce résultat nous résolvons le problème, resté longtemps ouvert, d'approximation par des graphes réguliers de tous les couplages singuliers aux sommets dans un graphe quantique. Nous présentons une construction dans laquelle les arêts sont disjointes et les paires d'extrémités ainsi obtenues sont raccordés par des arêtes additionnelles de longueur $2d$. Chaqune de ces arêtes additionnelles porte un potentiel δ et un potentiel vectoriel et ses extrémités sont couplés aux arêtes disjointes par des couplages δ. Nous montrons que lorsque d tend vers zéro et les potentiels ajoutés dépendent convenablement de d, la limite peut produire tout couplage singulier de sommets requis, et en outre que l'approximation converge dans le sens de la résolvante en norme.

Nous discutons aussi un autre type plus simple d'approximation où les arêts ne sont pas disjointes. On impose à la place un couplage δ au sommet et des interactions δ supplémentaires ainsi que des potentiels vectoriels placés sur les n arêtes émanant du sommet. Nous montrons que cet arrangement permet d'approximer une sous-famille à $3n$ paramètres d'opérateurs de Schrödinger pour des interactions δ et leurs paramètres de couplage, ainsi que les forces des potentiels vectoriels, convenablement choisis.

Ce type de conditions aux limites est utilisé pour examiner les propriétés de diffusion par des sommets singuliers de degrés 2 et 3. Nous identifions les composantes δ et δ' dans la condition de connection et nous montrons que les couplages entre chaque paire de lignes issues du sommet sont réglables individuellement ce qui pourrait permettre la conception de filtre quantique de type «aiguillage spectral».

Nous étudions aussi les operateurs de Schrödinger sur un graphe quantique infini en forme de chaîne composée de cercles identiques couplés aux points de contact par les interactions δ avec constante de couplage $\alpha \in \mathbb{R}$. Si le graphe est droit, c'est-à-dire périodique, l'hamiltonien a un spectre de bande avec le nombre infini de lacunes si $\alpha \neq 0$. Nous considérons une déformation «courbée» de la chaîne qui consiste en un changement de la position du point de contact entre deux cercles et on montre que cette déformation a pour conséquence la naissance de valeurs propres dans les lacunes spectrales. On analyse la dépendance de ces valeurs propres par rapport à α et à l'«angle de courbure», ainsi que celle des résonances du système créées par cette courbure.

Contents

Introduction

The concept of quantum mechanics on graphs was firstly used in the fifties of the twentieth century in the paper [RS53] where it had been suggested as a model to study the spectra of aromatic hydrocarbons. The basic idea is that the graph represents the configuration space of the system, in other words, motion of a quantum particle is confined to the graph. However, the public acceptance was at that time rather moderate; it was considered much more as a curiosity or an interesting textbook example than as a widely useful and practical model. That is why the theory was not significantly developed in the three following decades and the concept was almost forgotten.

On the other hand, the technology progressed in the second half of the twentieth century very fast. Over time a development of microfabrication techniques made it possible to produce graph-shaped structures of submicron sizes in big quantities. These structures, made of semiconductors, carbon and various other materials, were considered as being highly technologically important, what gave rise to a new branch of science, the nanotechnology.

It was in the eighties when it was realized that the thirty years old concept of quantum graphs is an extremely useful, powerful and elegant tool to study properties of nanostructures. There are two main aspects that make it so important, namely:

- a graph represents a natural model for a graph-like structure,
- these models are relatively simple from the mathematical point of view.

Let us briefly explain the second item. Since a graph may be considered as a quasi-one-dimensional variety, its spectral and scattering analysis is reduced to solving ordinary differential equations, and often simply to an algebraic problem. This is a significant simplification with respect to the two- or three-dimensional situation, where partial differential equations have to be solved.

With regard to the expansion of the nanotechnology expected for the near future, the importance and application potential of quantum graphs is going to grow rapidly, and their theory itself will probably widely develop. For now, despite of the significant progress that has been made in the last two decades, the theory is still far from being as complete as the theory of one-dimensional Schrödinger operators. There remain many open problems, often of a fundamental character, that will have to be solved.

In this thesis we address several of them. In particular, we are going to study

1. parametrization of vertex couplings,

2. the problem of meaning of quantum graph vertices,

3. scattering properties and classification of vertex couplings,

4. spectral properties of a perturbed periodic graph.

The results are based for the most part on four papers listed at the beginning of the Bibliography. Let us give an account how the thesis is organized.

In the first part we describe the results. We start with a summarization of basic notions and facts about quantum graphs in Chapter 1 (Preliminaries). We will accentuate the issue of vertex couplings and the formulation of boundary conditions, which form the central subject of this thesis. Then, in Chapters 2–5, we provide the reader with a brief, self-contained exposition of the work done. These chapters include all the needed notions and important claims, we explain there the results and the methods used. Each chapter is supplemented by notes which contextualize the problem solved.

On the other hand, proofs and other technical aspects of the arguments are in the first part mostly reduced to a presentation of their main steps, without going to technical details. For their complete versions we refer to the second part of the thesis, Appendices, where copies of the four papers on which the thesis is based are attached.

Part I

PRESENTATION OF THE RESULTS

Chapter 1

Preliminaries

We will give here a precise definition of a quantum graph and describe how boundary conditions at the vertices may be formulated. The chapter will be finished with several important examplex of vertex couplings.

1.1 Graph

A *graph* Γ is an ordered pair $\Gamma = (V, E)$, where

- V is a finite or countable set of *vertices*,
- E is a set of *edges*. We suppose that there is an injective map of the set E to the set $\binom{V}{2}$; the symbol $\binom{V}{2}$ stands here for the set of all two-element subsets of V. Usually the set of edges is identified with the corresponding subset of $\binom{V}{2}$.
  If $e = (v_1, v_2)$, we call v_1 and v_2 the *endpoints* of e.

Notice that the graphs we consider are undirected and our concept obviously excludes multiple edges and loops.

By a *degree* of a vertex $v \in V$, denoted by $\deg(v)$, we mean the number of outgoing edges, or in other words the number of edges containing v.

We say that Γ is a *metric graph*, if there is a map $\ell : E \to (0, +\infty]$; the number $\ell(e)$ is called the *length* of the edge e. An infinite length is allowed under the additional condition that at least one endpoint of e is of degree 1. Edges in metric graphs may be regarded not only as pairs of vertices, but also as linear varieties.

A *star graph* is a graph having n edges ($n \in \mathbb{N}$, $n \geq 2$) and $n+1$ vertices, where one vertex is of degree n and all the others of degree 1. It follows that all edges stem from the vertex of degree n, cf. Fig. 1.1. As before, the edges may be finite or infinite. The vertex of degree n is called center of the graph.

1.2 Quantum graph

We return now to the key idea of the quantum graph concept which has been mentioned already in the introduction, namely that the configuration space of the system is a graph.

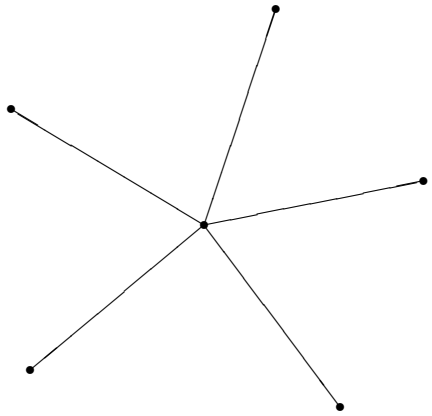

Figure 1.1: A star graph

Let us consider a free spinless particle whose motion is confined to a graph Γ having n edges $e_1, \ldots, e_n$ of the lengths $\ell(e_1), \ldots, \ell(e_n)$. A *wave function* Ψ of the system has then n components, $\Psi = (\psi_1, \psi_2, \ldots, \psi_n)^T$, and the corresponding Hilbert space $\mathcal{H}$ is given by $\bigoplus_{j=1}^n L^2(\ell(e_j))$. The Hamiltonian, denoted by H_Γ, acts as a minus second derivative on each wave function component, i.e.

$$H_\Gamma \begin{pmatrix} \psi_1 \\ \vdots \\ \psi_n \end{pmatrix} = \begin{pmatrix} -\psi_1'' \\ \vdots \\ -\psi_n'' \end{pmatrix} .$$

In this definition we neglect values of physical constants, i.e. we put $\hbar = 2m = 1$, because they will play no role in our considerations.

In the more general case when there are potentials $V_1, \ldots, V_n$ and vector potentials $A_1, \ldots, A_n$ imposed on the graph edges, the Hamiltonian action is given by

$$H_\Gamma \begin{pmatrix} \psi_1 \\ \vdots \\ \psi_n \end{pmatrix} = \begin{pmatrix} \left(-\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}x} - A_1\right)^2 \psi_1 + V_1 \cdot \psi_1 \\ \vdots \\ \left(-\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}x} - A_n\right)^2 \psi_n + V_n \cdot \psi_n \end{pmatrix} .$$

A *quantum graph* is a pair (Γ, H_Γ), where Γ is a graph and H_Γ a Hamiltonian on Γ.

1.3 Boundary conditions in quantum graph vertices

In the previous section we introduced Hamiltonian of a particle on a quantum graph and we described its action. In order to have the Hamiltonian fully defined, it is necessary to specify also boundary conditions at the vertices. Consider a vertex $v \in V$ of degree n, i.e. there are n edges going from v that may be without loss of generality enumerated as $e_1, \ldots, e_n$. Let us denote for all $j \in \hat{n}$ the wave function component on e_j by ψ_j and suppose that its variable x_j runs over the interval

$(0, \ell(e_j))$, where the value 0 corresponds to v and $\ell(e_j)$ to the other endpoint of the edge. By *boundary values* of the wave function in the vertex v we understand the two vectors Ψ_v and Ψ'_v (often denoted also as $\Psi(0)$ and $\Psi'(0)$) defined by

$$\Psi_v := \begin{pmatrix} \psi_1(0_+) \\ \vdots \\ \psi_n(0_+) \end{pmatrix}, \qquad \Psi'_v := \begin{pmatrix} \psi'_1(0_+) \\ \vdots \\ \psi'_n(0_+) \end{pmatrix},$$

i.e.

- Ψ_v is a vector from $\mathbb{C}^n$ which contains limits of the values of $\psi_1(x), \ldots, \psi_n(x)$ in the vertex v,
- Ψ'_v is a vector from $\mathbb{C}^n$ containing limits of the first derivatives of $\psi_1(x), \ldots, \psi_n(x)$ taken in the *outgoing* sense.

Since the Hamiltonian is a second-order linear operator, the boundary conditions in the vertex v of degree n have the form

$$A_v \Psi_v + B_v \Psi'_v = 0 \tag{1.1}$$

for certain $A_v, B_v \in \mathbb{C}^{n,n}$.

The boundary conditions have to be specified in such a way that the Hamiltonian H_Γ is a self-adjoint operator, or in physical terms that the probability currents at all the vertices are conserved. A standard form of the boundary conditions was derived by Kostrykin and Schrader in 1999 [KS99]; they showed that H_Γ is self-adjoint if and only if for every vertex $v \in V$ the matrices A_v and B_v satisfy the following two conditions:

$$\begin{aligned} &\bullet\ \operatorname{rank}(A_v|B_v) = \deg(v), \\ &\bullet\ \text{the product } A_v B_v^* \text{ is a self-adjoint matrix,} \end{aligned} \tag{1.2}$$

where the symbol $(A_v|B_v)$ denotes the matrix $\deg(v) \times 2\deg(v)$ with A_v and B_v forming first and second $\deg(v)$ columns, respectively. Boundary conditions (1.1) which comply with (1.2) may be called *admissible boundary conditions* and the corresponding vertex coupling *admissible vertex coupling*.

One can reformulate the statement in the following way.

(i) If the equality (1.1) represents boundary conditions in a vertex v of a quantum graph, the pair (A_v, B_v) satisfies (1.2).

(ii) For any vertex v of a quantum graph there exists a pair (A_v, B_v) such that (1.2) is satisfied.

It is obvious that also the statement

(iii) The pair (A_v, B_v) from *(ii)* is not unique.

holds, to see its validity consider a pair (CA_v, CB_v), where C is an arbitrary regular matrix from $\mathbb{C}^{\deg(v),\deg(v)}$. This pair may obviously replace (A_v, B_v), because

- $CA_v\Psi_v + CB_v\Psi'_v = 0$ is equivalent to (1.1),

- $\operatorname{rank}(CA_v|CB_v) = \deg(v)$ iff $\operatorname{rank}(A_v, B_v) = \deg(v)$,
- $CA_v(CB_v)^*$ is self-adjoint iff AB^* is.

In 2000, independently Harmer [Ha00] and Kostrykin & Schrader [KS00] have published a form of vertex boundary conditions that is unique. They showed that for any vertex coupling there is a unitary matrix $U_v \in \mathbb{C}^{\deg(v),\deg(v)}$, uniquely given by the formula $U_v = -(A_v + \mathrm{i}B_v)^{-1} \cdot (A_v - \mathrm{i}B_v)$, such that the matrices A_v and B_v in Equation (1.1) may acquire the form $A_v = U_v - I$, $B_v = \mathrm{i}(U_v + I)$, where I is the identity matrix $\deg(v) \times \deg(v)$. Conversely, for any $U_v \in \mathrm{U}(\deg(v))$, the boundary conditions

$$(U_v - I)\Psi_v + \mathrm{i}(U_v + I)\Psi_v' = 0 \tag{1.3}$$

determine an admissible vertex coupling, because the matrices $A_v = U_v - I$, $B_v = \mathrm{i}(U_v + I)$ satisfy (1.2) in consequence of unitarity of U_v.

It is appropriate to notice, however, that the condition (1.3) was known before in the general theory of self-adjoint extensions [GG91].

The formulation (1.3) of boundary conditions can be called a *parametrization* of the family of vertex couplings, since for any boundary conditions in a vertex of degree n there is exactly one matrix $U_v \in \mathrm{U}(n)$ complying with (1.3). Consequently, the family of vertex couplings in a vertex of degree n has n^2 real parameters, because the same is true for the group $\mathrm{U}(n)$. This fact is, however, well known already from the analysis of quantum graphs in terms of self-adjoint extensions [EŠ89].

Remark 1.3.1. The subscript v at the matrices A_v, B_v in (1.1) and (1.2), as well as at the matrix U_v in (1.3), may be dropped if there is no need to precize the vertex. In such a situation it is often more suitable to use the symbols $\Psi(0)$, $\Psi'(0)$ instead of Ψ_v, Ψ_v'.

1.4 Examples of vertex couplings

As we have seen in the previous section, the family of vertex couplings is very rich: if $\deg(v) = n$, it has n^2 real parameters. However, there are several types of couplings that are for certain reasons significant and have got special appellations. Let us list here the most important of them.

δ-interaction

We start with the prominent example of the δ-interaction (sometimes also called δ potential) which is characterized by the continuity of the wave function. The δ-interaction in the point $x = a$ is described by the relations

$$\psi(a_+) = \psi(a_-) =: \psi(a)\,, \qquad \psi'(a_+) - \psi'(a_-) = \alpha\psi(a)\,, \tag{1.4}$$

where $\alpha \in \mathbb{R} \cup \{+\infty\}$. The special case $\alpha = 0$ corresponds to a free motion and is sometimes called Kirchhoff boundary conditions, the case $\alpha = +\infty$ leads formally to the Dirichlet boundary conditions, i.e. $\psi(a_+) = \psi(a_-) = 0$, in this case the vertex may be regarded as n independent vertices of degree 1 with Dirichlet endpoints.

δ-coupling

The δ-coupling is a generalization of the δ-interaction for vertices of degree $n > 2$. It is described by the relations

$$\psi_j(0) = \psi_k(0) =: \psi(0)\,, \quad j,k \in \hat{n}\,, \qquad \sum_{j=1}^{n} \psi_j'(0) = \alpha\psi(0) \tag{1.5}$$

for $\alpha \in \mathbb{R} \cup \{+\infty\}$; the derivatives are taken in the outgoing sense. Similarly as in the case of the δ-interaction, $\alpha = 0$ corresponds to a free motion and $\alpha = +\infty$ to Dirichlet boundary conditions, i.e. the vertex may be regarded as n independent vertices of degree 1 with Dirichlet endpoints. We stress that it is the continuity of the wave function in the vertex which characterizes the δ-coupling and the δ-interaction and make them important. Both of them, the δ-interaction and the δ-coupling, are sometimes called *regular* in order to be distinguished from the other, *singular*, couplings that do not have this property of continuity.

We will show how (1.5) can be expressed in the form (1.1)&(1.2) and how the corresponding matrix U from (1.3) looks like. The natural way is to rewrite (1.5) in the following way:

$$\begin{pmatrix} 1 & -1 & 0 & 0 & \cdots & 0 \\ 1 & 0 & -1 & 0 & \cdots & 0 \\ 1 & 0 & 0 & -1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & 0 & 0 & 0 & \cdots & -1 \\ -\alpha & 0 & 0 & 0 & \cdots & 0 \end{pmatrix} \Psi(0) + \begin{pmatrix} 0 & 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 0 \\ 1 & 1 & 1 & 1 & \cdots & 1 \end{pmatrix} \Psi'(0) = 0 \tag{1.6}$$

The unitary matrix U needed for expressing the δ-coupling in the form (1.3) has the form $\frac{2}{n+\mathrm{i}\alpha}J - I$, where J denotes the $n \times n$ matrix whose all entries are equal to one. Hence $A = U - I = \frac{2}{n+\mathrm{i}\alpha}J - 2I$, $B = \frac{2\mathrm{i}}{n+\mathrm{i}\alpha}J$; we observe that these matrices are not real and their elements, compared to those of (1.6), complicated.

δ'-interaction

While the δ-interaction on a line is characterized by continuity of the wave function, the δ'-interaction requires continuity of the first derivative of the wave function, namely

$$\psi'(a_+) = \psi'(a_-) =: \psi'(a)\,, \qquad \psi(a_+) - \psi(a_-) = \beta\psi'(a)\,, \tag{1.7}$$

where $\beta \in \mathbb{R} \cup \{+\infty\}$. It is a counterpart of the δ-iteraction in the sense that the roles of values and derivatives in (1.7) are interchanged with respect to (1.4). The notion δ' is rather historical and not accurate; it has been proven in [Še86] that this interaction has little to do with the derivative of the δ-interaction. That is why some authors prefer the notion "ε-interaction" instead.

The δ'-interaction on the line has two possible analogues for $n > 2$, cf. [Ex95, Ex96a], namely the δ_s'-*coupling* and the δ'-*coupling*:

δ'_s-coupling

The δ'_s-coupling is an analogue of the δ'-interaction in the sense that it is a counterpart to (1.5) with the roles of $\Psi(0)$, $\Psi'(0)$ interchanged, i.e.

$$\psi'_j(0) = \psi'_k(0) =: \psi'(0)\,, \quad j,k \in \hat{n}\,, \qquad \sum_{j=1}^{n} \psi_j(0) = \beta\psi'(0)\,,$$

where $\beta \in \mathbb{R} \cup \{+\infty\}$; the special case $\beta = +\infty$ refers to full Neumann decoupling. This coupling may be expressed in a simple matrix form analogous to (1.6), it suffices to interchange $\Psi(0)$ and $\Psi'(0)$ and replace α by β. The corresponding unitary matrix needed for the form (1.3) is given by $U = I - \frac{2}{n-\mathrm{i}\beta}J$.

δ'-coupling

The δ'-coupling is an analogue of the δ'-interaction in the sense that when putting $n = 2$, one obtains exactly the δ'-interaction on a line. It is expressed by the conditions

$$\sum_{j=1}^{n} \psi'_j(0) = 0\,, \qquad \psi_j(0) - \psi_k(0) = \frac{\beta}{n}\left(\psi'_j(0) - \psi'_k(0)\right)\,, \qquad j,k \in \hat{n} \tag{1.8}$$

with $\beta \in \mathbb{R} \cup \{+\infty\}$; the case $\beta = +\infty$ again refers to full Neumann decoupling. It is easy to rewrite (1.8) into a matrix form analogous to (1.6), and as for the form (1.3), the corresponding matrix U is equal to $-\frac{n+\mathrm{i}\beta}{n-\mathrm{i}\beta}I + \frac{2}{n-\mathrm{i}\beta}J$.
Note that the special case $\beta = 0$ leads to the δ-coupling with parameter 0.

δ_p-coupling

Sometimes also the δ_p-coupling (or "permuted δ") is introduced as the counterpart to the δ'-coupling, i.e.

$$\sum_{j=1}^{n} \psi_j(0) = 0\,, \qquad \psi'_j(0) - \psi'_k(0) = \frac{\alpha}{n}\left(\psi_j(0) - \psi_k(0)\right)\,, \qquad j,k \in \hat{n}$$

with $\alpha \in \mathbb{R} \cup \{+\infty\}$; the value $\alpha = +\infty$ corresponds to the decoupled case with Dirichlet boundary conditions. It holds $U = \frac{n-\mathrm{i}\alpha}{n+\mathrm{i}\alpha}I - \frac{2}{n-\mathrm{i}\alpha}J$.
The special case $\alpha = 0$ is nothing but the δ'_s-coupling with parameter 0.

Remark 1.4.1. We observe that in all the above examples the matrices U are given as linear combinations of I and J. It can be easily shown, cf. [ET06], that this property is equivalent to the fact that the boundary conditions are invariant with respect to permutations of the edges.

Scale invariant coupling

The scale invariant subfamily of vertex couplings, introduced by Fülöp and Tsutsui in [FT00], comprises vertex couplings described by the boundary condition (1.1)&(1.2) such that both matrices A and B are singular, i.e.

$$\det(A) = \det(B) = 0\,.$$

Equivalently speaking, the numbers -1 and 1 are eigenvalues of the matrix U arising in the form (1.3). The boundary conditions can be in this case formulated as

$$A\Psi_v = 0\,, \qquad B\Psi'_v = 0,$$

or

$$(U-I)\Psi_v = 0\,, \qquad (U+I)\Psi'_v = 0\,,$$

i.e. the conditions for Ψ_v and for Ψ'_v are separable.

In the special case of the scale invariant interaction on the line the matrix U needed for the form (1.3) is given by

$$U = \begin{pmatrix} \cos\theta & \mathrm{e}^{\mathrm{i}\phi}\sin\theta \\ \mathrm{e}^{\mathrm{i}\phi}\sin\theta & -\cos\theta \end{pmatrix}$$

for $\theta, \phi \in \mathbb{R}$ (cf. [HC06]), and if the interaction is placed in the point $x = 0$, the boundary conditions may be written as

$$\psi(0_+) = \frac{\mathrm{e}^{\mathrm{i}\phi}}{\alpha}\psi(0_-)\,, \qquad \psi'(0_+) = \mathrm{e}^{\mathrm{i}\phi}\alpha\psi'(0_-)\,,$$

where $\alpha = -\mathrm{cotg}\,\frac{\theta}{2}$.

Chapter 2

Parametrization of vertex couplings in quantum graphs

In this chapter we present our results on parametrizations of vertex couplings in quantum graph vertices, namely we introduce two alternative ways how to express the boundary conditions. The essential part comes from the paper a copy of which is attached as Appendix A.

We begin the exposition with recalling the two classical forms of boundary conditions in a quantum graph vertex of degree n that we have introduced in Section 1.3, namely

(i) the standard form of Kostrykin and Schrader (1999),

$$A\Psi_v + B\Psi'_v = 0\,, \tag{2.1}$$

where

$$\begin{aligned} &\bullet\ \operatorname{rank}(A|B) = n, \\ &\bullet\ \text{the matrix } AB^* \text{ is self-adjoint,} \end{aligned} \tag{2.2}$$

and

(ii) its unique version of Harmer and Kostrykin & Schrader (2000),

$$(U - I)\Psi_v + \mathrm{i}(U + I)\Psi'_v = 0\,,$$

where

$$\bullet\ U \in \mathrm{U}(n)\,.$$

In what follows we will refer to *(i)* as to the *AB-form*, to *(ii)* as to the *U-form*. Recall that the U-form may be considered as a parametrization of all vertex couplings: any vertex coupling in a vertex of degree n corresponds, *via the matrix* U, to certain n^2-tuple of real parameters.

The natural question arising here is whether it is possible to find a *direct* parametrization, i.e. if one may write every element of A and B in terms of the n^2 real numbers parametrizing the coupling. Let us illustrate the problem on a simple example of $n = 2$:

Example. A general unitary matrix $U \in \mathrm{U}(2)$ can be parametrized by a four-tuple $(\theta_1, \theta_2, \theta_3, \theta_4) \in \mathbb{R}^4$ as

$$U = \mathrm{e}^{\mathrm{i}\theta_2} \cdot \begin{pmatrix} \mathrm{e}^{\mathrm{i}(\theta_3+\theta_4)} \cos\theta_1 & \mathrm{e}^{\mathrm{i}(\theta_3-\theta_4)} \sin\theta_1 \\ -\mathrm{e}^{\mathrm{i}(\theta_4-\theta_3)} \sin\theta_1 & \mathrm{e}^{-\mathrm{i}(\theta_3+\theta_4)} \cos\theta_1 \end{pmatrix} .$$

When we substitute this expression into the U-form and divide both sides of the equation by the factor $\mathrm{e}^{\mathrm{i}\theta_2}$, we obtain a direct parametrization of the family of vertex couplings in a vertex of degree 2:

$$\begin{pmatrix} \mathrm{e}^{\mathrm{i}(\theta_3+\theta_4)} \cos\theta_1 - \mathrm{e}^{-\mathrm{i}\theta_2} & \mathrm{e}^{\mathrm{i}(\theta_3-\theta_4)} \sin\theta_1 \\ -\mathrm{e}^{\mathrm{i}(\theta_4-\theta_3)} \sin\theta_1 & \mathrm{e}^{-\mathrm{i}(\theta_3+\theta_4)} \cos\theta_1 - \mathrm{e}^{-\mathrm{i}\theta_2} \end{pmatrix} \Psi_v + \\ + \mathrm{i} \begin{pmatrix} \mathrm{e}^{\mathrm{i}(\theta_3+\theta_4)} \cos\theta_1 + \mathrm{e}^{-\mathrm{i}\theta_2} & \mathrm{e}^{\mathrm{i}(\theta_3-\theta_4)} \sin\theta_1 \\ -\mathrm{e}^{\mathrm{i}(\theta_4-\theta_3)} \sin\theta_1 & \mathrm{e}^{-\mathrm{i}(\theta_3+\theta_4)} \cos\theta_1 + \mathrm{e}^{-\mathrm{i}\theta_2} \end{pmatrix} \Psi'_v = 0 .$$

Similarly as in the example one can proceed in the case of a general $n \in \mathbb{N}$, but the result is not very convenient for further use because of the expressions arising in the matrix elements which become long and complicated as n grows. Practical applications, for example the problem of approximations discussed further in Chapter 3, require rather a plain and transparent parametrization.

2.1 Motivation

In this work we suggest a different way how to parametrize matrices A and B. We will explain the idea first on a special subfamily of vertex couplings.

Let boundary conditions in the AB-form be given, and assume that B *is regular*. This assumption immediately implies that the condition $\mathrm{rank}(A|B) = n$ is satisfied, and also allows us to multiply both sides of the boundary conditions by B^{-1}:

$$B^{-1}A\Psi_v + I\Psi'_v = 0 .$$

The self-adjointness of AB^* is then equivalent to the self-adjointness of $B^{-1}AI^*$, i.e. of $B^{-1}A$. If we denote the s.a. matrix $-B^{-1}A$ (note the minus sign) as S and express Ψ'_v in terms of Ψ_v, we obtain the following form of boundary conditions:

$$\Psi'_v = S\Psi_v , \qquad S \text{ is self-adjoint} .$$

The relation between the n^2-tuple of real parameters and the coupling is now straighforward: if we denote the parameters by θ_{jk}, $j, k \in \hat{n}$, and put

$$\begin{aligned} \theta_{jj} &= S_{jj} , \\ \theta_{jk} &= \mathrm{Re}\,(S_{jk}) = \mathrm{Re}\,(S_{kj}) \quad \text{for } j < k , \\ \theta_{jk} &= -\mathrm{Im}\,(s_{jk}) = \mathrm{Im}\,(s_{kj}) \quad \text{for } j > k , \end{aligned}$$

the (j,k)-th element of the matrix S is given by

$$S_{jk} = \begin{cases} \theta_{jj} & \text{if } j = k , \\ \theta_{jk} + \mathrm{i}\theta_{kj} & \text{if } j < k , \\ \theta_{kj} - \mathrm{i}\theta_{jk} & \text{if } k < j . \end{cases}$$

The just demonstrated way of parametrization is

- unique,
- simple,
- but not universal: it does not incorporate boundary conditions with a singular matrix B.

In the next section we show how to deal with the general case $\mathrm{rank}(B) \leq n$.

2.2 ST-form

Before stating the main theorem of this section, introducing the promised alternative parametrization, we take note of one property which is common to both AB-form and U-form, namely their insensitivity to a particular edge numbering (by "numbering" of edges in the graph vertex of degree n we mean exclusively numbering by the elements of the set $\hat{n}$). If the edge numbering is permuted, one has just to replace the matrices A, B and U by $\tilde{A}, \tilde{B}$ and $\tilde{U}$, respectively, obtained by the appropriate rearrangement of columns and rows. In the theorem we will observe that this does not fully hold for our parametrization, cf. part (iii):

Theorem 2.2.1. *Let us consider a quantum graph vertex v of the degree n.*

(i) If $m \leq n$, $S \in \mathbb{C}^{m,m}$ is a self-adjoint matrix and $T \in \mathbb{C}^{m,n-m}$, then the equation

$$\begin{pmatrix} I^{(m)} & T \\ 0 & 0 \end{pmatrix} \Psi_v' = \begin{pmatrix} S & 0 \\ -T^* & I^{(n-m)} \end{pmatrix} \Psi_v \tag{2.3}$$

expresses admissible boundary conditions. This statement holds true for any numbering of the edges.

(ii) For any vertex coupling there exist a number $m \leq n$ and a numbering of edges such that the coupling is described by the boundary conditions (2.3) with the uniquely given matrices $T \in \mathbb{C}^{m,n-m}$ and self-adjoint $S \in \mathbb{C}^{m,m}$.

(iii) Consider a quantum graph vertex of the degree n with the numbering of the edges explicitly given; then there is a permutation $\Pi \in S_n$ such that the boundary conditions may be written in the modified form

$$\begin{pmatrix} I^{(m)} & T \\ 0 & 0 \end{pmatrix} \tilde{\Psi}_v' = \begin{pmatrix} S & 0 \\ -T^* & I^{(n-m)} \end{pmatrix} \tilde{\Psi}_v \tag{2.4}$$

for

$$\tilde{\Psi}_v = \begin{pmatrix} \psi_{\Pi(1)}(0) \\ \vdots \\ \psi_{\Pi(n)}(0) \end{pmatrix}, \qquad \tilde{\Psi}_v' = \begin{pmatrix} \psi'_{\Pi(1)}(0) \\ \vdots \\ \psi'_{\Pi(n)}(0) \end{pmatrix},$$

where the self-adjoint matrix $S \in \mathbb{C}^{m,m}$ and the matrix $T \in \mathbb{C}^{m,n-m}$ depend unambiguously on Π. This formulation of boundary conditions is in general not unique, since there may be different admissible permutations Π, but one can make it unique by choosing the lexicographically smallest permutation Π.

Proof. (A sketch; for the complete proof see Appendix A, Theorem 2.1.)

(i) It suffices to check that the matrices in (2.3) satisfy (2.2).

(ii) The key steps are the following:

1. Consider the boundary conditions in the AB-form and set $m = \mathrm{rank}(B)$.
2. Simultaneously permute the columns of A and B such that the first m columns of B are linearly independent; change properly the numbering.
3. Simultaneously permute the rows of A and B so that the first m rows of B are linearly independent.
4. From each of the last $n-m$ rows of the AB-form of the b.c. subtract such linear combination of the first m rows that all the last $n-m$ rows of B vanish.
5. Multiply the b. c. from left by appropriate regular matrix in order to obtain the $I^{(m)}$ block in B and the $I^{(n-m)}$ and the zero blocks in $-A$.
6. Substitute the final matrices A, B into AB^* and show that (2.2) is equivalent to the fact that the lower left block of $-A$ is the conjugate transpose of the upper right block of B.

(iii) The statement is an immediate consequence of (ii).

□

In the following we will call the form of boundary conditions (2.3) *ST-form*.

Remark 2.2.2. The expression (2.4) implies, in particular, that if B has not full rank, the number of real numbers parametrizing the vertex coupling (2.1) is reduced from n^2 to at most $m(2n-m) = n^2 - (n-m)^2$, where $m = \mathrm{rank}(B)$. Another reduction can come from a lower rank of the matrix A, as we will see in the following section.

Remark 2.2.3. In the proof of Theorem 2.2.1, claim (ii), we permuted columns and applied linear transformations to the rows of the system (2.1) with respect to the matrix B, but one can start by same right from the matrix A as well. In this way we would obtain similar boundary conditions as (2.3), only the vectors Ψ_v and Ψ'_v would be interchanged. Theorem 2.2.1 can be thus formulated with Equation (2.3) replaced by

$$\begin{pmatrix} I^{(\tilde{m})} & \tilde{T} \\ 0 & 0 \end{pmatrix} \Psi_v = \begin{pmatrix} \tilde{S} & 0 \\ -\tilde{T}^* & I^{(n-\tilde{m})} \end{pmatrix} \Psi'_v \,, \tag{2.5}$$

which we call the *reverse ST-form*. We accent the involved matrices S, T, as well as the number m, by tildas, since for a given vertex coupling they usually differ from those occuring in the standard ST-form (2.3).
Obviously, analogous remark can be made for Equation (2.4).

Let us point out main advantages and disadvantages of the formulations (2.3) and (2.4).

Advantages:

- Simple relation between the parameters and the boundary conditions,
- the matrices involved are often sparse, i.e. many of the matrix elements vanish,
- uniqueness.

Disadvantages:

- Structure depends on rank(B),
- vertex numbering is not fully permutable.

Remark 2.2.4. Another formulation of boundary conditions with a matrix structure singling out the regular part as in (2.4) has been derived in a different way by P. Kuchment in [Ku04]. Recall that in the setting analogous to ours he stated existence of an orthogonal projector P in $\mathbb{C}^n$ with the complementary projector $Q = Id - P$ and a self-adjoint operator L in $Q\mathbb{C}^n$ such that the boundary conditions may be written in the form

$$\begin{aligned} P\Psi_v &= 0 \\ Q\Psi'_v + LQ\Psi_v &= 0\,. \end{aligned} \tag{2.6}$$

Although the basic idea of Kuchment's formulation is close to the idea of the ST-form, there are significant differences, predetermining both formulations for different types of applications. We explain the main one. When the boundary conditions (2.6) are transformed into a matrix form, they consist of $2n$ linearly dependent equations. If a single group of n linearly indepent equations is extracted, one arrives at boundary conditions having the following structure:

$$\begin{pmatrix} \mathcal{A}_{11} & \mathcal{A}_{12} \\ \mathcal{A}_{21} & \mathcal{A}_{22} \end{pmatrix} \tilde{\Psi}_v + \begin{pmatrix} \mathcal{B}_{11} & \mathcal{B}_{12} \\ 0 & 0 \end{pmatrix} \tilde{\Psi}'_v = 0\,. \tag{2.7}$$

We see that in contrast to (2.4) where almost one half of the matrix elements vanished, there are generally no vanishing terms in (2.7) except the lower blocks of B, and moreover, the values of the coupling parameters are in (2.7) not obvious. On the other hand, the Kuchment's formulation in its original projector version (2.6) is probably more efficient in situations where the explicit values of the parameters play no role.

In the rest of the section we will derive the transformation relations between our matrices S and T and Kuchment's operators P, Q and LQ.
In the first step we separate the last $n-m$ conditions from the ST-form,

$$\begin{pmatrix} 0 & 0 \end{pmatrix} \Psi'_v = \begin{pmatrix} -T^* & I^{(n-m)} \end{pmatrix} \Psi_v\,,$$

this set of conditions obviously corresponds to $P\Psi_v = 0$. Consequently, the basis of the image of P is given as the linear span of the columns of the matrix $\mathcal{B}_P := \left(-T^*\, I^{(n-m)}\right)^* = \binom{-T}{I^{(n-m)}}$. Now we may employ the standard formula determining the orthogonal projector on a space given as the linear span of matrix columns:

$$P = \mathcal{B}_P \left(\mathcal{B}_P^* \mathcal{B}_P\right)^{-1} \mathcal{B}_P^* = \begin{pmatrix} T(I^{(n-m)} + T^*T)^{-1}T^* & -T(I^{(n-m)} + T^*T)^{-1} \\ -(I^{(n-m)} + T^*T)^{-1}T^* & (I^{(n-m)} + T^*T)^{-1} \end{pmatrix}.$$

Since the projector Q is orthogonal to P and $P+Q=Id$, the basis of Q is given by the columns of $\mathcal{B}_Q = \binom{I^{(m)}}{T^*}$ (since obviously $\mathrm{rank}(\mathcal{B}_P) = n-m$, $\mathrm{rank}(\mathcal{B}_Q) = m$ and all columns of $\mathcal{B}_Q$ are orthogonal to the columns of $\mathcal{B}_P$), hence

$$Q = \mathcal{B}_Q \left(\mathcal{B}_Q^* \mathcal{B}_Q\right)^{-1} \mathcal{B}_Q^* = \begin{pmatrix} (I^{(m)}+TT^*)^{-1} & (I^{(m)}+TT^*)^{-1}T \\ T^*(I^{(m)}+TT)^{-1} & T^*(I^{(m)}+TT^*)^{-1}T \end{pmatrix}.$$

To compute the operator LQ one has to realize that $Q\Psi_v' + LQ\Psi_v = 0$ corresponds to

$$\begin{pmatrix} I^{(m)} & T \end{pmatrix} \Psi_v' = \begin{pmatrix} S - CT^* & C \end{pmatrix} \Psi_v$$

for some $C \in \mathbb{C}^{m,n-m}$. Multiplying both sides of the equation by $\mathcal{B}_Q \left(\mathcal{B}_Q^* \mathcal{B}_Q\right)^{-1}$ we obtain

$$Q\Psi_v' = \begin{pmatrix} I^{(m)} \\ T^* \end{pmatrix} \left(I^{(m)} + TT^*\right)^{-1} \begin{pmatrix} S - CT^* & C \end{pmatrix} \Psi_v \,. \tag{2.8}$$

It follows from the second condition of (2.6) that the matrix on the RHS is equal to $-LQ$. We will find LQ in a block form $\begin{pmatrix} L_{11} & L_{12} \\ L_{21} & L_{22} \end{pmatrix}$, the blocks are of the same sizes as those of P and Q, see above. The blocks will be determined in the following two steps:

At first, we substitute the block form of L into $-LQ$ and compare the result with the matrix on the RHS of (2.8). This allowes one to eliminate C and obtain the equations

$$\left(I^{(m)} + TT^*\right)(L_{11} + L_{12}T^*) = S \quad \text{and} \quad L_{21} + L_{22}T^* = T^*(L_{11} + L_{12}T^*)\,. \tag{2.9}$$

Next, since the columns of $\mathcal{B}_P$ represent a basis of the image of P, and thus a basis of $\ker(Q)$, we have $LQ\mathcal{B}_P = 0$, i.e.

$$\begin{pmatrix} L_{11} & L_{12} \\ L_{21} & L_{22} \end{pmatrix} \begin{pmatrix} -T \\ I^{(n-m)} \end{pmatrix} = 0\,,$$

hence $L_{12} = L_{11}T$, $L_{22} = L_{21}T$. We substitute these two equalities into (2.9), and after a few manipulations we arrive at

$$\begin{aligned} LQ &= \\ &= -\begin{pmatrix} (I^{(m)}+TT^*)^{-1}S(I^{(m)}+TT^*)^{-1} & (I^{(m)}+TT^*)^{-1}S(I^{(m)}+TT^*)^{-1}T \\ T^*(I^{(m)}+TT^*)^{-1}S(I^{(m)}+TT^*)^{-1} & T^*(I^{(m)}+TT^*)^{-1}S(I^{(m)}+TT^*)^{-1}T \end{pmatrix}. \end{aligned}$$

2.3 Examples

We will demonstrate the application of the ST-form and its reverse version on the examplex of vertex couplings which have been introduced in Section 1.4. We consider a vertex of degree n and specify how the value m and the matrices S and T characterizing the coupling look like.

- **δ-coupling with parameter α**

The ST-form expressing the δ-coupling with parameter α is given by

$$\begin{pmatrix} 1 & 1 & 1 & \cdots & 1 \\ 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 0 \end{pmatrix} \Psi'_v = \begin{pmatrix} \alpha & 0 & 0 & \cdots & 0 \\ -1 & 1 & 0 & \cdots & 0 \\ -1 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ -1 & 0 & 0 & \cdots & 1 \end{pmatrix} \Psi_v \,.$$

In other words, it is characterized by the following m, S and T:

$$m = 1\,, \quad S = (\alpha) \in \mathbb{C}^{1,1}\,, \quad T = (1\ 1\ \cdots\ 1) \in \mathbb{C}^{1,n-1}.$$

- **δ'-coupling with parameter $\beta \neq 0$**

$$m = n\,, \quad S = \frac{1}{\beta}(nI - J) \in \mathbb{C}^{n,n}\,, \quad \text{the matrix } T \text{ is not present due to } m = n$$

- **scale invariant vertex coupling**

$$m \in \hat{n}\,, \quad S = 0 \in \mathbb{C}^{m,m}\,, \quad T \text{ arbitrary}$$

or $m = 0$.

As for the couplings of the type δ'_s and δ'_p, it is more efficient to express them in the reverse ST-form:

- **δ'_s-coupling with parameter β**

$$m = 1\,, \quad \tilde{S} = (\beta) \in \mathbb{C}^{1,1}\,, \quad \tilde{T} = (1\ 1\ \cdots\ 1) \in \mathbb{C}^{1,n-1}$$

- **δ'_p-coupling with parameter $\alpha \neq 0$**

$$m = n\,, \quad \tilde{S} = \frac{1}{\alpha}(nI - J) \in \mathbb{C}^{n,n}\,, \quad \tilde{T} \text{ is not present}$$

2.4 $PQRS$-form

In the previous section we have shown how the matrices A and B may be simultaneously decomposed into a 2×2 block form such that 3 of the 8 blocks were built of zeros. The sizes of the blocks were determined by the number $m = \operatorname{rank}(B)$. Below Theorem 2.2.1 there were two remarks that we are going to deal with now in more detail, namely

- Remark 2.2.2 saying that the number of real parameters of vertex couplings, being generally equal to n^2, reduces on condition that $\mathrm{rank}(B) < n$ or $\mathrm{rank}(A) < n$,
- Remark 2.2.3 mentioning that the decomposition may be done either with respect to B, or with respect to A.

Both the facts are related to the obvious asymmetry of the ST-form. In this section we aim to derive a version which is symmetric, we will call it the *$PQRS$-form*, and, inter alia, we will obtain a formula for the number of parameters of a vertex coupling in terms of the ranks $\mathrm{rank}(A)$ and $\mathrm{rank}(B)$.

Theorem 2.4.1. *Let us consider a quantum graph vertex V of a degree n.*

(i) Let

- *r_A, r_B be integers satisfying $0 \le r_A \le n$, $0 \le r_B \le n$,*
- *S be a self-adjoint matrix in $\mathbb{C}^{r_A+r_B-n, r_A+r_B-n}$,*
- *P, Q, and R be arbitrary matrices in $\mathbb{C}^{r_A+r_B-n, n-r_B}$, $Q \in \mathbb{C}^{n-r_A, n-r_B}$ and $R \in \mathbb{C}^{n-r_A, r_A+r_B-n}$, respectively.*

Then the equation

$$\begin{pmatrix} I^{(r_A+r_B-n)} & 0 & P \\ R & I^{(n-r_A)} & Q+RP \\ 0 & 0 & 0 \end{pmatrix} \Psi'_v = \begin{pmatrix} S & -SR^* & 0 \\ 0 & 0 & 0 \\ -P^* & -Q^* & I^{(n-r_B)} \end{pmatrix} \Psi_v \tag{2.10}$$

expresses admissible boundary conditions. This statement holds true for any numbering of the edges.

(ii) For any vertex coupling there exist numbers $0 \le r_A \le n$, $0 \le r_B \le n$ and a numbering of edges such that the coupling is described by the boundary conditions (2.3) with uniquely given matrices $P \in \mathbb{C}^{r_A+r_B-n, n-r_B}$, $Q \in \mathbb{C}^{n-r_A, n-r_B}$, $R \in \mathbb{C}^{n-r_A, r_A+r_B-n}$ and a regular *self-adjoint matrix $S \in \mathbb{C}^{r_A+r_B-n, r_A+r_B-n}$.*

(iii) Consider a quantum graph vertex of degree n with the numbering of the edges explicitly given. Then there is a permutation $\Pi \in S_n$ such that the boundary conditions may be written in the modified form

$$\begin{pmatrix} I^{(r_A+r_B-n)} & 0 & P \\ R & I^{(n-r_A)} & Q+RP \\ 0 & 0 & 0 \end{pmatrix} \tilde{\Psi}'_v = \begin{pmatrix} S & -SR^* & 0 \\ 0 & 0 & 0 \\ -P^* & -Q^* & I^{(n-r_B)} \end{pmatrix} \tilde{\Psi}_v \tag{2.11}$$

for

$$\tilde{\Psi}_v = \begin{pmatrix} \psi_{\Pi(1)}(0) \\ \vdots \\ \psi_{\Pi(n)}(0) \end{pmatrix}, \qquad \tilde{\Psi}'_v = \begin{pmatrix} \psi'_{\Pi(1)}(0) \\ \vdots \\ \psi'_{\Pi(n)}(0) \end{pmatrix},$$

where the regular self-adjoint matrix $S \in \mathbb{C}^{m,m}$ and the matrices $P \in \mathbb{C}^{r_A+r_B-n, n-r_B}$, $Q \in \mathbb{C}^{n-r_A, n-r_B}$, $R \in \mathbb{C}^{n-r_A, r_A+r_B-n}$ depend unambiguously on Π. This formulation of boundary conditions is in general not unique,

since there may be different admissible permutations Π*, but one can make it unique by choosing the lexicographically smallest possible permutation* Π.

Remark 2.4.2. The numbers r_A and r_B in the theorem are in fact equal to $\mathrm{rank}(A)$ and $\mathrm{rank}(B)$.

Proof. (Theorem 2.4.1)
We start with the claim (ii). Consider boundary conditions given in the form (2.3), i.e.

$$\begin{pmatrix} I^{(r_B)} & \mathcal{T} \\ 0 & 0 \end{pmatrix} \Psi'_v = \begin{pmatrix} \mathcal{S} & 0 \\ -\mathcal{T}^* & I^{(n-r_B)} \end{pmatrix} \Psi_v$$

where $r_B = \mathrm{rank}(B) \leq n$, $\mathcal{S} \in \mathbb{C}^{m,m}$ is a self-adjoint matrix and $\mathcal{T} \in \mathbb{C}^{m,n-m}$ is a general matrix.

If we denote $r_{\mathcal{S}} = \mathrm{rank}(\mathcal{S})$ and $r_A = \mathrm{rank}(A)$, we see that $r_A = r_{\mathcal{S}} + n - r_B$, hence

$$r_{\mathcal{S}} = r_A + r_B - n\,.$$

We may suppose without loss of generality that the first $r_A + r_B - n (= r_S)$ rows of S are linearly independent and the remaining $n - r_A$ rows are their linear combinations. If it is not the case, it obviously suffices to apply a simultaneous permutation on first r_B rows and columns of both matrices A and B and renumber the components of Ψ_v, Ψ'_v in the same manner. Now we decompose both matrices A, B in the following way:

$$\begin{pmatrix} I^{(r_A+r_B-n)} & 0 & P \\ 0 & I^{(n-r_A)} & Q \\ 0 & 0 & 0 \end{pmatrix} \Psi'_v = \begin{pmatrix} S_{11} & S_{21}^* & 0 \\ S_{21} & S_{22} & 0 \\ -P^* & -Q^* & I^{(n-r_B)} \end{pmatrix} \Psi_v \tag{2.12}$$

where

$$\begin{pmatrix} P \\ Q \end{pmatrix} = \mathcal{T}\,, \qquad \begin{pmatrix} S_{11} & S_{21}^* \\ S_{21} & S_{22} \end{pmatrix} = \mathcal{S}$$

and the sizes of all submatrices are determined by the blocks $I^{(r_A+r_B-n)}$, $I^{(n-r_A)}$ and $I^{(n-r_B)}$. Since the rows of $(S_{21}\ S_{22})$ are linear combinations of those of $(S_{11}\ S_{21}^*)$ (which are linearly independent), there is a unique matrix $-R \in \mathbb{C}^{n-r_A, r_A+r_B-n}$ such that

$$(S_{21}\ S_{22}) = -R\,(S_{11}\ S_{21}^*)\,. \tag{2.13}$$

In the next step we multiply the system (2.12) from the left by the matrix

$$\begin{pmatrix} I^{(r_A+r_B-n)} & 0 & 0 \\ R & I^{(n-r_A)} & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

to obtain

$$\begin{pmatrix} I^{(r_A+r_B-n)} & 0 & P \\ R & I^{(n-r_A)} & Q+RP \\ 0 & 0 & 0 \end{pmatrix} \Psi'_v = \begin{pmatrix} S_{11} & S_{21}^* & 0 \\ 0 & 0 & 0 \\ -P^* & -Q^* & I^{(n-r_B)} \end{pmatrix} \Psi_v\,. \tag{2.14}$$

We notice that (2.13) gives an explicit relation between S_{21} and S_{11} via the matrix R, namely

$$S_{21} = -RS_{11}\,.$$

We employ this fact to eliminate S_{21}^* from (2.14), then we rename S_{11} as S, and herewith we arrive at the sought final form of boundary conditions:

$$\begin{pmatrix} I^{(r_A+r_B-n)} & 0 & P \\ R & I^{(n-r_A)} & Q+RP \\ 0 & 0 & 0 \end{pmatrix} \Psi'_v = \begin{pmatrix} S & -SR^* & 0 \\ 0 & 0 & 0 \\ -P^* & -Q^* & I^{(n-r_B)} \end{pmatrix} \Psi_v\,. \quad (2.15)$$

It follows from the construction that the matrix $S \in \mathbb{C}^{r_A+r_B-n,r_A+r_B-n}$ is self-adjoint and regular, and $P \in \mathbb{C}^{r_A+r_B-n,n-r_B}$, $Q \in \mathbb{C}^{n-r_A,n-r_B}$, $R \in \mathbb{C}^{n-r_A,r_A+r_B-n}$ are general matrices of given sizes.

Thereby (ii) is proven. Since the claim (iii) can be obtained immediately from (ii) using a simultaneous permutation of elements in the vectors Ψ_v and Ψ'_v, it remains to prove (i). We have to show that the vertex coupling (2.1) with the matrices

$$A = \begin{pmatrix} -S & SR^* & 0 \\ 0 & 0 & 0 \\ P^* & Q^* & -I^{(n-r_B)} \end{pmatrix} \quad \text{and} \quad B = \begin{pmatrix} I^{(r_A+r_B-n)} & 0 & P \\ R & I^{(n-r_A)} & Q+RP \\ 0 & 0 & 0 \end{pmatrix}$$

conform with (1.2). We have

$$\operatorname{rank} \begin{pmatrix} -S & SR^* & 0 & I^{(r_A+r_B-n)} & 0 & P \\ 0 & 0 & 0 & R & I^{(n-r_A)} & Q+RP \\ P^* & Q^* & -I^{(n-r_B)} & 0 & 0 & 0 \end{pmatrix} =$$

$$= \operatorname{rank} \begin{pmatrix} I^{(r_A+r_B-n)} & 0 & 0 & -S & SR^* & P \\ R & I^{(n-r_A)} & 0 & 0 & 0 & Q+RP \\ 0 & 0 & -I^{(n-r_B)} & P^* & Q^* & 0 \end{pmatrix} = n$$

and

$$\begin{pmatrix} -S & SR^* & 0 \\ 0 & 0 & 0 \\ P^* & Q^* & -I^{(n-r_B)} \end{pmatrix} \cdot \begin{pmatrix} I^{(r_A+r_B-n)} & 0 & P \\ R & I^{(n-r_A)} & Q+RP \\ 0 & 0 & 0 \end{pmatrix}^* =$$

$$= \begin{pmatrix} -S & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix};$$

the latter matrix is self-adjoint since $S = S^*$, i.e. (2.2) is satisfied and (2.10) expresses admissible boundary conditions.

□

Remark 2.4.3. The assumption that S is regular can be dropped with the obvious consequence that we lose the uniqueness of R, cf. (2.13).

Remark 2.4.4. Similarly as in the case of the ST-form, there exists a projector formulation close to the $PQRS$-form, which was introduced in the work of Fulling, Kuchment and Wilson [FKW07]. The authors proved a theorem saying that for any vertex coupling in a vertex of degree n there are two orthogonal and mutually orthogonal projectors P, Q operating in $\mathbb{C}^n$ and an invertible self-adjoint operator Λ acting on the subspace $C\mathbb{C}^n$, where $C = 1 - P - Q$, such that the boundary conditions are equivalent to

$$\begin{aligned} P\Psi_v &= 0\,, \\ Q\Psi'_v &= 0\,, \\ C\Psi'_v &= \Lambda C\Psi_v\,. \end{aligned}$$

The relation between the $PQRS$-form and this decomposition is similar as the relation between the ST-form and the P. Kuchment's decomposition mentioned in Remark 2.2.4, cf. the detailed discussion ibid.

Number of parameters of vertex couplings

The whole family of vertex couplings in a vertex of degree n may be decomposed into disjoint subfamilies according to the pair $(\mathrm{rank}(A), \mathrm{rank}(B))$; the number of the subfamilies equals $\frac{(n+1)(n+2)}{2}$ by virtue of the condition $\mathrm{rank}(A|B) = n$. The $PQRS$-form indicates that such a decomposition is well-founded, which will be further confirmed in Chapter 4, where a classification of vertex couplings based on the values $\mathrm{rank}(A)$, $\mathrm{rank}(B)$ will be provided.

As we have already shown in Remark 2.2.2, if $\mathrm{rank}(B)$ is fixed and equal to $m \leq n$, the number of real parameters of the so obtained family of vertex couplings is equal to $n^2 - (n-m)^2$. The $PQRS$-form derived in this section allows us to go a step further and determine the number of parameters if both values $\mathrm{rank}(A)$, $\mathrm{rank}(B)$ are fixed. If we denote $r_A := \mathrm{rank}(A)$ and $r_B := \mathrm{rank}(B)$ and sum up the number of real parameters of the matrices P, Q, R, S involved in the $PQRS$-form (2.10), we arrive, after a simple manipulation, at the expression

$$n^2 - (n - r_A)^2 - (n - r_B)^2\,.$$

The formula shows in a very clear way how the number of parameters of the vertex coupling decreases with decreasing ranks of A and B.

Chapter 3

Approximations of singular vertex couplings in quantum graphs

The wave function coupling in the vertices is an essential component of quantum graph models. The most significant type, the δ-coupling together with its special case of free matching, is defined by the continuity of the wave function in the vertex. Let us take note of an important fact, namely that the δ-coupling has a simple physical meaning:

Theorem 3.0.5 (Ex96b)**.** *Let $H_\alpha(V)$ denote the Hamiltonian of a particle on a star graph with n infinite edges supporting potentials $V_1, \ldots, V_n$ and with the δ-coupling with parameter α in the center. Suppose that $V_j \in L^1_{\mathrm{loc}}(\mathbb{R}^+)$ are below bounded and $W_j \in L^1(\mathbb{R}^+)$ for $j = 1, \ldots, n$. Let us define the scaled potentials*

$$W_{\epsilon,j}(x) := \frac{1}{\epsilon} W_j\left(\frac{x}{\epsilon}\right), \qquad j = 1, \ldots, n\,.$$

Then

$$H_0(V + W_\epsilon) \to H_\alpha(V) \qquad \text{as } \epsilon \to 0_+$$

in the norm-resolvent sense, where $\alpha = \sum_{j=1}^n \int_0^{+\infty} W_j(x)\mathrm{d}x$.

In other words, the δ-coupling may be considered as a limit case of properly scaled regular potentials in the norm-resolvent sense, similarly as the Dirac delta function is a limit case of properly scaled regular functions in the sense of distributions. For this reason we call the δ-coupling a regular vertex coupling.

However, the subfamily of δ-couplings, parametrized by the value of its parameter, represents only a tiny subset of the whole family of vertex couplings. To a major part of the couplings, although they have been mathematically well defined for a decade, no simple explanation has been given for a long time, or even no explanation at all. They were accepted as being physically admissible, but nobody knew how to realize them. The question whether and in what sense one can approximate all the singular couplings by regular ones depending on suitable parameters had become a longstanding open problem.

In this work we present a solution. We propose such a construction, minimal in a natural sense using n^2 real parameters, and show that the closeness is achieved

in the norm-resolvent sense, so the convergence of all types of the spectra and the corresponding eigenprojections is guaranteed.

This chapter is based on results obtained in the papers attached as Appendix A and Appendix B.

3.1 Historical context

The key idea how to attempt the problem comes from a paper published by Cheon and Shigehara eleven years ago [CS98], in which the authors showed that a combination of regular point interactions on a line approaching each other with the coupling parameters scaled in a particular way with respect to the interaction distance can produce a singular point interaction. Three years later, in 2001, it was demonstrated [ENZ01] that the convergence in this model is norm-resolvent and the scaling choice is highly non-generic. The idea was then applied by Cheon and Exner to the simplest singular coupling, namely to the δ'_{s} one, in [CE04], and was demonstrated to work; the question was how much it can be extended. We examined it [ET07] and proved that with a larger number of regular interactions put on the edges one can approximate families described by $2n$ parameters *and not more*, we designed a concrete approximation arrangement and supported this construction by a proof of norm-resolvent convergence. At the same time we showed that changing locally the approximating graph topology one can deal with all the couplings invariant with respect to the time reversal which form an $\binom{n+1}{2}$-parameter subset, but our argument on this fact was formal, without a rigorous convergence proof.

It was clear that to proceed beyond the time-reversal symmetry one has to involve vector potentials similarly as it was done in the simplest situation in [SMMC99]. Here, in this thesis, we present such a construction which contains parameters breaking the symmetry and which at the same time is more elegant than that of [ET07] in the sense that the needed "ornamentation" of the graph is minimal: we disconnect the n edges at the vertex and join each pair of the so obtained free ends by an additional edge which shrinks to a point in the limit. The number of parameters leans on the decomposition $n^2 = n + 2\binom{n}{2}$, where the first summand, n, corresponds to δ couplings of the "outer" edge endpoints with those of the added shrinking ones. The second summand can be considered as $\binom{n}{2}$ times two parameters: one is a δ potential placed at the edge, the other is a vector potential supported by it. The main theorem of this chapter will show that the convergence of the approximation we propose is not only formal but it is valid also in the norm-resolvent sense.

3.2 The approximation arrangement

Our aim is to explain the meaning of vertex couplings using suitable approximations. It suffices to consider a prototypical example of this situation, namely a star graph with n semi-infinite edges and with a general vertex coupling in the center. We express the matching conditions in the vertex in the ST-form,

$$\begin{pmatrix} I^{(m)} & T \\ 0 & 0 \end{pmatrix} \Psi'_V = \begin{pmatrix} S & 0 \\ -T^* & I^{(n-m)} \end{pmatrix} \Psi_V \,; \tag{3.1}$$

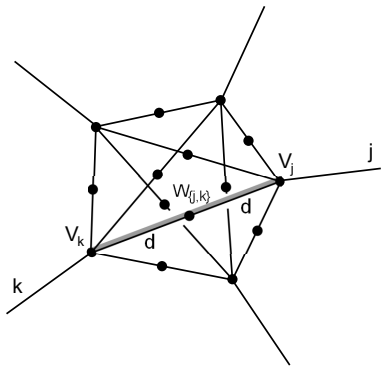

Figure 3.1: The scheme of the approximation. All inner links are of length $2d$. Some connection links may be missing if the conditions given in the text are not satisfied. The quantities corresponding to the index pair $\{j,k\}$ are marked, and the grey line symbolizes the vector potential $A_{(j,k)}(d)$.

note that the sensitivity of this formulation to the edge numbering plays no role, since one may rename the edges if necessary. As we will see below, the ST-form will help us significantly to simplify the design of the approximation arrangement and to achieve its minimality mentioned in the previous section.

It turns out that for notational purposes it is advantageous to adopt the following convention on a shift of the column indices of T:

Convention 3.2.1. *The lines of the matrix T are indexed from 1 to m, the columns are indexed from $m+1$ to n.*

We are going to show that the star graph with the singular vertex coupling given by the boundary conditions (3.1) may be understood as a limit case of certain family of graphs constructed only from edges connected by δ-couplings, δ-interactions, and supporting constant vector potentials. The detailed description of our approximating model follows, cf. Fig. 3.2.

- We take n halflines, each parametrized by $x \in [0, +\infty)$, with the endpoints denoted as V_j, and put a δ-coupling (to the edges specified below) with the parameter $v_j(d)$ at the point V_j for all $j \in \hat{n}$.

- Certain pairs V_j, V_k of halfline endpoints will be joined by edges of the length $2d$, and the center of each such joining segment will be denoted as $W_{\{j,k\}}$. For each pair $\{j,k\}$, the points V_j and V_k, $j \neq k$, are joined if one of the following three conditions is satisfied (keep in mind Convention 3.2.1):

  (1) $j \in \hat{m}$, $k \geq m+1$, and $T_{jk} \neq 0$ (or $j \geq m+1$, $k \in \hat{m}$, and $T_{kj} \neq 0$),

  (2) $j,k \in \hat{m}$ and $(\exists l \geq m+1)(T_{jl} \neq 0 \wedge T_{kl} \neq 0)$,

  (3) $j,k \in \hat{m}$, $S_{jk} \neq 0$, and the previous condition is not satisfied.

  We remark that in this step we take advantage of the structure of the ST-form.

- At each point $W_{\{j,k\}}$ we place a δ-interaction with a parameter $w_{\{j,k\}}(d)$. From now on we use the following convention: the connecting edges of the length $2d$ are considered as composed of two line segments of the length d, on each of them the variable runs from 0 (corresponding to the point $W_{\{j,k\}}$) to d (corresponding to the point V_j or V_k).

- On each connecting segment described above we put a vector potential which is constant on the whole line between the points V_j and V_k. We denote the potential strength between the points $W_{\{j,k\}}$ and V_j as $A_{(j,k)}(d)$, and between the points $W_{\{j,k\}}$ and V_k as $A_{(k,j)}(d)$. It follows from the continuity that $A_{(k,j)}(d) = -A_{(j,k)}(d)$ for any pair $\{j,k\}$.

The values of $v_j(d)$, $w_{\{j,k\}}(d)$ and $A_{(j,k)}(d)$ in terms of the parameter d depend on the vertex coupling we approximate. For deriving them we have applied the method which was used for the first time in [CS98, SMMC99] for the case of a point interaction on the line. We explain the main idea. We consider the approximating system and perform the following steps.

1. Expand all the wave function components at the vertices V_j, $W_{\{j,k\}}$ into Taylor polynomials.

2. Write down the conditions expressing the δ-couplings and δ-interactions at all vertices.

3. Take into account the vector potentials on the connecting edges, using the following Lemma (cf. Appendix A, Lemma 3.2 and its proof):

   Lemma 3.2.2. *Let us consider a line parametrized by the variable $x \in (0, L)$, $L \in (0, +\infty) \cup \{+\infty\}$, and let H denote a Hamiltonian of a particle on this line interacting with a potential V,*

   $$H = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V\,, \tag{3.2}$$

   sufficiently regular to make H self-adjoint. We denote by $\psi^{s,t}$ the solution of $H\psi = k^2\psi$ with the boundary values $\psi^{s,t}(0) = s$, $\psi^{s,t\prime}(0) = t$. Consider the same system with a vector potential A added, again sufficiently regular; the Hamiltonian is consequently given by

   $$H_A = \left(-\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}x} - A\right)^2 + V\,. \tag{3.3}$$

   Let $\psi_A^{s,t}$ denote the solution of $H_A\psi = k^2\psi$ with the same boundary values as before, i.e. $\psi_A^{s,t}(0) = s$, $\psi_A^{s,t\prime}(0) = t$. Then the function $\psi_A^{s,t}$ can be expressed as

   $$\psi_A^{s,t}(x) = \mathrm{e}^{\mathrm{i}\int_0^x A(z)\mathrm{d}z} \cdot \psi^{s,t}(x) \qquad \textit{for all} \quad x \in (0, L)\,.$$

4. Employ results of previous steps to relate the values and derivatives at the points V_j and $W_{\{j,k\}}$.

5. Using convenient elimination express the relation between $\Psi(0) := (\psi_1(0_+), \ldots, \psi_n(0_+))$ and $\Psi'(0) := (\psi_1'(0_+), \ldots, \psi_n'(0_+))$, where ψ_j $(j \in \hat{n})$ denotes the wave function component on the j-th half line.

6. Require that $\Psi(0)$ and $\Psi'(0)$ satisfy *in the limit* $d \to 0_+$ the boundary conditions (3.1). This step gives a set of conditions on $v_j(d)$, $w_{\{j,k\}}(d)$ and $A_{(j,k)}(d)$. Now it suffices to find expressions for these quantities such that the conditions will be fulfilled at the same time, cf. below.

Detailed calculation can be found in Appendix A. Here we state only the final expressions, obtained in the last step. They make use of the symbols N_j and $\langle c \rangle$ defined in the following way:

- $N_j \subset \hat{n}$ stands for the set containing indices of all the edges that are joined to the j-th one by a connecting segment, i.e.

$$\begin{aligned} N_j =& \{k \in \hat{m} |\, S_{jk} \neq 0\} \cup \{k \in \hat{m} |\, (\exists l \geq m+1)(T_{jl} \neq 0 \wedge T_{kl} \neq 0)\} \\ & \cup \{k \geq m+1 |\, T_{jk} \neq 0\} \qquad \text{for } j \in \hat{m}\,, \\ N_j =& \{k \in \hat{m} |\, T_{kj} \neq 0\} \qquad \text{for } j \geq m+1\,. \end{aligned}$$

- $\langle \cdot \rangle$ denotes the map from $\mathbb{C}$ into $\mathbb{R}$ acting as follows: if $c \in \mathbb{C}$, then

$$\langle c \rangle = \begin{cases} |c| & \text{if } \operatorname{Re} c \geq 0\,, \\ -|c| & \text{if } \operatorname{Re} c < 0\,. \end{cases}$$

Now we proceed to the sought parameters of approximating system.

- $v_j(d)$ is given by

$$v_j(d) = \begin{cases} S_{jj} - \frac{\#N_j}{d} - \sum_{k=1}^{m} \left\langle S_{jk} + \frac{1}{d} \sum_{l=m+1}^{n} T_{jl}\overline{T_{kl}} \right\rangle + \\ \qquad + \frac{1}{d} \sum_{l=m+1}^{n} (1 + \langle T_{jl} \rangle) \langle T_{jl} \rangle \qquad \text{if } j \in \hat{m}\,, \\ \frac{1}{d} \left(1 - \#N_j + \sum_{h=1}^{m} \langle T_{hj} \rangle\right) \qquad \text{if } j \geq m+1\,. \end{cases} \tag{3.4}$$

- For all j, $w_{\{j,k\}}(d)$ is given by

$$w_{\{j,k\}}(d) = \begin{cases} -\frac{1}{d} \left(2 + \frac{1}{\left\langle d \cdot S_{jk} + \sum_{l=m+1}^{n} T_{jl}\overline{T_{kl}} \right\rangle}\right) & \text{if } k \in N_j \cap \hat{m}\,, \\ \frac{1}{d} \left(-2 + \frac{1}{\langle T_{jk} \rangle}\right) & \text{if } k \in N_j \backslash \hat{m}\,. \end{cases} \tag{3.5}$$

- For all j, $A_{(j,k)}(d)$ is given by

$$A_{(j,k)}(d) = \begin{cases} \frac{1}{2d} \arg \left(d \cdot S_{jk} + \sum_{l=m+1}^{n} T_{jl}\overline{T_{kl}}\right) \\ \qquad \text{if } k \in N_j \cap \hat{m} \wedge \operatorname{Re} \left(d \cdot S_{jk} + \sum_{l=m+1}^{n} T_{jl}\overline{T_{kl}}\right) \geq 0\,, \\ \frac{1}{2d} \left[\arg \left(d \cdot S_{jk} + \sum_{l=m+1}^{n} T_{jl}\overline{T_{kl}}\right) - \pi\right] \\ \qquad \text{if } k \in N_j \cap \hat{m} \wedge \operatorname{Re} \left(d \cdot S_{jk} + \sum_{l=m+1}^{n} T_{jl}\overline{T_{kl}}\right) < 0\,, \\ \frac{1}{2d} \arg T_{jk} \qquad \text{if } k \in N_j \backslash \hat{m} \wedge \operatorname{Re} T_{jk} \geq 0\,, \\ \frac{1}{2d} (\arg T_{jl} - \pi) \qquad \text{if } k \in N_j \backslash \hat{m} \wedge \operatorname{Re} T_{jl} < 0\,. \end{cases} \tag{3.6}$$

If the parameters of the δ-couplings and δ-interactions $v_j(d)$, $w_{\{j,k\}}(d)$ and the strengths of the vector potentials $A_{(j,k)}(d)$ are chosen according to the formulae above, one may expect that the smaller the value d is, the closer the approximating system to the approximated system is. In the following we are going to give a clear meaning to this convergence.

3.3 The norm-resolvent convergence

In the previous section we have shown that any vertex coupling in the center of a star graph may be regarded as a limit of a certain family of graphs supporting nothing but δ-couplings, δ-interactions and constant vector potentials. The parameter values of all the δ's and the vector potentials have been derived using a method devised originally in [CS98, SMMC99] for the case of a generalized point interaction on the line. In this section we are going to show that the Hamiltonian of the approximating system converges to the Hamiltonian of the approximated system *in the norm-resolvent sense*, with the natural consequences for the convergence of eigenvalues, eigenfunctions, etc.

We denote the Hamiltonian of the star graph Γ with the coupling (3.1) at the vertex as H^{Ad} (referring to the *a*pproximate*d* system), and H_d^{Ag} will stand for the *a*pproximating family of graphs that has been constructed in the previous section.

Our aim is to establish a convergence of H_d^{Ag} to H^{Ad} for $d \to 0_+$. Both H^{Ad} and H_d^{Ag} are unbounded operators, therefore we will examine and compare their resolvents. Let the symbols $R^{\mathrm{Ad}}(k^2)$ and $R_d^{\mathrm{Ag}}(k^2)$ denote the resolvents of H^{Ad} and H_d^{Ag} at the points k^2 from the resolvent set. Needless to say, the operators act on different spaces: $R^{\mathrm{Ad}}(k^2)$ on $L^2(G)$, where $G = (\mathbb{R}^+)^n$ corresponds to the star graph Γ, and $R_d^{\mathrm{Ag}}(k^2)$ on $L^2(G_d)$, where

$$G_d = (\mathbb{R}^+)^n \oplus (0,d)^{\sum_{j=1}^n N_j} .$$

In order to be able to compare them, we need to identify $R^{\mathrm{Ad}}(k^2)$ with the orthogonal sum

$$R_d^{\mathrm{Ad}}(k^2) = R^{\mathrm{Ad}}(k^2) \oplus 0 ,$$

where 0 is a zero operator acting on the space $L^2\left((0,d)^{\sum_{j=1}^n N_j}\right)$ which is removed in the limit. Then both the operators $R_d^{\mathrm{Ad}}(k^2)$ and $R_d^{\mathrm{Ag}}(k^2)$ are defined as acting on functions from $L^2(G_d)$ which are vector functions with $n + \sum_{j=1}^n N_j$ components; we will index the components by the set

$$\mathcal{I} = \hat{n} \cup \{\, (l,h) |\ l \in \hat{n}, h \in N_l \} .$$

Let us now use this setting to state the main theorem of this chapter.

Theorem 3.3.1. *Let $v_j(d)$, $w_{\{j,k\}}(d)$ and $A_{(j,k)}(d)$, where $j \in \hat{n}$, $k \in N_j$, depend on d according to* (3.4), (3.5) *and* (3.6), *respectively. Then the family H_d^{Ag} converges to H_d^{Ad} in the norm-resolvent sense as $d \to 0_+$, i.e.*

$$\lim_{d \to 0_+} \left\| R_d^{\mathrm{Ag}}(k^2) - R_d^{\mathrm{Ad}}(k^2) \right\| = 0 ,$$

where $\|\cdot\|$ is the L^2-norm in G_d.

Proof. The proof is very long and is contained in Appendix A, cf. Theorem 4.1. Here we briefly describe its main steps.

1. Computation of $R^{\mathrm{Ad}}(k^2)$ and $R_d^{\mathrm{Ag}}(k^2)$:
   i. Decompose both graphs, approximating and approximated, into individual edges, posing the Dirichlet boundary conditions at the endpoints,
   ii. compute the resolvents of the both decomposed systems,
   iii. employ Krein's formula to obtain expressions for $R^{\mathrm{Ad}}(k^2)$ and $R_d^{\mathrm{Ag}}(k^2)$; this step gives the expressions for the resolvents *up to certain coefficients*,
   iv. require that if $R^{\mathrm{Ad}}(k^2)$ and $R_d^{\mathrm{Ag}}(k^2)$ are applied to an arbitrary Ψ from $L^2(G)$ and $L^2(G_d)$, respectively, the image lies in the domain of H^{Ad} and H_d^{Ag}, respectively; hence compute the unknown coefficients introduced in the previous step.
2. Identification of $R^{\mathrm{Ad}}(k^2)$ with $R_d^{\mathrm{Ad}}(k^2)$.
3. Computation of the difference $\left\| R_d^{\mathrm{Ag}}(k^2) - R_d^{\mathrm{Ag}}(k^2) \right\|_2^2$, where $\|\cdot\|_2$ denotes the Hilbert-Schmidt norm in $L^2(G_d)$.
4. $\|\cdot\| \leq \|\cdot\|_2$.

□

Since for some applications it may be useful to know how quickly the term $\left\| R_d^{\mathrm{Ag}}(k^2) - R_d^{\mathrm{Ad}}(k^2) \right\|$ approaches zero if $d \to 0_+$, we add the following remark.

Remark 3.3.2. *(The rate of convergence.)*
If the assumptions of Theorem 3.3.1 are satisfied, there is a number $K > 0$ independent of d such that

$$\left\| R_d^{\mathrm{Ag}}(k^2) - R_d^{\mathrm{Ad}}(k^2) \right\| \leq K \cdot \sqrt{d}\,.$$

3.4 Approximations without added edges

The approximation arrangement studied in the previous section was leaning on additional connecting lines supporting δ-interactions and vector potentials. One may, however, wonder whether it is possible to construct an approximating graph without added edges, i.e. where the δ-interactions and vector potentials are supported by the half lines of the star graph themselves. We refer in advance to Fig. 3.2 which illustrates the idea.

When we were recalling the evolution of the problem of approximations, cf. Section 3.1, we mentioned that the first constructions had been done just in this way. In this section we will see that such simple approximations have a very limited use and cannot approximate a general vertex coupling.

This sort of approximation arrangements is one of the topics which were studied in my master thesis. I have investigated approximating graphs supporting the δ-coupling at the center and the δ-interactions on the lines, but no vector potentials

were considered. During my PhD study we have written and published a paper [ET07] based on these results, its copy is attached in Appendix B. Later we realized, however, that the results could be extended using the vector potentials placed on the edges. The aim of this section is to present this generalized solution on the background of Appendix B.

We begin with recalling the main results of the paper. We present them in the form of basic steps, followed by brief expository comments.

1. At first we have explored limits of the considered approximation.

   In Proposition 3.1 of Appendix B and its proof we found that the class of the vertex couplings that can be approximated using the δ-interactions placed on the edges of the star graph and the δ-coupling placed at the center depend on at most $2n$ parameters (or less), no matter how large the number of the δ-interactions is. Moreover, we obtained a description of this class using the U-form; we showed that the matrix U has to be of the type

   $$U = \frac{2i}{\rho + \mathrm{i}\left(1 + \sum_{\ell=2}^{n} \frac{1}{c_\ell^2 + t_\ell^2}\right)} D^{(1)} J D^{(1)} - D^{(2)}\,, \tag{3.7}$$

   where

   $$D^{(1)} = \operatorname{diag}\left(\mathrm{e}^{-\mathrm{i}\theta}, \frac{1}{c_2 + \mathrm{i}t_2}, \frac{1}{c_3 + \mathrm{i}t_3}, \ldots, \frac{1}{c_n + \mathrm{i}t_n}\right),$$
   $$D^{(2)} = \operatorname{diag}\left(\mathrm{e}^{-2\mathrm{i}\theta}, \frac{c_2 - \mathrm{i}t_2}{c_2 + \mathrm{i}t_2}, \frac{c_3 - \mathrm{i}t_3}{c_3 + \mathrm{i}t_3}, \ldots, \frac{c_n - \mathrm{i}t_n}{c_n + \mathrm{i}t_n}\right)$$

   and J is a matrix $n \times n$ all of whose elements are equal to 1. The $2n$ real parameters determining U are then $\theta, c_2, c_3, \ldots, c_n, t_2, t_3, \ldots t_n, \rho$.

2. Secondly, we designed the approximating settlement.

   Knowing that the maximum number of parameters which can be achieved in this way is bounded by $2n$, we were naturally lead to the idea of placing two δ-interactions at each of the n half lines. In our considerations we left out the case $n = 2$ which had been discussed in the paper [SMMC99].

   The designed approximating graph has the following structure, cf. Fig. 3.2:

   - There is a δ-coupling with parameter $u(d)$ in the star centre,
   - on each half line there is a δ-interaction with parameter $v_j(d)$, where j is the half line index, at a distance $D(d)$ from the centre,
   - each half line supports another δ-interaction with parameter $w_j(d)$ at the distance $D(d) + d$ from the centre.

3. Thirdly, we determined the values of the parameters $u(d)$, $v_j(d)$ and $w_j(d)$, as well as the dependence of $D(d)$ on d.

   We employed the boundary conditions in the vertices where the δ-coupling and the δ-interactions are placed, as well as asymptotic expansions of the wave

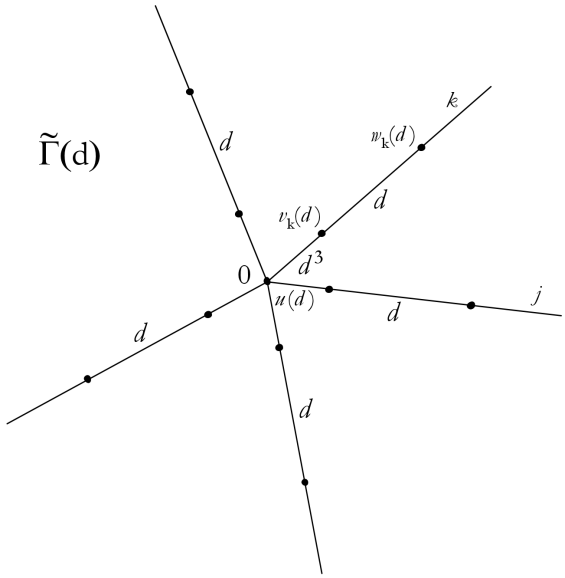

Figure 3.2: Scheme of a $2n$-parameter approximation

function components in their neighbourhoods. In this way (cf. Appendix B, Section 3.2 for details) we obtained expressions for $u(d)$, $v_j(d)$ and $w_j(d)$ and found that $D(d)$ could be chosen as d^3. A heuristic argument showed that this choice of the parameters realizes an approximation of the $2n$-parameter family which was found in the first step as maximal achievable.

4. Finally, we proved the norm-resolvent convergence.

   Let the center of the graph Γ support a coupling which fall within the family that has been found in the first step; we denote the corresponding Hamiltonian by $H^{\vec{\theta}}$, where $\vec{\theta} \in \mathbb{R}^{2n}$ is the vector of parameters. Let $H^{u,\vec{v},\vec{w}}(d)$ denote the Hamiltonian of the approximating family constructed above.

   Theorem 3.4.1. *Let $u(d)$, $v_j(d)$ and $w_j(d)$, $j \in \hat{n}$ properly depend on d. Then $H^{u,\vec{v},\vec{w}}(d)$ converges to $H^{\vec{\theta}}$ in the norm-resolvent sense as $d \to 0_+$.*

Vector potentials

Now we explain how this result can be extended if vector potentials are involved. It immediately follows from Lemma 3.2.2 that a vector potential A supported by the interval $(0, a)$ shifts the phase of the wave function, as well as the phase of its derivative, after the point $x = a$ by the factor $\mathrm{e}^{\mathrm{i}\int_0^a A(x)\mathrm{d}x}$. It is an important fact that only the integral of A is of significance, not the A itself. Therefore, a vector potential placed on one edge can increase the number of parameters of approximable couplings by 1, but cannot increase it by more; if vector potentials are placed on all edges, then the number of so gainable parameters equals n.

Specifically, if we consider the approximating graph with two δ-interactions on the half lines which has been constructed above (cf. Fig. 3.2) and place a constant

vector potential of the strength A_j/d at the segment (d^3, d^3+d) on the j-th half line for each $j \in \hat{n}$, the values of $\psi_j(d^3+d)$ and $\psi_j'(d^3+d_+)$ change to $\psi_j^A(d^3+d) = \mathrm{e}^{\mathrm{i}A_j}\psi_j(d^3+d)$ and $\psi_j^{A\prime}(d^3+d_+) = \mathrm{e}^{\mathrm{i}A_j}\psi_j'(d^3+d_+)$, respectively. The choice of how the vector potential depends on d ensures that the phase shift factors remain constant when d approaches zero, therefore in the limit

$$\begin{pmatrix} \psi_1^A(0_+) \\ \vdots \\ \psi_n^A(0_+) \end{pmatrix} = \begin{pmatrix} \mathrm{e}^{\mathrm{i}A_1}\psi_1(0_+) \\ \vdots \\ \mathrm{e}^{\mathrm{i}A_n}\psi_n(0_+) \end{pmatrix}, \qquad \begin{pmatrix} \psi_1^{A\prime}(0_+) \\ \vdots \\ \psi_n^{A\prime}(0_+) \end{pmatrix} = \begin{pmatrix} \mathrm{e}^{\mathrm{i}A_1}\psi_1'(0_+) \\ \vdots \\ \mathrm{e}^{\mathrm{i}A_n}\psi_n'(0_+) \end{pmatrix}.$$

If we denote $D_A = \mathrm{diag}\left(\mathrm{e}^{\mathrm{i}A_1}, \ldots, \mathrm{e}^{\mathrm{i}A_n}\right)$, we have

$$\Psi_A(0) = D_A\Psi(0)\,, \qquad \Psi_A'(0) = D_A\Psi'(0)\,.$$

Let $\tilde{\Gamma}(d)$ denote the approximating graph without vector potentials that we have described in the step 2 above, cf. Fig. 3.2. Suppose that the limiting case for $d \to 0_+$ corresponds to a star graph with the vertex coupling which is determined by the boundary conditions

$$(U-I)\Psi(0) + \mathrm{i}(U+I)\Psi'(0) = 0\,,$$

where U is a unitary matrix belonging to the class described by (3.7).

Let now $\tilde{\Gamma}_A(d)$ denote the approximating graph obtained from $\tilde{\Gamma}(d)$ by adding the constant vector potential A_j/d at (d^3, d^3+d) on the j-th half line for all $j \in \hat{n}$, as described above. With regard to our discussion, the limiting case of $\tilde{\Gamma}_A(d)$ for $d \to 0_+$ corresponds to the vertex coupling determined by the boundary conditions

$$(U-I)D_A\Psi(0) + \mathrm{i}(U+I)D_A\Psi'(0) = 0\,.$$

When we multiply the last equation by D_A^{-1} from the left, we obtain

$$\left(D_A^{-1}UD_A - I\right)\Psi(0) + \mathrm{i}\left(D_A^{-1}UD_A + I\right)\Psi'(0) = 0$$

and can make the conclusion:

Proposition 3.4.2. *The most general vertex coupling, approximable with the help of the δ-interactions and vector potentials placed on the edges of the original star graph, is described by the unitary matrix U_A which depend on $3n$ real parameters $\theta, c_2, c_3, \ldots, c_n, t_2, t_3, \ldots t_n, \rho$, $A_1, \ldots, A_n$ and is given by*

$$U_A = \frac{2i}{\rho + \mathrm{i}\left(1 + \sum_{\ell=2}^n \frac{1}{c_\ell^2+t_\ell^2}\right)} D_A^{-1}D^{(1)}JD^{(1)}D_A - D^{(2)}\,,$$

where $D^{(1)}$, $D^{(2)}$, J are matrices defined above (cf. Equation (3.7)),
$D_A = \mathrm{diag}\left(\mathrm{e}^{\mathrm{i}A_1}, \ldots, \mathrm{e}^{\mathrm{i}A_n}\right)$.

One can also prove the norm-resolvent convergence of such approximation:

Let

- $H^{\vec{\theta_A}}$ denote the Hamiltonian of a star graph with a vertex coupling belonging to the family described in Proposition 3.4.2 in the centre, the vector $\vec{\theta_A}$ represents the corresponding coupling parameters, i.e.
  $\vec{\theta_A} = (\theta, c_2, c_3, \ldots, c_n, t_2, t_3, \ldots t_n, \rho, A_1, \ldots, A_n) \in \mathbb{R}^{3n}$,
- $H^{u,\vec{v},\vec{w},\vec{A}}(d)$ denote the Hamiltonian of the approximating graph constructed above.

Theorem 3.4.3. *Let $u(d)$, $v_j(d)$ and $w_j(d)$ properly depend on d, $A_j(d) = \frac{A_j}{d}$ $(j \in \hat{n})$. Then $H^{u,\vec{v},\vec{w},\vec{A}}(d)$ converges to $H^{\vec{\theta_A}}$ in the norm-resolvent sense as $d \to 0_+$.*

Proof.
- The proof makes use of Krein's formula,
- its structure is similar to the one of Theorem 4.1 from Appendix B, but slightly more complicated due to the vector potentials,
- the effect of the vector potentials can be treated in the same way as in the proof of Theorem 3.3.1 formulated in the last section, see its detailed version in Appendix A, proof of Theorem 4.1.

□

Chapter 4

Spectral filtering in quantum Y-junction

The ST-form of boundary conditions, derived in Chapter 2, helped us in Chapter 3 to construct an approximation of a general singular vertex coupling. Now we will take advantage of the ST-form once again. It turns out that it helps to classify singular vertices and examine their scattering properties. The results presented in this chapter come from the paper a copy of which is attached as Appendix C.[1]

4.1 Scattering matrix

Consider a quantum particle on a star graph with n half lines. We denote $\Psi = (\psi_1, \dots, \psi_n)^T$ the vector of wave function components. The system is specified by boundary conditions in the vertex,

$$A\Psi(0) + B\Psi'(0) = 0\,, \tag{4.1}$$

where $\Psi(0)$ stands for $(\psi_1(0_+), \dots, \psi_n(0_+))^T$ and $\Psi'(0)$ for $(\psi_1'(0_+), \dots, \psi_n'(0_+))^T$ (the derivatives are taken in the outgoing sense). Let us recall that in the ST-form (2.3), which is a special formulation of the boundary conditions (4.1), the matrices A and B acquire the form

$$A = -\begin{pmatrix} S & 0 \\ -T^* & I^{(n-r_B)} \end{pmatrix}, \quad B = \begin{pmatrix} I^{(r_B)} & T \\ 0 & 0 \end{pmatrix},$$

$r_B = \mathrm{rank}(B)$. In Chapter 3 we have introduced also the reverse ST-form (2.5), which is characterized by

$$A = \begin{pmatrix} I^{(r_A)} & \tilde{T} \\ 0 & 0 \end{pmatrix}, \quad B = -\begin{pmatrix} \tilde{S} & 0 \\ -\tilde{T}^* & I^{(n-r_A)} \end{pmatrix};$$

$r_A = \mathrm{rank}(A)$. In this chapter we will use exclusively these two formulations.

[1] To be consistent with the other chapters we use here a notation that slightly differs from the one employed in Appendix C.

Let $\Psi^{(j)} = \left(\psi_1^{(j)}, \dots, \psi_n^{(j)}\right)^T$ be the scattering solution for incoming wave entering from j-th line with the wave number k. Then it holds

$$\psi_i^{(j)}(x_i) = \begin{cases} e^{-\mathrm{i}kx_i} + \mathcal{R}_i e^{\mathrm{i}kx_i} & (i = j)\,, \\ \mathcal{T}_{ij}\, e^{\mathrm{i}kx_i} & (i \neq j)\,, \end{cases}$$

where $\mathcal{R}_i$ represents the reflection amplitude for i-th line and $\mathcal{T}_{ij}$ the transmission amplitude from j-th to i-th line.

The scattering matrix $\mathcal{S}(k)$ (which is not to be confused with the sub-matrix S appearing in the ST-form) is given by

$$\mathcal{S}(k) = \begin{pmatrix} \mathcal{R}_1(k) & \mathcal{T}_{12}(k) & \cdots & \mathcal{T}_{1n}(k) \\ \mathcal{T}_{21}(k) & \mathcal{R}_2(k) & \cdots & \mathcal{T}_{2n}(k) \\ \vdots & & & \vdots \\ \mathcal{T}_{n1}(k) & \mathcal{T}_{n2}(k) & \cdots & \mathcal{R}_n(k) \end{pmatrix}$$

and can be computed as

$$\mathcal{S}(k) = -(A + \mathrm{i}kB)^{-1}(A - \mathrm{i}kB)\,. \tag{4.2}$$

It is easy to check that if the matrices A and B occurring in (4.1) interchange their positions, the scattering matrix $\mathcal{S}_d(k)$ corresponding to the so obtained "swapped" boundary conditions (the "dual" scattering matrix) is given by $\mathcal{S}_d(k) = -\mathcal{S}(-1/k)$.

It is useful for our next considerations to mention how the transmission amplitudes look like for the δ-interaction, δ'-interaction and scale invariant interaction:

- δ-interaction with parameter α: $\mathcal{T}_{ij}(k) = \frac{2k}{2k+\mathrm{i}\alpha}$,
  hence $\mathcal{T}_{ij}(0) = 0, \quad \mathcal{T}_{ij}(+\infty) = 1$
- δ'-interaction with parameter β: $\mathcal{T}_{ij}(k) = \frac{-2}{2-\mathrm{i}k\beta}$,
  hence $\mathcal{T}_{ij}(0) = -1, \quad \mathcal{T}_{ij}(+\infty) = 0$
- scale invariant interaction with parameters α, ϕ: $\mathcal{T}_{ij}(k) = \frac{2\alpha}{1+\alpha^2}\mathrm{e}^{\mathrm{i}\phi} = \text{const.}$

The terms $\mathcal{T}_{ij}(0)$ and $\mathcal{T}_{ij}(+\infty)$ are here considered conventionally as *limits*, as well as in the rest of the chapter.

4.2 Classification in the case $n = 2$. Transmission amplitudes

We present first the results for the known case of $n = 2$, namely, the *point interaction on a line*, in order to see the effectiveness of the ST-form in identifying the physical content of the singular vertex. The classification will be done with respect to $\mathrm{rank}(B)$ and $\mathrm{rank}(A)$. It is useful to notice that if $\mathrm{rank}(B)$ is fixed, the value $\mathrm{rank}(A)$ is uniquely related to $\mathrm{rank}(S)$ by the equality $\mathrm{rank}(A) = n - \mathrm{rank}(B) + \mathrm{rank}(S)$, and has to be greater or equal to $n - \mathrm{rank}(B)$.

- $\mathrm{rank}(B) = 0$

The ST-form gives $A = -I$, hence

$$0 = \Psi(0)\,,$$

which obviously defines disjoint Dirichlet boundaries $\psi_1(0_+) = \psi_2(0_+) = 0$.

- $\operatorname{rank}(B) = 1$

$$\begin{pmatrix} 1 & t \\ 0 & 0 \end{pmatrix} \Psi'(0) = \begin{pmatrix} s & 0 \\ -\bar{t} & 1 \end{pmatrix} \Psi(0)$$

This case can be separated into two situations:

  - $s = 0$, i.e. $\operatorname{rank}(A) = 1$
    It represents the scale invariant interaction, cf. Section 2.3.

  - $s \neq 0$, i.e. $\operatorname{rank}(A) = 2$
    We note at first that the special case $t = 1$ corresponds to the δ-interaction with parameter s (cf. Sect. 2.3). For a general value of t, the substitution of the matrices A and B into (4.2) leads to the following formula for the transmission amplitude,
$$\mathcal{T}_{12}(k) = \frac{2kt}{k(1 + |t|^2) + \mathrm{i}s},$$
    showing the low wave number blockade ($\mathcal{T}_{12}(0) = 0$) and asymptotically constant high wave number transparency ($\mathcal{T}_{12}(+\infty) = \frac{2t}{1+|t|^2}$), which becomes the perfect transparency $\mathcal{T}_{12}(+\infty) = 1$ for $t = 1$. We conclude that the coupling corresponding to $\operatorname{rank}(B) = 1$ can be viewed as a combination of δ and scale invariant interactions.

- $\operatorname{rank}(B) = 2$

The ST-form gives $B = I$, $A = -S$, hence

$$\Psi'(0) = \begin{pmatrix} s_{11} & s_{12} \\ \overline{s_{12}} & s_{22} \end{pmatrix} \Psi(0)\,.$$

We divide the explanation into three situations according to $\operatorname{rank}(A)$ $(= \operatorname{rank}(S))$.

  - $\operatorname{rank}(A) = \operatorname{rank}(S) = 0$, i.e. $S = 0$
    We get $\Psi'(0) = 0$, which represents disjoint Neumann boundaries $\psi_1'(0_+) = \psi_2'(0_+) = 0$.

  - $\operatorname{rank}(A) = \operatorname{rank}(S) = 1$, i.e. S is a singular nonzero matrix.
    In this case it is convenient to employ the reverse ST-form,
$$\begin{pmatrix} \tilde{s} & 0 \\ -\overline{\tilde{t}} & 1 \end{pmatrix} \Psi'(0) = \begin{pmatrix} 1 & \tilde{t} \\ 0 & 0 \end{pmatrix} \Psi(0)\,,$$
    whence we see immediately that $\tilde{t} = 1$ represents the δ'-interaction. Generally, the transmission amplitude is given by
$$\mathcal{T}_{12}(k) = \frac{-2\tilde{t}}{\big(1 + |\tilde{t}|^2\big) - \mathrm{i}k\tilde{s}},$$
    which shows both the high wave number blockade, $\mathcal{T}_{12}(+\infty) = 0$, and low wave number pass filtering behavior, $\mathcal{T}_{12}(0) = \frac{-2\tilde{t}}{1+|\tilde{t}|^2}$. Therefore this case can be viewed as the δ'-interaction amended by the scale invariant interaction.

- $\operatorname{rank}(A) = \operatorname{rank}(S) = 2$, i.e. S is regular.
  The transmission amplitude is here given by

$$\mathcal{T}_{12}(k) = \frac{2ks_{12}}{\mathrm{i}k^2 - k\,\mathrm{tr}[S] - \mathrm{i}\det[S]}$$

  and shows both low-wave number and high-wave number blockade: $\mathcal{T}_{12}(0) = 0$, $\mathcal{T}_{12}(+\infty) = 0$. This indicates a combinations of δ and δ' interactions.

In summary, the ranks of the matrices B and A are the determining factors of physical contents of the point interactions.

4.3 The case $n = 3$ ("Y-junction")

We now examine the quantum Y-junction, namely, the singular vertex of degree $n = 3$. We will again express the transmission amplitudes between each two lines outgoing from the vertex in terms of the parameters involved in the ST-form or the reverse ST-form.

We start with an explanation of *"pure δ-like"* and *"pure δ'-like"* connection between two lines coupled in a vertex. In idealized limit, two lines i and j are identified as having "pure δ-like" connections when we have

$$\mathcal{T}_{ij}(0) = 0, \quad \text{and} \quad \mathcal{T}_{ij}(+\infty) \in \mathbb{C}\,;$$

conversely, i and j are identified as "pure δ'-like" if we have

$$\mathcal{T}_{ij}(0) \in \mathbb{C}, \quad \text{and} \quad \mathcal{T}_{ij}(+\infty) = 0\,.$$

However, since the quantum flux can circumvent direct blocking between i and j through indirect path $i \to k \to j$, strict conditions $\mathcal{T}_{ij}(0) = 0$ for δ-like and $\mathcal{T}_{ij}(+\infty) = 0$ for δ'-like connection are to be breached when other types of connections are present among other lines, and therefore, zeros for $\mathcal{T}_{ij}$ need to be replaced by *small* numbers, $\mathcal{T}_{ij} \approx 0$ in above conditions. General characterization of pure δ-like connection as high-pass frequency filter and pure δ'-like connection as low-pass filter is still valid.

As in the case of $n = 2$, the boundary conditions are classified according to the values of $\operatorname{rank}(B)$ and $\operatorname{rank}(A)$. We will present the main results of Appendix C, Section 4, where the full study can be found, i.e. the classification, expressions for transmission and reflexion amplitudes, graphs illustrating squared absolute values of the amplitudes in dependence on k, as well as expository remarks.

- $\operatorname{rank}(B) = 0$

In the ST-form we have $A = -I$, hence

$$0 = \Psi(0)\,.$$

This case corresponds to disconnected Dirichlet boundaries $\psi_1(0_+) = \psi_2(0_+) = \psi_3(0_+) = 0$.

- $\operatorname{rank}(B) = 1$

$$\begin{pmatrix} 1 & t_2 & t_3 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \Psi'(0) = \begin{pmatrix} s & 0 & 0 \\ -\overline{t_2} & 1 & 0 \\ -\overline{t_3} & 0 & 1 \end{pmatrix} \Psi(0)$$

It holds $\operatorname{rank}(A) = \operatorname{rank}(S) + 2$, thus there are two possible values of $\operatorname{rank}(A)$, namely 2 and 3.

  - $\operatorname{rank}(A) = 2$, i.e. $\operatorname{rank}(S) = 0$
    Since $S = 0$, this case represents the scale invariant coupling (cf. Section 2.3).
  - $\operatorname{rank}(A) = 3$, i.e. $\operatorname{rank}(S) = 1$
    - The special situation $T = (1\ 1)$ corresponds to the δ-coupling.
    - For a general T, the transmission coefficients, given by

$$\begin{aligned} \mathcal{T}_{31}(k) &= \frac{2\overline{t_3}k}{\mathrm{i}s + (1 + |t_2|^2 + |t_3|^2)k}\,, \\ \mathcal{T}_{12}(k) &= \frac{2t_2k}{\mathrm{i}s + (1 + |t_2|^2 + |t_3|^2)k}\,, \\ \mathcal{T}_{23}(k) &= \frac{2\overline{t_2}t_3k}{\mathrm{i}s + (1 + |t_2|^2 + |t_3|^2)k}\,, \end{aligned}$$

      show the high wave number pass filtering behaviour

$$\mathcal{T}_{ij}(0) = 0, \quad \mathcal{T}_{ij}(+\infty) \in \mathbb{C}\,,$$

      which is a hallmark of pure δ connections between all branches (see Fig. 4.1).

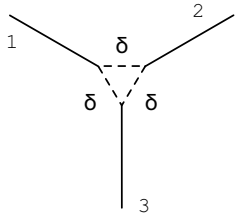

Figure 4.1: Pure δ type connection between all lines, obtained from the ST-form with $\operatorname{rank}(B) = 1$ and $\operatorname{rank}(A) = 3$.

- $\operatorname{rank}(B) = 2$

We have $\operatorname{rank}(A) = \operatorname{rank}(S) + 1$ and three possible values of $\operatorname{rank}(A)$.

  - $\operatorname{rank}(A) = 1$, i.e. $\operatorname{rank}(S) = 0$
    This situation represents a scale invariant interaction between the lines 1–3 and a scale invariant interaction between the lines 2–3.

- $\mathrm{rank}(A) = 2$, i.e. $\mathrm{rank}(S) = 1$
  This case is of special interest. It can be shown, cf. Appendix C, Sect. 4.3.2, that the proper choice of parameters enables one to construct the following two types of junctions:
  - a junction with pure δ-like connections between the lines $3-1$ and between $2-3$, and a pure δ'-like connection between the lines $1-2$ (see Fig. 4.2, left),
  - a junction with pure δ'-like connections between the lines $1-2$ and between $2-3$, and a pure δ-like connection between lines the $3-1$ (see Fig. 4.2, right).

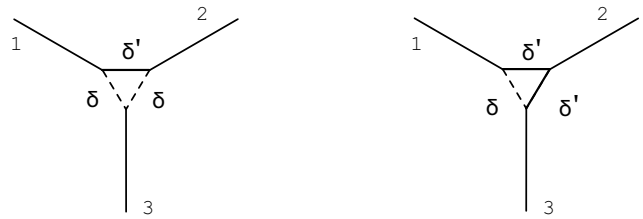

Figure 4.2: Mixed type vertex coupling obtained from the ST-form with $\mathrm{rank}(B) = 2$ and $\mathrm{rank}(A) = 2$: connections δ–δ–δ' (left) and δ'–δ'–δ (right).

We refer also to Appendix C, Figs. 4 and 5, where the transmission and reflexion amplitudes are plotted in a concrete setting. The graphs clearly illustrate the filtering behaviour of both the connections δ–δ–δ' and δ'–δ'–δ.

Other facts concerning the case $\mathrm{rank}(B) = 2 = \mathrm{rank}(A) = 2$ can be found in Appendix C. Generally speaking, it represents a mixture of δ and δ' connections, and the two pure connections $\delta - \delta - \delta'$ and $\delta' - \delta' - \delta$ described above are its limiting cases.

- $\mathrm{rank}(A) = 3$, i.e. $\mathrm{rank}(S) = 2$
  This case corresponds to a general combination of δ and δ' interactions between each two half lines. If $T = (t_1\ t_2)^T$ denotes the matrix $T \in \mathbb{C}^{2,1}$ occuring in the ST-form, it can be shown that

$$\mathcal{T}_{ij}(0) = 0 \quad \text{for all } i \text{ and } j\,,$$
$$\mathcal{T}_{31}(+\infty) \propto \overline{t_1}\,, \quad \mathcal{T}_{12}(+\infty) \propto \overline{t_2} t_1\,, \quad \mathcal{T}_{23}(+\infty) \propto t_2\,.$$

  We observe the zero energy blockade $\mathcal{T}_{ij}(0) = 0$ for all i and j which guarantees the presence of a δ-like connection between all the lines. The high energy blockade $\mathcal{T}_{ij}(+\infty) = 0$, determining the presence or absence of a δ'-like component, is controlled by the elements of T.

- $\mathrm{rank}(B) = 3$

We have $B = I$, $A = -S$ and the ST-form $\Psi'(0) = S\Psi(0)$. There are four possible values of $\mathrm{rank}(A)$ $(= \mathrm{rank}(S))$:

- $\mathrm{rank}(A) = \mathrm{rank}(S) = 0$, i.e. $S = 0$
  This situation corresponds to disjoint Neumann condition $\varphi_1'(0_+) = \varphi_2'(0_+) = \varphi_3'(0_+) = 0$.

- $\mathrm{rank}(A) = \mathrm{rank}(S) = 1$
  It is useful to rewrite the boundary conditions in the reverse ST-form

$$\begin{pmatrix} \tilde{s} & 0 & 0 \\ -\overline{\tilde{t}_2} & 1 & 0 \\ -\overline{\tilde{t}_3} & 0 & 1 \end{pmatrix} \Psi'(0) = \begin{pmatrix} 1 & \tilde{t}_2 & \tilde{t}_3 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \Psi(0)\,;$$

  the transmission amplitudes are then given by

$$\mathcal{T}_{31}(k) = \frac{-2\overline{\tilde{t}_3}}{-\mathrm{i}\tilde{s}k + (1 + |\tilde{t}_2|^2 + |\tilde{t}_3|^2)}\,,$$
$$\mathcal{T}_{12}(k) = \frac{-2\tilde{t}_2}{-\mathrm{i}\tilde{s}k + (1 + |\tilde{t}_2|^2 + |\tilde{t}_3|^2)}\,,$$
$$\mathcal{T}_{23}(k) = \frac{-2\overline{\tilde{t}_2}\tilde{t}_3}{-\mathrm{i}\tilde{s}k + (1 + |\tilde{t}_2|^2 + |\tilde{t}_3|^2)}$$

  and satisfy $\mathcal{T}_{ij}(+\infty) = 0$ and $\mathcal{T}_{ij}(0) \in \mathbb{C}$. The special choice $T = (\tilde{t}_2\ \tilde{t}_3) = (1\ 1)$ leads to the δ_s'-coupling (cf. Sect. 2.3), for a general T we get the δ_s'-coupling mixed with the scale invariang coupling. See Fig. 4.3.

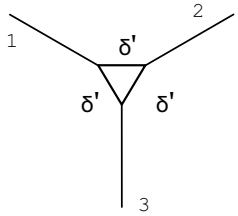

Figure 4.3: Pure δ' type connection between all lines, obtained from the ST-form with $\mathrm{rank}(B) = 3$ and $\mathrm{rank}(A) = 1$.

- $\mathrm{rank}(A) = \mathrm{rank}(S) = 2$
  The calculation again simplifies when the reverse ST-form is used; we skip technical details, since they are similar to the previous cases and can be found in Section 4.4.3 of Appendix C. This situation is dual to the one of $\mathrm{rank}(B) = 2$, $\mathrm{rank}(A) = 3$: the transmission amplitudes now satisfy

$$\mathcal{T}_{ij}(+\infty) = 0 \quad \text{for all } i \text{ and } j\,,$$
$$\mathcal{T}_{31}(0) \propto \overline{\tilde{t}_1}\,, \quad \mathcal{T}_{12}(0) \propto \overline{\tilde{t}_2}\tilde{t}_1\,, \quad \mathcal{T}_{23}(0) \propto \tilde{t}_2\,,$$

  where $(\tilde{t}_1\ \tilde{t}_2)^T$ is the matrix $\tilde{T}$ from the reverse ST-form. The transmission amplitudes show the high energy blockade $\mathcal{T}_{ij}(+\infty) = 0$ for all i and j, guaranteeing the presence of δ'-like connection between all lines. The zero energy expressions $\mathcal{T}_{ij}(0)$ are proportional to $\tilde{t}_1$ and $\tilde{t}_2$, i.e. the presence or absence of the δ-like component is controlled by the parameters of the coupling.

- $\mathrm{rank}(A) = \mathrm{rank}(S) = 3$
  When the ranks of the matrices A and B are both equal to $n = 3$, we have the generic connection condition for a quantum particle residing on joint three lines, namely the combinations of δ and δ' interactions.
  The transmission amplitudes are given by

$$\mathcal{T}_{ij}(k) = \frac{-2\mathrm{i}k^2 s_{ij} + 2k\det[\mathcal{S}(j,i)]}{k^3 + \mathrm{i}k^2\mathrm{tr}[S] - k\sum_{i=1}^{3}\det[\mathcal{S}(i,i)] - \mathrm{i}\det[S]}\,, \quad i,j \in \hat{3}\,,\ i \neq j\,,$$

  hence $\mathcal{T}_{ij}(0) = \mathcal{T}_{ij}(+\infty) = 0$ for all $i \neq j$. This signifies the guaranteed presence of both δ-like and δ'-like components in all connections.

  This expression, along with the analogous expression for $n = \mathrm{rank}(A) = \mathrm{rank}(B) = 2$ case, invites an easy straightforward extension to general n.

4.4 Summary

Our main finding is the fact that in a quantum Y-junction the couplings between each pair of outgoing lines are individually tunable. The ST-form of vertex boundary condition is found to be instrumental in identifying the type of coupling between each two outgoing lines. The ranks of matrices A and B represent crucial quantities to identify the physics of singular vertex.

Specifically, the pure δ-type coupling is constructed from $\mathrm{rank}(B) = 1$ boundary condition, while the pure δ'-type coupling is constructed from $\mathrm{rank}(A) = 1$.

Boundary conditions corresponding to $\mathrm{rank}(A) = \mathrm{rank}(B) = 2$ include both δ–δ–δ' type and δ'–δ'–δ type singular connections as limiting cases for a proper choice of parameter values. These types of singular vertices enable spectral filtering of quantum waves.

The treatment can be extended to quantum singular vertex of degrees $n \geq 4$ once the need of detail analysis is required as a model of quantum single electron devices. We hope that this work will become a stepping stone for such extensions. Obviously, the experimental realization and demonstration with quantum wires and quantum dots are highly desired. For that purpose, a construction of a real-world approximation of singular vertices, which has been examined also in the previous chapter, will become crucial.

Chapter 5

Spectrum of a bent chain graph

One of the frequent questions in the theory of quantum graphs concerns relations between the geometry of a graph Γ and spectral properties of a Schrödinger operator supported by Γ. Put like that, the question allows different interpretations. On one hand, we can have in mind the intrinsic geometry of Γ which enters the problem through the adjacency matrix of the graph and the lengths of its edges. On the other hand, quite often one thinks of Γ as of a subset of $\mathbb{R}^n$ with the geometry inherited from the ambient space. In that case geometric perturbations can acquire a rather illustrative meaning and one can ask in which way they influence spectral properties of a quantum particle "living" on Γ; in this context one can think of graphs which are "bent", locally "protruded" or "squeezed", etc.

The aim of this chapter is to analyze the influence of a "bending" deformation on a graph which exhibits a one-dimensional periodicity. Without striving for generality we will discuss in detail a simple nontrivial example in which the unperturbed system is a "chain graph" consisting of an array of rings of the same radius, cf. Fig. 5.1, connected through their touching points. We suppose that there is δ-coupling in the

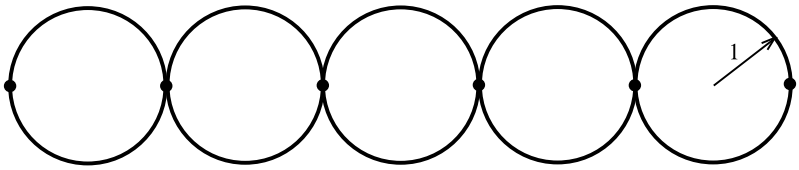

Figure 5.1: The unperturbed chain graph

vertices, let us recall that it is characterized by the conditions

$$\psi_j(0) = \psi_k(0) =: \psi(0)\,, \quad j,k \in \hat{n}\,, \qquad \sum_{j=1}^{n} \psi_j'(0) = \alpha\psi(0)\,, \tag{5.1}$$

cf. (1.5), where $\hat{n} = \{1, 2, \ldots, n\}$ is the index set numbering the edges emanating from the vertex and $\alpha \in \mathbb{R}$ is the coupling constant which is supposed to be the same at every vertex of the chain. In our case it holds $n = 4$.

The geometric perturbation to consider is the simplest possible bending of such a chain obtained by a shift of one of the contact points, as sketched in Fig. 5.2, which is parametrized by the bending angle ϑ characterizing the ratio of the two edges constituting the perturbed ring. Our aim is to show that the bending gives

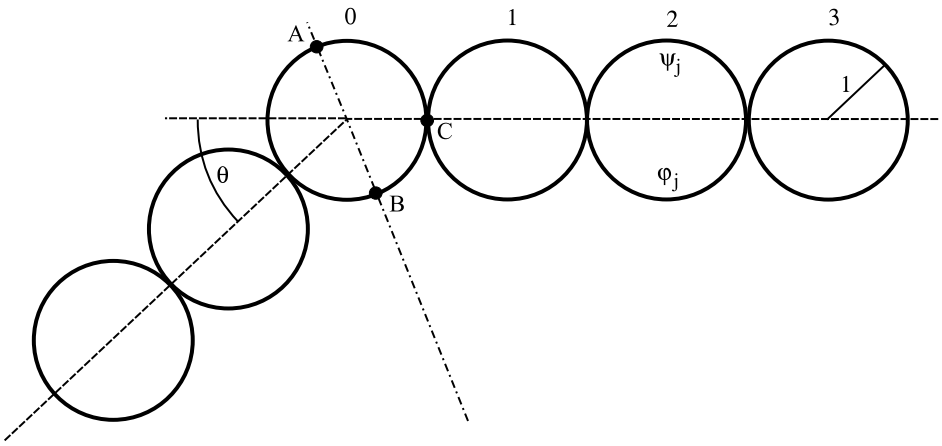

Figure 5.2: A bent graph

rise to eigenvalues in the gaps of the unperturbed spectrum and to analyze how they depend on ϑ. At the same time the bent chain will exhibit resonances and we will discuss behaviour of the corresponding poles.

5.1 An infinite periodic chain

We begin with the analysis of the straight chain. Consider a periodic graph Γ_0 as sketched in Fig. 5.1; without loss of generality we may suppose that the circumference of each ring is 2π. The state Hilbert space of a nonrelativistic and spinless particle living on Γ_0 is $L^2(\Gamma_0)$. We suppose that the particle is free, i.e. its Hamiltonian, denoted by H_0, acts as the negative Laplacian on each graph link, $\psi_j \mapsto -\psi_j''$, and its domain consists of all functions from $W^{2,2}_{\mathrm{loc}}(\Gamma_0)$ which satisfy the boundary conditions (5.1) at the vertices of Γ_0.

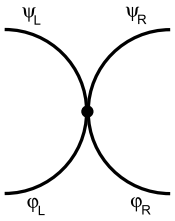

Figure 5.3: Elementary cell of the periodic system

In view of the periodicity of Γ_0 (the elementary cell is depicted in the Fig. 5.3), we find the spectral bands of H_0 using Bloch-Floquet decomposition. The result is formulated in the following theorem.

Theorem 5.1.1. *The spectrum of H_0 consists of infinitely degenerate eigenvalues equal to n^2 with $n \in \mathbb{N}$, and absolutely continuous spectral bands with the following properties:*

If $\alpha > 0$, then every spectral band is contained in an interval $(n^2, (n+1)^2]$ with $n \in \mathbb{N}$. Its upper edge coincides with the value $(n+1)^2$, the lower one with the squared solution of

$$\left| \cos k\pi + \frac{\alpha}{4} \cdot \frac{\sin k\pi}{k} \right| = 1 \quad \wedge \quad k \in (n, n+1)\,. \tag{5.2}$$

If $\alpha < 0$, then in each interval $[n^2, (n+1)^2)$ with $n \in \mathbb{N}$ there is exactly one spectral band the lower edge of which coincides with n^2, the upper one with the squared solution of (5.2). In addition, there is a spectral band with the lower edge (being the overall spectral threshold) equal to $-\kappa^2$, where κ is the largest solution of

$$\left| \cosh \kappa\pi + \frac{\alpha}{4} \cdot \frac{\sinh \kappa\pi}{\kappa} \right| = 1\,. \tag{5.3}$$

The position of the upper edge of this band depends on α. If $-8/\pi < \alpha < 0$, then it is equal to k^2, where k is the solution of

$$\cos k\pi + \frac{\alpha}{4} \cdot \frac{\sin k\pi}{k} = -1$$

contained in $(0,1)$. On the other hand, for $\alpha < -8/\pi$ the upper edge is negative, equal to $-\kappa^2$ with κ being the smallest solution of (5.3). For $\alpha = -8/\pi$ it equals zero.

Finally, in the case $\alpha = 0$ it holds $\sigma(H_0) = [0, +\infty)$.

Proof. Cf. Appendix D, Theorem 2.4. □

We remark that the Bloch-Floquet decomposition does not work in the situation $k \in \mathbb{N}$, but it is straightforward to check that k^2 is then an eigenvalue, and moreover, that it has infinite multiplicity. One can construct an eigenfunction which is supported by a single circle, namely $\psi(x) = \sin kx$ with $x \in [0, \pi]$ on the upper semicircle and $\varphi(x) = -\sin kx$ with $x \in [0, \pi]$ on the lower one.

Remark 5.1.2. The condition (5.2) reminds us of the corresponding condition in the Kronig-Penney model with the distance between the interaction sites equal to π, cf. [AGHH05], the only difference being that the coupling constant is halved, $\frac{\alpha}{2}$ instead of α. In contrast to that, the point spectrum of the KP model is empty. These facts are easy to understand if we realize that our model has the up-down mirror symmetry, and thus H_0 decomposes into a symmetric and antisymmetric part. The former is unitarily equivalent to the KP model with modified coupling, the latter corresponds to functions vanishing at the vertices, having thus a pure point spectrum. Looking ahead, we remark that the bending perturbation breaks this mirror symmetry.

5.2 Perturbed system and its spectrum

In this section we will analyze the discrete spectrum due to a local perturbation. Let us suppose that the straight chain of the previous section suffers a bending perturbation as shown in Figure 5.2. We call the perturbed graph Γ_ϑ; it differs from Γ_0 by replacing the arc lengths π of a fixed ring, conventionally numbered as zero, by $\pi \pm \vartheta$. The bending angle ϑ is supposed to take values from $(0, \pi)$, regardless of the fact that for $\vartheta \geq 2\pi/3$ it is not possible to consider Γ_ϑ as embedded in the plane as sketched — one can certainly realize such a "bending" in an alternative way, for instance, by deforming the selected ring.

The state Hilbert space of the perturbed system is $L^2(\Gamma_\vartheta)$, and its Hamiltonian, denoted by H_ϑ, is obtained by a natural modification of H_0. To determine its spectrum, we take advantage of the mirror symmetry of Γ_ϑ – the axis of symmetry is drawn in Fig. 5.2. It justifies one to reduce the operator H_ϑ by parity subspaces into a direct sum of an even part, H^+, and odd one, H^-; for the sake of simplicity we drop the subscript ϑ.

All the components of the wave function at energy $k^2 \neq 0$ are linear combinations of $\mathrm{e}^{\pm \mathrm{i}kx}$. As we have said, we use the ring labelling with zero corresponding to the perturbed one; the mirror symmetry allows us to study a half of the system only, say, with non-negative indices. The wave function on each ring is a pair of functions ψ_j and φ_j, where j is the circle index, ψ_j corresponds to the upper semicircle and φ_j to the lower one,

$$\begin{aligned} \psi_j(x) &= C_j^+ \mathrm{e}^{\mathrm{i}kx} + C_j^- \mathrm{e}^{-\mathrm{i}kx}, \quad x \in [0, \pi]\,, \\ \varphi_j(x) &= D_j^+ \mathrm{e}^{\mathrm{i}kx} + D_j^- \mathrm{e}^{-\mathrm{i}kx}, \quad x \in [0, \pi] \end{aligned} \tag{5.4}$$

for $j \in \mathbb{N}$. The situation is different in the case $j = 0$ where the variables run over modified intervals,

$$\begin{aligned} \psi_0(x) &= C_0^+ \mathrm{e}^{\mathrm{i}kx} + C_0^- \mathrm{e}^{-\mathrm{i}kx}, \quad x \in \left[\frac{\pi - \vartheta}{2}, \pi\right], \\ \varphi_0(x) &= D_0^+ \mathrm{e}^{\mathrm{i}kx} + D_0^- \mathrm{e}^{-\mathrm{i}kx}, \quad x \in \left[\frac{\pi + \vartheta}{2}, \pi\right]. \end{aligned}$$

There are δ-couplings with the parameter α in the points of contact, i.e.

$$\psi_j(0) = \varphi_j(0)\,, \qquad \psi_j(\pi) = \varphi_j(\pi) \tag{5.5}$$

and

$$\psi_j(0) = \psi_{j-1}(\pi)\,, \tag{5.6}$$

$$\psi_j'(0) + \varphi_j'(0) - \psi_{j-1}'(\pi) - \varphi_{j-1}'(\pi) = \alpha \cdot \psi_j(0)\,. \tag{5.7}$$

Substituting (5.4) into (5.5) we obtain

$$C_j^+ \cdot \sin k\pi = D_j^+ \cdot \sin k\pi \quad \text{and} \quad C_j^- \cdot \sin k\pi = D_j^- \cdot \sin k\pi\,,$$

thus for $k \notin \mathbb{N}$ we have $C_j^+ = D_j^+$ and $C_j^- = D_j^-$. As for the case $k \in \mathbb{N}$, it is easy to see that squares of integers are infinitely degenerate eigenvalues and the

eigenfunctions can be supported by any ring with the exception of the zeroth one, cf. also the previous section. From now on, we suppose $k \notin \mathbb{N}$.

Using the coupling conditions (5.6) and (5.7), we arrive at a "transfer matrix" relation between coefficients of the neighbouring rings,

$$\begin{pmatrix} C_j^+ \\ C_j^- \end{pmatrix} = \underbrace{\begin{pmatrix} \left(1+\frac{\alpha}{4\mathrm{i}k}\right)\mathrm{e}^{\mathrm{i}k\pi} & \frac{\alpha}{4\mathrm{i}k}\mathrm{e}^{-\mathrm{i}k\pi} \\ -\frac{\alpha}{4\mathrm{i}k}\mathrm{e}^{\mathrm{i}k\pi} & \left(1-\frac{\alpha}{4\mathrm{i}k}\right)\mathrm{e}^{-\mathrm{i}k\pi} \end{pmatrix}}_{M} \cdot \begin{pmatrix} C_{j-1}^+ \\ C_{j-1}^- \end{pmatrix}, \tag{5.8}$$

valid for all $j \geq 2$. Of course, the matrix M depends on α and k.

So far we have excluded $k = 0$. In this case the expressions for the wave function components are of the type $C_j^+ \cdot x + C_j^- \cdot 1$, and in the same way as above we find the matrix M corresponding to $k = 0$:

$$M = \begin{pmatrix} 1+\frac{\alpha\pi}{2} & \frac{\alpha}{2} \\ \pi & 1 \end{pmatrix}.$$

For any $k^2 \notin \mathbb{N}^2$, we can express the coefficients C_j^+, C_j^- for every $j \in \mathbb{N}$:

$$\begin{pmatrix} C_j^+ \\ C_j^- \end{pmatrix} = M^{j-1} \cdot \begin{pmatrix} C_1^+ \\ C_1^- \end{pmatrix}. \tag{5.9}$$

It is an important fact that $\det(M) = 1$ – it implies that the eigenvalues of M, denoted by λ_1, λ_2, conform to exactly one of the following three cases:

(i) $\lambda_1, \lambda_2 \in \mathbb{R}$, $\quad |\lambda_1| > 1 > |\lambda_2| \quad$ (or $|\lambda_2| > 1 > |\lambda_1|$),

(ii) $\lambda_1 = \lambda_2 = \pm 1$,

(iii) $\lambda_1, \lambda_2 \in \mathbb{C}\backslash\mathbb{R}$, $\quad |\lambda_1| = |\lambda_2| = 1$.

Note that if $p_M(\lambda) = 0$ is the characteristic equation of M, the value of its discriminant $D_\alpha(k)$ (which depends on both α and k) distinguishes the situations *(i)*-*(iii)*: *(i)* corresponds to $D_\alpha(k) > 0$, *(ii)* to $D_\alpha(k) = 0$, *(iii)* to $D_\alpha(k) < 0$.

We bear in mind that the wave function components on the j-th ring for both $H^\pm$, as well as on the $(-j)$-th by the mirror symmetry, are determined by C_j^+ and C_j^-, and thus by C_1^+, C_1^- by virtue of (5.9).

Now the key idea comes. Suppose that $(C_1^+, C_1^-)^T$ is an eigenvector of M corresponding to an eigenvalue λ. Then:

$$\begin{aligned} |\mu| < 1 \quad &\Rightarrow \quad \left\|(C_j^+, C_j^-)^T\right\| \text{ decays exponentially with respect to } j, \\ |\mu| > 1 \quad &\Rightarrow \quad \left\|(C_j^+, C_j^-)^T\right\| \text{ grows exponentially with respect to } j, \\ |\mu| = 1 \quad &\Rightarrow \quad \left\|(C_j^+, C_j^-)^T\right\| \text{ is independent of } j. \end{aligned}$$

Hence we immediately conclude:

- If $(C_1^+, C_1^-)^T$ has a non-vanishing component related to an eigenvalue of M of modulus larger than one, it determines neither an eigenfunction, nor a generalized eigenfunction of $H^\pm$.

- If $(C_1^+, C_1^-)^T$ is an eigenvector of the matrix M with modulus less than one, then this vector, together with (5.9) and (5.6), determines an eigenfunction and the corresponding energy k^2 belongs to the point spectrum of the operator $H^\pm$.

- If $(C_1^+, C_1^-)^T$ is a linear combination of eigenvectors of M with moduli equal to one, then this vector determines a generalized eigenfunction and the corresponding energy k^2 belongs to the continuous spectrum of $H^\pm$.

Next steps are now obvious. To examine the *eigenvalues* of $H^\pm$ for a fixed α, we

1. use the boundary conditions determining H^+ and H^- to compute $(C_1^+, C_1^-)^T$,
2. examine the range of k's, for which it holds $D_\alpha(k) > 0$,
3. for such k compute $v_\alpha(k)$ - the eigenvector of M corresponding to the eigenvalue of modulus less than one,
4. find k for which the vectors $v_\alpha(k)$ and $(C_1^+, C_1^-)^T$ are linearly dependent.

The study of *continuous spectrum* of $H^\pm$ is much simpler, it suffices to determine k satisfying $D_\alpha(k) \leq 0$. Performing that, one find that the perturbation does not affect the spectral bands, which is, of course, obvious from general principles: Using the natural identification of $L^2(\Gamma_0)$ and $L^2(\Gamma_\vartheta)$ we see that H_0 and H_ϑ differ by a shift of the point where a boundary condition is applied, hence their resolvent difference has a finite rank (in fact, rank two). Consequently, their essential spectra coincide and each spectral gap of H_0 contains at most two eigenvalues of H_ϑ, see [We80, Sec. 8.3, Cor. 1].

Following the way described above, one arrives at the spectral conditions (k, κ are positive numbers):

$$k^2 \in \sigma_{\mathrm{p}}(H^+) \quad \Leftrightarrow$$

$$\cos k\vartheta = -\cos k\pi + \frac{\sin^2 k\pi}{\frac{\alpha}{4k}\sin k\pi \pm \sqrt{\left(\cos k\pi + \frac{\alpha}{4k}\sin k\pi\right)^2 - 1}}\,, \quad (5.10)$$

$$-\kappa^2 \in \sigma_{\mathrm{p}}(H^+) \quad \Leftrightarrow$$

$$\cosh \kappa\vartheta = -\cosh \kappa\pi - \frac{\sinh^2 \kappa\pi}{\frac{\alpha}{4\kappa}\sinh \kappa\pi \pm \sqrt{\left(\cosh \kappa\pi + \frac{\alpha}{4\kappa}\sinh \kappa\pi\right)^2 - 1}}\,, \quad (5.11)$$

$$k^2 \in \sigma_{\mathrm{p}}(H^-) \quad \Leftrightarrow$$

$$-\cos k\vartheta = -\cos k\pi + \frac{\sin^2 k\pi}{\frac{\alpha}{4k}\sin k\pi \pm \sqrt{\left(\cos k\pi + \frac{\alpha}{4k}\sin k\pi\right)^2 - 1}}\,, \quad (5.12)$$

$$-\kappa^2 \in \sigma_{\mathrm{p}}(H^-) \quad \Leftrightarrow$$

$$-\cosh\kappa\vartheta = -\cosh\kappa\pi - \frac{\sinh^2\kappa\pi}{\frac{\alpha}{4\kappa}\sinh\kappa\pi \pm \sqrt{\left(\cosh\kappa\pi + \frac{\alpha}{4\kappa}\sinh\kappa\pi\right)^2 - 1}} \tag{5.13}$$

with the signs in the denominators given by the signs of $\cos k\pi + \frac{\alpha}{4k}\sin k\pi$ and $\cosh\kappa\pi + \frac{\alpha}{4\kappa}\sinh\kappa\pi$, respectively. Note that the conditions (5.11) and (5.13) are obtained by substituting $k = \mathrm{i}\kappa$ into (5.10) and (5.12), respectively.

Conditions (5.10)–(5.13) provide a characterization of $\sigma_{\mathrm{p}}(H^+)$ and $\sigma_{\mathrm{p}}(H^-)$ which we formulate in two theorems below. We use the symbol G_n denoting the spectral gap adjacent to n^2, $n \in \mathbb{N}$; the exceptional case is $n = 1$ if $\alpha > 0$: since for $\alpha > 0$ there are two gaps adjacent to 1, we specify that G_1 denotes the gap *above* 1.

Proposition 5.2.1.

- *Let $n \in \mathbb{N}$. H^+ has at least one eigenvalue in G_n except for the case when ϑ satisfies $\cos n\vartheta = (-1)^{n-1}$, or equivalently, except for the angles $\vartheta = \frac{n+1-2\ell}{n}\pi$, $\ell = 1, \ldots, \lfloor\frac{n+1}{2}\rfloor$.*
- *If $\alpha \geq 0$, H^+ has no negative eigenvalues.*
- *If $\alpha < 0$, H^+ has at least one negative eigenvalue which lies under the lowest spectral band and above the number $-\kappa_0^2$, where κ_0 is the (unique) solution of $\kappa \cdot \tanh\kappa\pi = -\alpha/2$.*

Proposition 5.2.2.

- *Let $n \in \mathbb{N}$. H^- has at least one eigenvalue in G_n except for the case when $\vartheta = \frac{n-2\ell}{n}\pi$, $\ell = 0, \ldots, \lfloor\frac{n}{2}\rfloor$.*
- *If $\alpha \geq 0$, H^- has no negative eigenvalues.*

Both statements are derived in Appendix D.

Remark 5.2.3. The eigenvalues of H^+ and H^- may coincide and in this case they become a single eigenvalue of multiplicity two. It happens for the eigenvalues k^2 such that

$$k \cdot \tan k\pi = \frac{\alpha}{2}\,.$$

5.3 Resonances and analyticity

The added eigenvalues are not the only consequence of the chain bending. If one investigates all solutions of (5.10) and (5.12), i.e. not only the real ones corresponding to $\sigma_p(H^+)$ and $\sigma_p(H^-)$, one obtains imaginary solutions which describe *resonances* of the system. More precisely speaking, this approach leads to the *resolvent resonances*; the notion of resonances in the system can be introduced in several ways, which are, however, mutually equivalent, cf. [EL07].

We start with investigation of the analyticity of resonances and eigenvalues with respect to the bending angle ϑ. At first we rewrite the condition (5.10) as

$$\frac{\alpha}{2k}(1+\cos k\vartheta\cos k\pi)(\cos k\vartheta+\cos k\pi) = \sin k\pi\cdot(1+2\cos k\vartheta\cos k\pi+\cos^2 k\vartheta)\,; \tag{5.14}$$

it can be checked (Appendix D, Proposition 4.1) that for non-integer values of k the formulations are equivalent. Similarly, (5.12) may be rewriten as

$$\frac{\alpha}{2k}(1-\cos k\vartheta\cos k\pi)(-\cos k\vartheta+\cos k\pi)=\sin k\pi\cdot(1-2\cos k\vartheta\cos k\pi+\cos^2 k\vartheta)\,. \tag{5.15}$$

Now we can prove the analyticity of the solutions:

Proposition 5.3.1.
- *Curves given by the implicit equation* (5.14) *(corresponding to H^+) are analytic everywhere except at $(\vartheta,k)=(\frac{n+1-2\ell}{n}\pi,n)$, where $n\in\mathbb{N}$, $\ell\in\mathbb{N}$, $\ell\le\lfloor\frac{n+1}{2}\rfloor$. Moreover, the real solution in every G_n is given by a function $\vartheta\mapsto k$ which is analytic, except at the points $\frac{n+1-2\ell}{n}\pi$.*
- *Curves given by Equation* (5.15) *(corresponding to H^-) are analytic everywhere except at $(\vartheta,k)=(\frac{n-2\ell}{n}\pi,n)$, where $n\in\mathbb{N}$, $\ell\in\mathbb{N}_0$, $\ell\le\lfloor\frac{n}{2}\rfloor$. Moreover, the real solution in every G_n is given by a function $\vartheta\mapsto k$ which is analytic, except at the points $\frac{n-2\ell}{n}\pi$.*

Proof. Cf. Appendix D, Prop. 4.2. □

The numerical solution of the spectral condition for different signs of the coupling constant and the real parts of the resonances of the system are illustrated in Figs. 4–6 in Appendix D. We refer also to Fig. 7 ibidem visualizing the imaginary parts corresponding to the situation of Fig. 4.

The above results raise naturally the question about the behaviour of the curves at the singular points

$$(\vartheta,k)=\left(\frac{n+1-2\ell}{n}\pi,n\right)\quad\text{with}\quad n\in\mathbb{N},\,\ell\in\mathbb{N},\,\ell\le\left\lfloor\frac{n+1}{2}\right\rfloor,$$

corresponding to H^+, and

$$(\vartheta,k)=\left(\frac{n-2\ell}{n}\pi,n\right)\quad\text{with}\quad n\in\mathbb{N},\,\ell\in\mathbb{N}_0,\,\ell\le\left\lfloor\frac{n}{2}\right\rfloor,$$

corresponding to H^-, i.e. at the points where the curves touch the band edges and where the eigenvalues and resonances may cross. We examine the asymptotic behaviour at these points and look how many curves "stem" from them. Since the results for H^+ and H^- are similar, we will concentrate mainly on the case of H^+.

The idea consists in taking $k_0\in\mathbb{N}$ and $\vartheta_0:=\frac{n+1-2\ell}{n}\pi$ for some $\ell\in\mathbb{N}$, and substituting

$$k:=k_0+\varepsilon,\qquad \vartheta:=\vartheta_0+\delta$$

into (5.14). The theory of algebroidal functions and Newton polygon here leads to the result saying that there are exactly three types of solutions:

- $\varepsilon=\sqrt[3]{\frac{\alpha}{4}\frac{k_0}{\pi}}\delta^{4/3}$ (a real solution corresponding to the spectrum),
- $\varepsilon=\mathrm{e}^{\pm\mathrm{i}\frac{2}{3}\pi}\sqrt[3]{\frac{\alpha}{4}\frac{k_0}{\pi}}\delta^{4/3}$ (imaginary solutions corresponding to resonances).

Let us remark that since (5.14) has a symmetry with respect to the complex conjugation of k, the imaginary solutions come in pairs. This is why we find pairs of curves outside from the real plane, conventionally just one of them is associated with a resonance.

Combining this fact with the previous results, we infer that the complete graph of solutions of (5.14) has the following structure:

- It consists of curves that are analytic and not intersecting, except at the points $(\vartheta, k) = (\frac{n+1-2\ell}{n}\pi, n)$, where $n \in \mathbb{N}$, $\ell \in \mathbb{N}$, $\ell \leq \left[\frac{n+1}{2}\right]$; these are the only ramification points.
- The real curves branches join the points $(\frac{n+1-2\ell}{n}\pi, n)$ and $(\frac{n+1-2\ell-2}{n}\pi, n)$, i.e. the consecutive points on the lines $k = n \in \mathbb{N}$.
- The curves branches outside the plane $\mathrm{Im}\,(k) = 0$ join the points $(\frac{\ell}{n-\ell}\pi, n-\ell)$ and $(\frac{\ell+1}{n-\ell-1}\pi, n-\ell-1)$, i.e. the consecutive points laying on the hyperbolas $(\vartheta+\pi)\cdot k = n\cdot\pi$, $k \in \mathbb{R}$, $n \in \mathbb{N}$, n odd, cf. Fig. 7 in Appendix D.

This characterization allows one to precize the description of the point spectrum provided in Proposition 5.2.1.

Theorem 5.3.2.
- *Let $n \in \mathbb{N}$. If $\vartheta = \frac{n+1-2\ell}{n}\pi$, $\ell = 1, \ldots, \lfloor\frac{n+1}{2}\rfloor$, then the operator H^+ has no eigenvalue in G_n. Otherwise H^+ has in G_n exactly one eigenvalue of multiplicity 1.*
- *If $\alpha \geq 0$, H^+ has no negative eigenvalues.*
- *If $\alpha < 0$, H^+ has exactly one negative eigenvalue which lies under the lowest spectral band and above the number $-\kappa_0^2$, where κ_0 is the (unique) solution of $\kappa \cdot \tanh \kappa\pi = -\alpha/2$.*

The next theorem, based on Equation (5.3), characterizes the behaviour of eigenvalues in the vicinity of the singular points.

Theorem 5.3.3. *If $n \in \mathbb{N}$ and $\ell \in \mathbb{N}$ such that $\ell \leq \lfloor\frac{n+1}{2}\rfloor$, then the curve of eigenvalues of H^+ behaves in the neighbourhood of the point $(\vartheta, k) = (\frac{n+1-2\ell}{n}\pi, n)$ asymptotically as*

$$k \approx k_0 + \sqrt[3]{\frac{\alpha}{4}\frac{k_0}{\pi}}\,|\vartheta - \vartheta_0|^{4/3}\,.$$

The statement is valid for the particular case $\vartheta_0 = 0$, $k_0 \in \mathbb{N}$ as well, provided the band edge k_0 is odd.

However, H^+ has an eigenvalue near $\vartheta_0 = 0$ also in the gaps adjacent to even numbers. In these cases the curve starts at the point $(0, k_0)$ for k_0 being the solution of $|\cos k\pi + \frac{\alpha}{4k}\sin k\pi| = 1$ in $(n, n+1)$, n even, and its asymptotic behaviour of k for ϑ close to zero is different, namely:

Theorem 5.3.4. *Suppose that $n \in \mathbb{N}$ is even and k_0 is as described above, i.e. k_0^2 is the right endpoint of the spectral gap adjacent to n^2. Then the behaviour of the solution of (5.14) in the neighbourhood of $(0, k_0)$ is given by*

$$k = k_0 - C_{k_0,\alpha}\cdot\vartheta^4 + \mathcal{O}(\vartheta^5)\,,$$

where $C_{k_0,\alpha} := \frac{k_0^2}{8\pi}\cdot\left(\frac{\alpha}{4}\right)^3 (k_0\pi + \sin k_0\pi)^{-1}$.

Proof. Cf. Appendix D, Theorem 5.1. □

The analogous asymptotic behaviour applies to k^2, the energy distance of the eigenvalue from the band edge is again proportional to ϑ^4 in the leading order. Notice that this is true in any spectral gap, but of course, the error term depends in general on the gap index.

We refrain from discussing in detail the odd part H^- of the Hamiltonian. The corresponding results are practically the same, the only difference is that the roles of the even and odd gaps are interchanged. Let us directly formulate the analogy to 5.3.2:

Theorem 5.3.5.
- *Let $n \in \mathbb{N}$. If $\vartheta = \frac{n-2\ell}{n}\pi$, $\ell = 1, \ldots, \lfloor \frac{n}{2} \rfloor$, then the operator H^- has no eigenvalue in G_n. Otherwise H^- has in G_n exactly one eigenvalue of multiplicity 1. These eigenvalues are positive except the one in G_1, which may be negative if $\alpha < -8/\pi$ and θ is sufficiently small.*

- *If $\alpha \geq 0$, H^- has no negative eigenvalues.*

Most of what we have discussed above modifies easily to the case of attractive coupling with the obvious changes: for $\alpha < 0$ the spectral gaps lay now *below* the numbers n^2, $n \in \mathbb{N}$. Of particular interest is the spectral gap adjacent to the value one, because with the increase of $|\alpha|$ its lower edge moves towards zero and may become negative for $|\alpha|$ large enough. The even part H^+ has similar properties as before: the eigenvalue curve goes from $(0,1)$ to (π, k_0), where $k_0 \in (0,1)$, and there are two complex conjugated branches with $\mathrm{Re}\,(k) > 0$ one of which describes a resonance.

However, the odd part H^- requires a more detailed examination. We know that there is an eigenvalue curve going to the point $[\pi, 1]$. If the entire spectral gap is above zero, this curve joins it with $[0, k_0^2]$, where k_0^2 is the lower edge of the gap. On the other hand, if $|\alpha|$ is large enough, the eigenvalue curve starts from $[0, -\kappa_0^2]$ where $-\kappa_0^2$ is again the lower gap edge; to show that even in this case the curve joins the points $[0, -\kappa_0^2]$ and $[\pi, 1]$ analytically, it suffices to show that the solutions of (5.15) with the negative sign preserves analyticity when it crosses the line $k^2 = 0$. This statement together with a proof can be found in Appendix D. Of course, the claim can be obtained also by means of the analytic perturbation theory [Ka66].

Finally, note that by Proposition 5.3.1 the solutions of both (5.14) and (5.15) are analytic in the whole open halfplane $\mathrm{Re}\,(k) < 0$, and consequently, no resonance curves can be found there.

Remarks

- The spectral and resonance properties due geometric perturbations hold probably much more generally.

- One may interpret the chain graph alternatively as a *decoration* of a simple array-type graph. The results say that *a local modification* of the decoration can produce a discrete spectrum in the gaps and also resonances.

- There is an interesting parallel between the quantum graphs discussed here and *quantum waveguides*. Although the nature of the two systems is very different, in both there exist bound states below the essential spectrum threshold due to a local bend. Moreover, in the case of Dirichlet quantum waveguides, the binding energy for a gentle bend is proportional to the fourth power of the bending angle [DE95], i.e. has exactly the same behaviour as described by Theorem 5.3.4.
  For quantum waveguides with mixed boundary conditions it was shown [Ji06] that the effect of *binding through bending* is present for any repulsive boundary. In our case an eigenvalue below the lowest band exists whenever $\alpha \neq 0$ which inspires another look at the waveguide case. It appears that the argument of [Ji06] works again and proves the existence of curvature-induced bound states in all cases except the Neumann boundary which is an analogue of the case $\alpha = 0$ here.

Conclusion and outlook

The main outcome of the present work is an extension of the knowledge of the properties of quantum graph vertices. This was done in three areas, which we will summarize now.

Parametrization of boundary conditions

We have introduced an alternative way how the boundary conditions in quantum graph vertices may be expressed and parametrized, namely the ST-form with its reverse version, and the $PQRS$-form. Their main advantages, namely the clearness in which the parameters occur in the boundary conditions and the large number of the vanishing matrix elements, makes our parametrizations effective for many applications. The ST-form turned out to be an excellent formulation for dealing with two problem listed below, and recently we realized that the solution of another problem, namely the spectral analysis of an infinite two-dimensional lattice, also simplifies when the ST-form is employed.

Meaning of vertex couplings

Another result of the thesis shows that any singular vertex coupling can be approximated by a graph in which the vertex is replaced by a local graph structure in combination with local regular interactions and local magnetic fields. This finding not only helps to understand the meaning of vertex couplings, but also opens way to constructing "structured" vertices tailored to the desired conductivity properties, even tunable ones, if the interactions are controlled by gate electrodes.

The problem of understanding vertex couplings has one more aspect. The approximating object needs not to be a graph but can be another geometrical structure. A lot of attention was paid in the physics community to the situation of "fat graphs", or networks of this tubes built around the graph skeleton. The point is that the two approaches can be combined, for instance, by "lifting" the graph results to fat graphs. In this way approximations to δ and δ'_{s} couplings by suitable families of Schrödinger operators on such manifolds with Neumann boundaries were recently demonstrated in [EP08]. The results of this paper can be similarly "lifted" to manifolds; that will be the subject of a subsequent work.

Properties of quantum branchings

> We have studied the scattering at singular vertices of degree 2 (an interaction on the line), and especially 3 (the Y-junction). The classification that we have obtained using the ST-form helps to understand physical properties of quantum graph vertices. We have also shown that the couplings between each pair of outgoing lines of the Y-junction are individually tunable, which de facto enables a design of quantum spectral branch-filters. In this work we were concerned in the case $n \leq 3$ only, where n denotes the degree of the vertex, however, our approach is applicable to vertices of higher degrees once the need arises.

The last result is related to the theory of *periodic graphs with locally compact perturbations*:

We have examined an example of a bent infinite chain and provided a detailed description of its spectrum and resonances in dependence on the bending angle. Among others we have found that the perturbation produces eigenvalues in a way surprisingly similar to bent waveguides, which are systems of a very different nature. This result supports the presumption that there are deep connections between quantum graphs and more-dimensional systems, so far hidden and waiting for their discovery. Quantum graphs might then become also an efficient "laboratory" in which properties of other, more complex structures are investigated. This would yet more raise their applicability.

List of symbols

$\mathbb{R}$	...	set of real numbers
$\mathbb{R}^+$, $\mathbb{R}^-$	...	set of positive numbers, set of negative numbers
$\mathbb{R}_0^+$	...	set of non-negative numbers
$\mathbb{C}$	...	set of complex numbers
$\mathbb{C}^{k,l}$	...	set of complex matrices with k rows and l columns
$\mathbb{N}$, $\mathbb{N}_0$	...	set of positive integers, set of non-negative integers
$\hat{n}$	...	set $\{1, 2, \ldots, n\}$
$\mathrm{Re}\, x$, $\mathrm{Im}\, x$	...	real part of the number x, imaginary part of x
x_j	...	j-th component of the vector x
a_{ij}	...	(i,j)-th element of the matrix A
A_{ij}	...	(i,j)-th block of the matrix A or (i,j)-th element of A
$A(i,j)$	...	i,j-minor of the square matrix A
A^T	...	transpose of the matrix A
A^*	...	conjugate transpose of the matrix A
$A_{i\bullet}$, $A_{\bullet j}$	...	i-th row of the matrix A, j-th column of A
$\mathrm{rank}(A)$	...	rank of the matrix A
$\mathrm{diag}\,(a_1, \ldots, a_n)$	...	diagonal matrix with the diagonal elements $a_1, \ldots, a_n$
$\mathrm{U}(n)$	...	unitary group of the degree n
$f(x_+)$	...	right-sided limit of the function f at the point x (similarly $f(x_-)$ - left-sided limit)
$\mathcal{H}$	...	a Hilbert space
$(f,g)_{\mathcal{H}}$	...	scalar product of f, g in the space $\mathcal{H}$
$L^2(M)$	...	Hilbert space of square-integrable functions on a set M with respect to the Lebesgue measure on M
$\|f\|$	...	Hilbert space norm of f
$\|f\|_2$	...	Hilbert-Schmidt norm of f
$R_H(k)$	...	resolvent of the operator H at the point k
$\sigma(H)$	...	spectrum of the operator H
$\sigma_{\mathrm{p}}(H)$	...	point spectrum of the operator H

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Part II

APPENDICES

Appendix A

Approximation of a general singular vertex coupling in quantum graphs

Approximation of a general singular vertex coupling in quantum graphs

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Abstract

The longstanding open problem of approximating all singular vertex couplings in a quantum graph is solved. We present a construction in which the edges are decoupled; an each pair of their endpoints is joined by an edge carrying a δ potential and a vector potential coupled to the "loose" edges by a δ coupling. It is shown that if the lengths of the connecting edges shrink to zero and the potentials are properly scaled, the limit can yield any prescribed singular vertex coupling, and moreover, that such an approximation converges in the norm-resolvent sense.

Key words: singular quantum interaction, solvable quantum model, quantum wires
PACS: 03.65.-w, 03.65.Db, 73.21.Hb

1. Introduction

While the origin of the idea to investigate quantum mechanics of particles confined to a graph was conceived originally to address to a particular physical problem, namely the spectra of aromatic hydrocarbons [RS53], the motivation was quickly lost and for a long time the problem remained rather an obscure textbook example. This changed in the last two decades when the progress of microfabrication techniques made graph-shaped structures of submicron sizes technologically important. This generated an intense interest to investigation of quantum graph models which went beyond the needs of practical applications, since these models proved to be an excellent laboratory to study various properties of quantum systems. The literature on quantum graphs is nowadays huge; we limit ourselves to mentioning the recent volume [AKST08] where many concepts are discussed and a rich bibliography can be found.

The essential component of quantum graph models is the wavefunction coupling in the vertices. While often the most simple matching conditions (dubbed free, Kirchhoff, or Neumann) or the slightly more general δ coupling in which the functions are continuous in the vertex are

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used, these cases represent just a tiny subset of all admissible couplings. The family of the latter is determined by the requirement that the corresponding Hamiltonian is a self-adjoint operator, or in physical language, that the probability current is conserved at the vertices. It is not difficult to find all the admissible conditions mathematically; if the vertex joins n edges they contain n^2 free parameters, and with exception of the one-parameter subfamily mentioned above they are all singular in the sense that the wavefunctions are discontinuous at the vertex.

What is much less clear is the physical meaning of such conditions. It is longstanding open problem whether and in what sense one can approximate all the singular couplings by regular ones depending on suitable parameters, and the aim of the present paper is to answer this question by presenting such a construction, minimal in a natural sense using n^2 real parameters, and to show that the closeness is achieved in the norm-resolvent sense, so the convergence of all types of the spectra and the corresponding eigenprojections is guaranteed.

The key idea comes from a paper of one of us with Shigehara [CS98] which showed that a combination of regular point interactions on a line approaching each other with the coupling scaled in a particular way w.r.t. the interaction distance can produce a singular point interaction. Later it was demonstrated [ENZ01] that the convergence in this model is norm-resolvent and the scaling choice is highly non-generic. The idea was applied by two of us to the simplest singular coupling, the so-called $\delta'_{\rm s}$, in [CE04] and was demonstrated to work; the question was how much it can be extended. Two other of us examined it [ET07] and found that with a larger number of regular interactions one can deal with families described by $2n$ parameters, and changing locally the approximating graph topology one can deal with all the couplings invariant with respect to the time reversal which form an $\binom{n+1}{2}$-parameter subset.

It was clear that to proceed beyond the time-reversal symmetry one has to involve vector potentials similarly as it is was done in the simplest situation in [SMMC99]. In this paper we present such a construction which contains parameters breaking the symmetry and which at the same time is more elegant than that of [ET07] in the sense that the needed "ornamentation" of the graph is minimal: we disconnect the n edges at the vertex and join each pair of the so obtained free ends by an additional edge which shrinks to a point in the limit. The number of parameters leans on the decomposition $n^2 = n + 2\binom{n}{2}$, where the first summand, n, corresponds to δ couplings of the "outer" edge endpoints with those of the added shrinking ones. The second summand can be considered as $\binom{n}{2}$ times two parameters: one is a δ potential placed at the edge, the other is a vector potential supported by it.

Our result shows that any singular vertex coupling can be approximated by a graph in which the vertex is replaced by a local graph structure in combination with local regular interactions and local magnetic fields. This opens way to constructing "structured" vertices tailored to the desired conductivity properties, even tunable ones, if the interactions are controlled by gate electrodes, however, we are not going to elaborate such approximations further in this paper.

We have to note for completeness that the problem of understanding vertex couplings has also other aspects. The approximating object needs not to be a graph but can be another geometrical structure. A lot of attention was paid to the situation of "fat graphs", or networks of this tubes built around the graph skeleton. The two approaches can be combined, for instance, by "lifting" the graph results to fat graphs. In this way approximations to δ and $\delta'_{\rm s}$ couplings by suitable families of Schrödinger operators on such manifolds with Neumann boundaries were recently demonstrated in [EP08]. The results of this paper can be similarly "lifted" to manifolds; that will be the subject of a subsequent work.

Let us review briefly the contents of the paper. In the next section we gather the needed

preliminary information. We review the information about vertex couplings and derive a new parametrization of a general coupling suitable for our purposes. In Section 3 we describe in detail the approximation sketched briefly above and show that on a heuristic level it converges to a chosen vertex coupling. Finally, in the last section we present and prove our main result showing that the said convergence is not only formal but it is valid also in the norm-resolvent sense.

2. Vertex coupling in quantum graphs

Let us first recall briefly a few basic notions; for a more detailed discussion we refer to the literature given in the introduction. The object of our interest are Schrödinger operators on metric graphs. A graph is conventionally identified with a family of vertices and edges; it is metric if each edge can be equipped with a distance, i.e. to be identified with a finite or semi-infinite interval.

We regard such a graph Γ with edges $E_1, \dots, E_n$ as a configuration space of a quantum mechanical system, i.e. we identify the orthogonal sum $\mathcal{H} = \bigoplus_{j=1}^n L^2(E_j)$ with the state Hilbert space and the wave function of a spinless particle "living" on Γ can be written as the column $\Psi = (\psi_1, \psi_2, \dots, \psi_n)^T$ with $\psi_j \in L^2(E_j)$. In the simplest case when no external fields are present the system Hamiltonian acts as $(H_\Gamma \Psi)_j = -\psi_j''$, with the domain consisting of functions from $W^{2,2}(\Gamma) := \bigoplus_{j=1}^n W^{2,2}(E_j)$. Not all such functions are admissible, though, in order to make the operator self-adjoint we have to require that appropriate boundary conditions are satisfied at the vertices of the graph.

We restrict our attention to the physically most interesting case when the boundary conditions are *local*, coupling values of the functions and derivatives is each vertex separately. Our aim is explain the meaning of a general vertex coupling using suitable approximations; the local character means that we can investigate how such a system behaves in the vicinity of a single vertex. A prototypical example of this situation is a *star graph* with one vertex in which a finite number of semi-infinite edges meet; this is the case we will mostly have in mind in the following.

Let us thus consider a graph vertex V of degree n, i.e. with n edges connected at V. We denote these edges by $E_1, \dots, E_n$ and the components of the wave function values at them by $\psi_1(x_1), \dots, \psi_n(x_n)$. We choose the coordinates at the edges in such a way that $x_j \geq 0$ for all $j = 1, \dots, n$, and the value $x_j = 0$ corresponds to the vertex V. For notational simplicity we put $\Psi_V = (\psi_1(0), \dots, \psi_n(0))^T$ and $\Psi_V' = (\psi_1'(0), \dots, \psi_n'(0))^T$. Since our Hamiltonian is a second-order differential operator, the sought boundary conditions will couple the above boundary values, their most general form being

$$A\Psi_V + B\Psi_V' = 0\,, \tag{1}$$

where A and B are complex $n \times n$ matrices.

To ensure self-adjointness of the Hamiltonian, which is in physical terms equivalent to conservation of the probability current at the vertex V, the matrices A and B cannot be arbitrary but have to satisfy the following two conditions,

$$\begin{aligned} &\bullet\ \operatorname{rank}(A|B) = n, \\ &\bullet\ \text{the matrix } AB^* \text{ is self-adjoint,} \end{aligned} \tag{2}$$

where $(A|B)$ denotes the $n \times 2n$ matrix with A, B forming the first and the second n columns, respectively, as stated for the first time by Kostrykin and Schrader [KS99]. The relation (1)

together with conditions (2) (for brevity, we will write (1)&(2)) describe all possible vertex boundary conditions giving rise to a self-adjoint Hamiltonian; we will speak about *admissible boundary conditions*.

On the other hand, it is obvious that the formulation (1)&(2) is non-unique in the sense that different pairs (A_1, B_1), (A_2, B_2) may define the same vertex coupling, as A, B can be equivalently replaced by CA, CB for any regular matrix $C \in \mathbb{C}^{n,n}$. To overcome this ambiguity, Harmer [Ha00], and independently Kostrykin and Schrader [KS00] proposed a unique form of the boundary conditions (1), namely

$$(U - I)\Psi_V + \mathrm{i}(U + I)\Psi'_V = 0\,, \tag{3}$$

where U is a unitary $n \times n$ matrix. Note that in a more general context such conditions were known before [GG91], see also [FT00].

The natural *parametrization* (3) of the family of vertex couplings has several advantages in comparison to (1)&(2), besides its uniqueness it also makes obvious how "large" the family is: since the unitary group $U(n)$ has n^2 real parameters, the same is true for vertex couplings in a quantum graph vertex of the degree n. Of course, this fact is also clear if one interprets the couplings from the viewpoint of self-adjoint extensions [EŠ89].

On the other hand, among the disadvantages of the formulation (3) one can mention its complexity: vertex couplings that are simple from the physical point of view may have a complicated description when expressed in terms of the condition (3). As an example, let us mention in the first place the δ-coupling with a parameter $\alpha \in \mathbb{R}$, characterized by relations

$$\psi_j(0) = \psi_k(0) =: \psi(0)\,, \quad j,k = 1\ldots,n\,, \qquad \sum_{j=1}^{n} \psi'_j(0) = \alpha\psi(0)\,, \tag{4}$$

for which the matrix U used in (3) has entries given by

$$U_{jk} = \frac{2}{n + \mathrm{i}\alpha} - \delta_{jk}\,, \tag{5}$$

δ_{jk} being the Kronecker delta. When we substitute (5) into (3) and compare with (4) rewritten into a matrix form (1), we observe that the first formulation is not only more complicated with respect to the latter, but also contains complex values whereas the latter does not. This is a reason why it is often better to work with simpler expressions of the type (1)&(2). Another aspect of this parametrization difference concerns the meaning of the parameters. Since the n^2 ones mentioned earlier are "encapsulated" in a unitary matrix, it is difficult to understand which role each of them plays.

On the other hand, both formulations (1)&(2) and (3) have a common feature, namely that they have a form insensitive to a particular edge numbering. If the edges are permuted one has just to replace the matrices A, B and U by $\tilde{A}, \tilde{B}$ and $\tilde{U}$, respectively, obtained by the appropriate rearrangement of rows and columns. This may hide different ways in which the edges are coupled; it is easy to see that a particular attention should be paid to "singular" situations when the matrix U has eigenvalue(s) equal to ± 1.

Since the type of the coupling will be important for the approximation we are going to construct, we will rewrite the vertex coupling conditions in another form which is again simple and unique but requires an appropriate edge numbering. This will be done in Theorem 2.1, before

stating it we introduce several symbols that will be employed in the further text, namely

$$\begin{aligned} \mathbb{C}^{k,l} &- \text{the set of complex matrices with } k \text{ rows and } l \text{ columns,} \\ \hat{n} &- \text{the set } \{1, 2, \ldots, n\}, \\ I^{(n)} &- \text{the identity matrix } n \times n. \end{aligned}$$

To be precise, let us remark that the term "numbering" with respect to the edges connected in the graph vertex of the degree n means strictly numbering by the elements of the set $\hat{n}$.

Theorem 2.1. *Let us consider a quantum graph vertex V of the degree n.*

(i) If $m \le n$, $S \in \mathbb{C}^{m,m}$ is a self-adjoint matrix and $T \in \mathbb{C}^{m,n-m}$, then the equation

$$\begin{pmatrix} I^{(m)} & T \\ 0 & 0 \end{pmatrix} \Psi'_V = \begin{pmatrix} S & 0 \\ -T^* & I^{(n-m)} \end{pmatrix} \Psi_V \tag{6}$$

expresses admissible boundary conditions. This statement holds true for any numbering of the edges.

(ii) For any vertex coupling there exist a number $m \le n$ and a numbering of edges such that the coupling is described by the boundary conditions (6) *with the uniquely given matrices $T \in \mathbb{C}^{m,n-m}$ and self-adjoint $S \in \mathbb{C}^{m,m}$.*

(iii) Consider a quantum graph vertex of the degree n with the numbering of the edges explicitly given; then there is a permutation $\Pi \in S_n$ such that the boundary conditions may be written in the modified form

$$\begin{pmatrix} I^{(m)} & T \\ 0 & 0 \end{pmatrix} \tilde{\Psi}'_V = \begin{pmatrix} S & 0 \\ -T^* & I^{(n-m)} \end{pmatrix} \tilde{\Psi}_V \tag{7}$$

for

$$\tilde{\Psi}_V = \begin{pmatrix} \psi_{\Pi(1)}(0) \\ \vdots \\ \psi_{\Pi(n)}(0) \end{pmatrix}, \qquad \tilde{\Psi}'_V = \begin{pmatrix} \psi'_{\Pi(1)}(0) \\ \vdots \\ \psi'_{\Pi(n)}(0) \end{pmatrix},$$

where the self-adjoint matrix $S \in \mathbb{C}^{m,m}$ and the matrix $T \in \mathbb{C}^{m,n-m}$ depend unambiguously on Π. This formulation of boundary conditions is in general not unique, since there may be different admissible permutations Π, but one can make it unique by choosing the lexicographically smallest permutation Π.

Proof. The claim (iii) is an immediate consequence of (ii) using a simultaneous permutation of elements in the vectors Ψ_V and Ψ'_V, so we have to prove the first two. As for (i), we have to show that the vertex coupling (1) with matrices

$$A = \begin{pmatrix} -S & 0 \\ T^* & -I^{(n-m)} \end{pmatrix} \quad \text{and} \quad B = \begin{pmatrix} I^{(n)} & T \\ 0 & 0 \end{pmatrix},$$

conform with (2). We have

$$\operatorname{rank} \begin{pmatrix} -S & 0 & I^{(m)} & T \\ T^* & -I^{(n-m)} & 0 & 0 \end{pmatrix} = \operatorname{rank} \begin{pmatrix} I^{(m)} & 0 & -S & T \\ 0 & -I^{(n-m)} & T^* & 0 \end{pmatrix} = n$$

and

$$\begin{pmatrix} -S & 0 \\ T^* & -I^{(n-m)} \end{pmatrix} \cdot \begin{pmatrix} I^{(n)} & T \\ 0 & 0 \end{pmatrix}^* = \begin{pmatrix} -S & 0 \\ 0 & 0 \end{pmatrix};$$

the latter matrix is self-adjoint since $S = S^*$, thus (2) is satisfied.

Now we proceed to (ii). Consider a quantum graph vertex of the degree n with an arbitrary fixed vertex coupling. Let Ψ_V and Ψ'_V denote the vectors of values and derivatives of the wave function components at the edge ends; the order of the components is arbitrary but fixed and the same for both vectors. We know that the coupling can be described by boundary conditions (1) with some $A, B \in \mathbb{C}^{n,n}$ satisfying (2). Our aim is to find a number $m \leq n$, a certain numbering of the edges and matrices S and T such that the boundary conditions (1) are equivalent to (6). Moreover, we have to show that such a number m is the only possible and that S, T depend uniquely on the edge numbering.

When proceeding from (1) to (6), we may use exclusively manipulations that do not affect the meaning of the coupling, namely

- simultaneous permutation of columns of the matrices A, B combined with corresponding simultaneous permutation of components in Ψ_V and Ψ'_V,
- multiplying the system from left by a regular matrix.

We see from (6) that m is equal to the rank of the matrix applied at Ψ'_V. We observe that the rank of this matrix, as well as of that applied at Ψ_V, is not influences by any of the manipulations mentioned above, hence it is obvious that $m = \mathrm{rank}(B)$ and that such a choice is the only possible, i.e. m is unique.

Since $\mathrm{rank}(B) = m$ with $m \in \{0, \ldots, n\}$, there is an m-tuple of linearly independent columns of the matrix B; suppose that their indices are $j_1, \ldots, j_m$. We permute simultaneously the columns of B and A so that those with indices $j_1, \ldots, j_m$ are now at the positions $1, \ldots, m$, and the same we do with the components of the vectors Ψ_V, Ψ'_V. Labelling the permuted matrices A, B and vectors Ψ_V, Ψ'_V with tildes, we get

$$\tilde{A}\tilde{\Psi}_V + \tilde{B}\tilde{\Psi}'_V = 0\,. \tag{8}$$

Since $\mathrm{rank}(\tilde{B}) = \mathrm{rank}(B) = m$, there are m rows of $\tilde{B}$ that are linearly independent, let their indices be $i_1, \ldots, i_m$, and $n - m$ rows that are linear combinations of the preceding ones. First we permute the rows in (8) so that those with indices $i_1, \ldots, i_m$ are put to the positions $1, \ldots, m$; note that it corresponds to a matrix multiplication of the whole system (8) by a permutation matrix (which is regular) from the left, i.e. an authorized manipulation. In this way we pass from $\tilde{A}$ and $\tilde{B}$ to matrices which we denote as $\check{A}$ and $\check{B}$; it is obvious that this operation keeps the first m columns of the matrix $\check{B}$ linearly independent.

In the next step we add to each of the last $n - m$ rows of $\check{A}\tilde{\Psi}(0) + \check{B}\tilde{\Psi}'(0) = 0$ such a linear combination of the first m rows that all the last $n - m$ rows of $\check{B}$ vanish. This is possible, because the last $n - m$ lines of $\check{B}$ are linearly dependent on the first m lines. It is easy to see that it is an authorized operation, not changing the meaning of the boundary conditions; the resulting matrices at the LHS will be denoted as $\hat{B}$ and $\hat{A}$, i.e.

$$\hat{A}\tilde{\Psi}_V + \hat{B}\tilde{\Psi}'_V = 0\,. \tag{9}$$

From the construction described above we know that the matrix $\hat{B}$ has a block form,

$$\hat{B} = \begin{pmatrix} \hat{\mathcal{B}}_{11} & \hat{\mathcal{B}}_{12} \\ 0 & 0 \end{pmatrix},$$

where $\hat{\mathcal{B}}_{11} \in \mathbb{C}^{m,m}$ and $\hat{\mathcal{B}}_{12} \in \mathbb{C}^{m,n-m}$; the square matrix $\hat{\mathcal{B}}_{11} \in \mathbb{C}^{m,m}$ is regular, because its columns are linearly independent. We proceed by multiplying the system (9) from the left by the matrix

$$\begin{pmatrix} \hat{\mathcal{B}}_{11}^{-1} & 0 \\ 0 & I^{(n-m)} \end{pmatrix},$$

arriving at boundary conditions

$$\begin{pmatrix} \mathcal{A}_{11} & \mathcal{A}_{12} \\ \mathcal{A}_{21} & \mathcal{A}_{22} \end{pmatrix} \tilde{\Psi}_V + \begin{pmatrix} I^{(m)} & \mathcal{B}_{12} \\ 0 & 0 \end{pmatrix} \tilde{\Psi}'_V = 0\,, \tag{10}$$

where $\mathcal{B}_{12} = \hat{\mathcal{B}}_{11}^{-1}\hat{\mathcal{B}}_{12}$.

Boundary conditions (10) are equivalent to (1), therefore they have to be admissible. In other words, the matrices $\begin{pmatrix} \mathcal{A}_{11} & \mathcal{A}_{12} \\ \mathcal{A}_{21} & \mathcal{A}_{22} \end{pmatrix}$ and $\begin{pmatrix} I^{(m)} & \mathcal{B}_{12} \\ 0 & 0 \end{pmatrix}$ have to satisfy both the conditions (2), which we are now going to verify. Let us begin with the second one. We have

$$\begin{pmatrix} \mathcal{A}_{11} & \mathcal{A}_{12} \\ \mathcal{A}_{21} & \mathcal{A}_{22} \end{pmatrix} \cdot \begin{pmatrix} I^{(m)} & 0 \\ \mathcal{B}_{12}^* & 0 \end{pmatrix} = \begin{pmatrix} \mathcal{A}_{11} + \mathcal{A}_{12}\mathcal{B}_{12}^* & 0 \\ \mathcal{A}_{21} + \mathcal{A}_{22}\mathcal{B}_{12}^* & 0 \end{pmatrix}$$

and this matrix is self-adjoint if and only if $\mathcal{A}_{11} + \mathcal{A}_{12}\mathcal{B}_{12}^*$ is self adjoint and $\mathcal{A}_{21} + \mathcal{A}_{22}\mathcal{B}_{12}^* = 0$. We infer that $\mathcal{A}_{21} = -\mathcal{A}_{22}\mathcal{B}_{12}^*$, hence condition (10) acquires the form

$$\begin{pmatrix} \mathcal{A}_{11} & \mathcal{A}_{12} \\ -\mathcal{A}_{22}\mathcal{B}_{12}^* & \mathcal{A}_{22} \end{pmatrix} \tilde{\Psi}_V + \begin{pmatrix} I^{(m)} & \mathcal{B}_{12} \\ 0 & 0 \end{pmatrix} \tilde{\Psi}'_V = 0\,. \tag{11}$$

The first one of the conditions (2) says that

$$\operatorname{rank} \begin{pmatrix} \mathcal{A}_{11} & \mathcal{A}_{12} & I^{(m)} & \mathcal{B}_{12} \\ -\mathcal{A}_{22}\mathcal{B}_{12}^* & \mathcal{A}_{22} & 0 & 0 \end{pmatrix} = n\,,$$

hence $\operatorname{rank}\left(-\mathcal{A}_{22}\mathcal{B}_{12}^* | \mathcal{A}_{22}\right) = n - m$. Since $\left(-\mathcal{A}_{22}\mathcal{B}_{12}^* | \mathcal{A}_{22}\right) = -\mathcal{A}_{22} \cdot \left(\mathcal{B}_{12}^* | I^{(n-m)}\right)$ we obtain the condition $\operatorname{rank}(\mathcal{A}_{22}) = n - m$, i.e. $\mathcal{A}_{22}$ must be a regular matrix. It allows us to multiply the equation (11) from the left by the matrix

$$\begin{pmatrix} I^{(m)} & -\mathcal{A}_{12}\mathcal{A}_{22}^{-1} \\ 0 & -\mathcal{A}_{22}^{-1} \end{pmatrix},$$

which is obviously well-defined and regular; this operation leads to the condition

$$\begin{pmatrix} \mathcal{A}_{11} + \mathcal{A}_{12}\mathcal{B}_{12}^* & 0 \\ \mathcal{B}_{12}^* & -I^{(n-m)} \end{pmatrix} \tilde{\Psi}_V + \begin{pmatrix} I^{(m)} & \mathcal{B}_{12} \\ 0 & 0 \end{pmatrix} \tilde{\Psi}'_V = 0\,.$$

If follows from our previous considerations that the square matrix $\mathcal{A}_{11} + \mathcal{A}_{12}\mathcal{B}_{12}^*$ is self-adjoint. If we denote it as $-S$, rename the block $\mathcal{B}_{12}$ as T and transfer the term containing $\tilde{\Psi}'_V$ to the right hand side, we arrive at boundary conditions

$$\begin{pmatrix} I^{(m)} & T \\ 0 & 0 \end{pmatrix} \tilde{\Psi}'_V = \begin{pmatrix} S & 0 \\ -T^* & I^{(n-m)} \end{pmatrix} \tilde{\Psi}_V\,. \tag{12}$$

The order of components in $\tilde{\Psi}_V$ and $\tilde{\Psi}'_V$ determines just the appropriate numbering, in other words, the vectors $\tilde{\Psi}_V$ and $\tilde{\Psi}'_V$ represent exactly what we understood by Ψ_V and Ψ'_V in the formulation of the theorem.

Finally, the uniqueness of the matrices S and T with respect to the choice of the permutation Π is a consequence of the presence of the blocks $I^{(m)}$ and $I^{(n-m)}$. First of all, the block $I^{(n-m)}$ implies that there is only one possible T, otherwise the conditions for $\tilde{\psi}'_{m+1}, \ldots, \tilde{\psi}'_n$ would change, and next, the block $I^{(m)}$ together with the uniqueness of T implies that there is only one possible S, otherwise the conditions for $\tilde{\psi}_1, \ldots, \tilde{\psi}_m$ would change. □

Remark 2.2. The expression (7) implies, in particular, that if B has not full rank, the number of real numbers parametrizing the vertex coupling (1) is reduced from n^2 to at most $m(2n-m) = n^2 - (n-m)^2$, where $m = \mathrm{rank}(B)$. Another reduction can come from a lower rank of the matrix A.

Remark 2.3. The procedure of permuting columns and applying linear transformations to the rows of the system (1) has been done with respect to the matrix B, but one can start by same right from the matrix A as well. In this way we would obtain similar boundary conditions as (6), only the vectors Ψ_V and Ψ'_V would be interchanged. Theorem 2.1 can be thus formulated with Equation (6) replaced by

$$\begin{pmatrix} I^{(m)} & T \\ 0 & 0 \end{pmatrix} \Psi_V = \begin{pmatrix} S & 0 \\ -T^* & I^{(n-m)} \end{pmatrix} \Psi'_V \,.$$

For completeness' sake we add that another possible forms of Equation (6) in Theorem 2.1 are

$$\begin{pmatrix} S & 0 \\ -T^* & I^{(n-m)} \end{pmatrix} \Psi_V + \begin{pmatrix} I^{(m)} & T \\ 0 & 0 \end{pmatrix} \Psi'_V = 0$$

and

$$\begin{pmatrix} I^{(m)} & T \\ 0 & 0 \end{pmatrix} \Psi_V + \begin{pmatrix} S & 0 \\ -T^* & I^{(n-m)} \end{pmatrix} \Psi'_V = 0 \,;$$

having the standardized form $A\Psi_V + B\Psi'_V = 0$, last two formulations may be sometimes more convenient than (6).
Obviously, an analogous remark can be made for Equation (7).

Remark 2.4. A formulation of boundary conditions with a matrix structure singling out the regular part as in (7) has been derived in a different way by P. Kuchment [Ku04]. Recall that in the setting analogous to ours he stated existence of an orthogonal projector P in $\mathbb{C}^n$ with the complementary projector $Q = Id - P$ and a self-adjoint operator L in $Q\mathbb{C}^n$ such that the boundary conditions may be written in the form

$$\begin{aligned} P\Psi_V &= 0 \\ Q\Psi'_V + LQ\Psi_V &= 0 \,. \end{aligned} \tag{13}$$

Let us briefly explain how P. Kuchment's form differs from (7). When transformed into a matrix form, (13) consists of two groups of n linearly dependent equations. If we then naturally extract a single group of n linearly indepent ones, we arrive at a condition with a structure similar to (11), i. e. the upper right submatrix standing at Ψ'_V is generally a *nonzero* matrix $m \times (n-m)$. In other words, whilst P. Kuchment aimed to decompose the boundary conditions with respect to

two complementary orthogonal projectors, our aim was to obtain a unique matrix form with as many vanishing terms as possible; the form (6) turned out to have a highly suitable structure for solving the problem of approximations that we are going to analyze in the rest of the paper.

To conclude this introductory section, let us summarize main advantages and disadvantages of the conditions (6) and (7). They are unique and exhibit a simple and clear correspondence between the parameters of the coupling and the entries of matrices in (6), furthermore, the matrices in (6) are relatively sparse. On the negative side, the structure of matrices in (6) depends on rank(B) and the vertex numbering is not fully permutable.

3. The approximation arrangement

We have argued above that due to a local character one can consider a single-vertex situation, i.e. star graph, when asking about the meaning of the vertex coupling. In this section we consider such a quantum graph with general matching conditions and show that the singular coupling may be understood as a limit case of certain family of graphs constructed only from edges connected by δ-couplings, δ-interactions, and supporting constant vector potentials.

Following the above discussion, one may consider the boundary conditions of the form (6), renaming the edges if necessary. It turns out that for notational purposes it is advantageous to adopt the following convention on a shift of the column indices of T:

Convention 3.1. *The lines of the matrix T are indexed from 1 to m, the columns are indexed from $m+1$ to n.*

Now we can proceed to the description of our approximating model. Consider a star graph with n outgoing edges coupled in a general way given by the condition (7). The approximation in question looks as follows (cf. Fig.1):

- We take n halflines, each parametrized by $x \in [0, +\infty)$, with the endpoints denoted as V_j, and put a δ-coupling (to the edges specified below) with the parameter $v_j(d)$ at the point V_j for all $j \in \hat{n}$.
- Certain pairs V_j, V_k of halfline endpoints will be joined by edges of the length $2d$, and the center of each such joining segment will be denoted as $W_{\{j,k\}}$. For each pair $\{j,k\}$, the points V_j and V_k, $j \neq k$, are joined if one of the following three conditions is satisfied (keep in mind Convention 3.1):
  (1) $j \in \hat{m}$, $k \geq m+1$, and $T_{jk} \neq 0$ (or $j \geq m+1$, $k \in \hat{m}$, and $T_{kj} \neq 0$),
  (2) $j,k \in \hat{m}$ and $(\exists l \geq m+1)(T_{jl} \neq 0 \wedge T_{kl} \neq 0)$,
  (3) $j,k \in \hat{m}$, $S_{jk} \neq 0$, and the previous condition is not satisfied.
- At each point $W_{\{j,k\}}$ we place a δ interaction with a parameter $w_{\{j,k\}}(d)$. From now on we use the following convention: the connecting edges of the length $2d$ are considered as composed of two line segments of the length d, on each of them the variable runs from 0 (corresponding to the point $W_{\{j,k\}}$) to d (corresponding to the point V_j or V_k).
- On each connecting segment described above we put a vector potential which is constant on the whole line between the points V_j and V_k. We denote the potential strength between the points $W_{\{j,k\}}$ and V_j as $A_{(j,k)}(d)$, and between the points $W_{\{j,k\}}$ and V_k as $A_{(k,j)}(d)$. It follows from the continuity that $A_{(k,j)}(d) = -A_{(j,k)}(d)$ for any pair $\{j,k\}$.

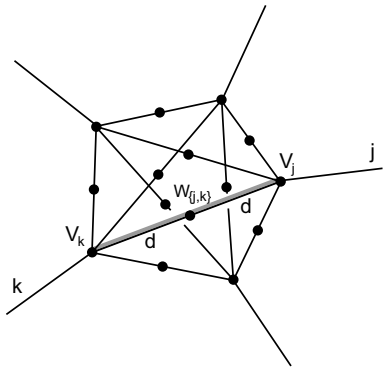

Figure 1: The scheme of the approximation. All inner links are of length $2d$. Some connection links may be missing if the conditions given in the text are not satisfied. The quantities corresponding to the index pair $\{j,k\}$ are marked, and the grey line symbolizes the vector potential $A_{(j,k)}(d)$.

The choice of the dependence of $v_j(d)$, $w_{\{j,k\}}(d)$ and $A_{(j,k)}(d)$ on the parameter d is crucial for the approximation and will be specified later.

It is useful to introduce the set $N_j \subset \hat{n}$ containing indices of all the edges that are joined to the j-th one by a connecting segment, i.e.

$$\begin{aligned} N_j =& \{k \in \hat{m} |\, S_{jk} \neq 0\} \cup \{k \in \hat{m} |\, (\exists l \geq m+1)(T_{jl} \neq 0 \wedge T_{kl} \neq 0)\} \\ & \cup \{k \geq m+1 |\, T_{jk} \neq 0\} \qquad \text{for } j \in \hat{m} \\ N_j =& \{k \in \hat{m} |\, T_{kj} \neq 0\} \qquad \text{for } j \geq m+1 \end{aligned} \tag{14}$$

The definition of N_j has these two trivial consequences, namely

$$k \in N_j \Leftrightarrow j \in N_k \tag{15}$$

$$j \geq m+1 \Rightarrow N_j \subset \hat{m} \tag{16}$$

For the wave function components on the edges we use the following symbols:

- the wave function on the j-th half line is denoted by ψ_j,
- the wave function on the line connecting points V_j and V_k has two components: the one on the line between $W_{\{j,k\}}$ and V_j is denoted by $\varphi_{(j,k)}$, the one on the half between the middle and the endpoint of the k-th half line is denoted by $\varphi_{(k,j)}$. We remind once more the way in which the variable x of $\varphi_{(j,k)}$ and $\varphi_{(k,j)}$ is considered: it grows from 0 at the point $W_{\{j,k\}}$ to d at the point V_j or V_k, respectively.

Next we describe how the δ couplings involved look like; for simplicity we will refrain from indicating in the boundary conditions the dependence of the parameters u, v_j, $w_{\{j,k\}}$ on the distance d.

The δ interaction at the edge connecting the j-th and k-th half line (of course, for $j,k \in \hat{n}$ such that $k \in N_j$ only) is expressed through the conditions

$$\begin{aligned} \varphi_{(j,k)}(0) = \varphi_{(k,j)}(0) =: \varphi_{\{j,k\}}(0)\,, \\ \varphi'_{(j,k)}(0_+) + \varphi'_{(k,j)}(0_+) = w_{\{j,k\}}\varphi_{\{j,k\}}(0)\,, \end{aligned} \tag{17}$$

the δ coupling at the endpoint of the j-th half line ($j \in \hat{n}$) means

$$\begin{aligned} &\psi_j(0) = \varphi_{(j,k)}(d) \quad \text{for all } k \in N_j\,, \\ &\psi_j'(0) - \textstyle\sum_{k\in N_j} \varphi'_{(j,k)}(d) = v_j \psi_j(0)\,. \end{aligned} \tag{18}$$

Further relations which will help us to find the parameter dependence on d come from Taylor expansion. Consider first the case without any added potential,

$$\begin{aligned} &\varphi_{(j,k)}(d) = \varphi_{\{j,k\}}(0) + d\,\varphi'_{(j,k)}(0) + O(d^2)\,, \\ &\varphi'_{(j,k)}(d) = \varphi'_{(j,k)}(0) + O(d)\,, \quad j,k \in \hat{n}\,. \end{aligned} \tag{19}$$

To take the effect of added vector potentials into account, the following lemma will prove useful:

Lemma 3.2. *Let us consider a line parametrized by the variable $x \in (0, L)$, $L \in (0, +\infty) \cup \{+\infty\}$, and let H denote a Hamiltonian of a particle on this line interacting with a potential V,*

$$H = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V\,, \tag{20}$$

sufficiently regular to make H self-adjoint. We denote by $\psi^{s,t}$ the solution of $H\psi = k^2\psi$ with the boundary values $\psi^{s,t}(0) = s$, $\psi^{s,t\prime}(0) = t$. Consider the same system with a vector potential A added, again sufficiently regular; the Hamiltonian is consequently given by

$$H_A = \left(-\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}x} - A\right)^2 + V\,. \tag{21}$$

Let $\psi_A^{s,t}$ denote the solution of $H_A\psi = k^2\psi$ with the same boundary values as before, i.e. $\psi_A^{s,t}(0) = s$, $\psi_A^{s,t\prime}(0) = t$. Then the function $\psi_A^{s,t}$ can be expressed as

$$\psi_A^{s,t}(x) = \mathrm{e}^{\mathrm{i}\int_0^x A(z)\mathrm{d}z} \cdot \psi^{s,t}(x) \qquad \textit{for all} \quad x \in (0, L)\,.$$

Proof. The aim is to prove that

$$-\psi^{s,t\prime\prime} + V\psi^{s,t} = k^2\psi^{s,t} \quad \wedge \quad \psi^{s,t}(0) = s \quad \wedge \quad \psi^{s,t\prime}(0) = t$$

implies

$$\left(-\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}x} - A\right)^2 \left(\mathrm{e}^{\mathrm{i}\int_0^x A(z)\mathrm{d}z} \cdot \psi^{s,t}\right) + V \cdot \mathrm{e}^{\mathrm{i}\int_0^x A(z)\mathrm{d}z} \cdot \psi^{s,t} = k^2 \mathrm{e}^{\mathrm{i}\int_0^x A(z)\mathrm{d}z} \cdot \psi^{s,t}$$

and $\psi_A^{s,t}(0) = s$, $\psi_A^{s,t\prime}(0) = t$. The last part is obvious, since the exponential factor involved is equal to one, hence it suffices to prove the displayed relation. It is straightforward that the Hamiltonian H_A acts generally as

$$H_A = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + 2\mathrm{i}A\frac{\mathrm{d}}{\mathrm{d}x} + \mathrm{i}A' + A^2 + V\,.$$

We substitute $\mathrm{e}^{\mathrm{i}\int_0^x A(z)\mathrm{d}z} \cdot \psi^{s,t}$ for ψ, obtaining

$$\begin{aligned} \left[H_A\left(\mathrm{e}^{\mathrm{i}\int_0^x A(z)\mathrm{d}z} \cdot \psi^{s,t}\right)\right](x) = &-\frac{\mathrm{d}^2}{\mathrm{d}x^2}\left(\mathrm{e}^{\mathrm{i}\int_0^x A(z)\mathrm{d}z} \cdot \psi^{s,t}\right)(x) + \\ &+ 2\mathrm{i}A(x)\frac{\mathrm{d}}{\mathrm{d}x}\left(\mathrm{e}^{\mathrm{i}\int_0^x A(z)\mathrm{d}z} \cdot \psi^{s,t}\right)(x) + \left(\mathrm{i}A'(x) + A(x)^2 + V(x)\right)\mathrm{e}^{\mathrm{i}\int_0^x A(z)\mathrm{d}z} \cdot \psi^{s,t}(x)\,. \end{aligned}$$

Now we express the derivatives applying the formula $\frac{\mathrm{d}}{\mathrm{d}x}\int_0^x A(z)\mathrm{d}z = A(x)$. Most of the terms then cancel, it remains only

$$\left[H_A\left(\mathrm{e}^{\mathrm{i}\int_0^x A(z)\mathrm{d}z}\cdot\psi^{s,t}\right)\right](x) = \mathrm{e}^{\mathrm{i}\int_0^x A(z)\mathrm{d}z}\cdot\left(-\psi^{s,t\prime\prime}(x) + V(x)\cdot\psi^{s,t}(x)\right).$$

Due to the assumption $-\psi^{s,t\prime\prime} + V\psi^{s,t} = k^2\psi^{s,t}$, we have

$$\left[H_A\left(\mathrm{e}^{\mathrm{i}\int_0^x A(z)\mathrm{d}z}\cdot\psi^{s,t}\right)\right](x) = k^2\mathrm{e}^{\mathrm{i}\int_0^x A(z)\mathrm{d}z}\cdot\psi^{s,t}(x)\,,$$

what we have set out to prove. □

The lemma says that adding a vector potential on an edge of a quantum graph has a very simple effect of changing the phase of the wave function by the value $\int_0^x A(z)\mathrm{d}z$. We will work in this paper with the special case of constant vector potentials on the connecting segments of the lengths $2d$, hence the phase shift will be given here as a product of the value A and the length in question.

Lemma 3.2 has the following very useful consequence.

Corollary 3.3. *Consider a quantum graph vertex with n outgoing edges indexed by* $1,\dots,n$ *and parametrized by* $x\in(0,L_j)$*. Suppose that there is a* δ *coupling with the parameter* α *at the vertex, and moreover, that there is a constant vector potential* A_j *on the* j*-th edge for all* $j\in\hat{n}$*. Let* ψ_j *denote the wave function component on the* j*-the edge. Then the boundary conditions acquire the form*

$$\psi_j(0) = \psi_k(0) =: \psi(0) \qquad \textit{for all} \quad j,k\in\hat{n}\,, \tag{22}$$

$$\sum_{j=1}^n \psi_j'(0) = \left(\alpha + \mathrm{i}\sum_{j=1}^n A_j\right)\psi(0)\,, \tag{23}$$

where $\psi_j(0)$*,* $\psi_j'(0)$*, etc., stand for the one-sided (right) limits at* $x=0$*.*

In other words the effect of the vector potentials on the boundary conditions corresponding to a "pure" δ coupling is the following:

- the continuity is not affected,
- the coupling parameter is changed from α to $\alpha + \mathrm{i}\sum_{j=1}^n A_j$.

Proof. Consider first the situation without any vector potentials. If ψ_j^0, $j\in\hat{n}$, denote the wave function components corresponding to this case, the boundary conditions expressing the δ coupling have the form (4), i.e.

$$\begin{gathered}\psi_j^0(0) = \psi_k^0(0) =: \psi^0(0) \qquad \text{for all} \quad j,k\in\hat{n}\,,\\ \textstyle\sum_{j=1}^n \psi_j^{0\prime}(0) = \alpha\psi^0(0)\,.\end{gathered} \tag{24}$$

If there are vector potentials on the edges, A_j on the j-th edge, one has in view of the previous lemma, $\psi_j(x) = \mathrm{e}^{\mathrm{i}A_jx}\psi_j^0(x)$, i.e.

$$\psi_j^0(x) = \mathrm{e}^{-\mathrm{i}A_jx}\psi_j(x)\,,$$

$$\psi_j^{0\prime}(x) = \frac{\mathrm{d}}{\mathrm{d}x}\left(\mathrm{e}^{-\mathrm{i}A_jx}\psi_j(x)\right) = \mathrm{e}^{-\mathrm{i}A_jx}\psi_j{}'(x) - \mathrm{i}A_j\cdot\mathrm{e}^{-\mathrm{i}A_jx}\psi_j(x)\,.$$

Thence we express $\psi_j^0(0)$ and $\psi_j^{0\prime}(0)$: they are equal to

$$\psi_j^0(0) = \psi_j(0)\,,$$
$$\psi_j^{0\prime}(0) = \psi_j{}'(0) - \mathrm{i}A_j\psi_j(0)\,;$$

substituting them to (24) we obtain

$$\psi_j(0) = \psi_k(0) =: \psi(0) \qquad \text{for all} \quad j,k \in \hat{n}\,,$$
$$\sum_{j=1}^{n} \left(\psi_j'(0) - \mathrm{i}A_j \cdot \psi_j(0)\right) = \alpha\psi(0)\,.$$

The first line expresses the continuity of the wavefunction in the vertex supporting the δ coupling in the same way as in the absence of vector potentials, whereas the second line shows how the condition for the sum of the derivatives is changed. With the continuity in mind, we may replace $\psi_j(0)$ by $\psi(0)$ obtaining

$$\sum_{j=1}^{n} \psi_j'(0) = \left(\alpha + \mathrm{i}\sum_{j=1}^{n} A_j\right)\psi(0)\,,$$

which finishes the proof. □

Recall that approximating we are constructing supposes that constant vector potentials are added on the joining edges. If an edge of the length $2d$ joins the endpoints of the j-th and k-th half line, there is a constant vector potential of the value $A_{(j,k)}(d)$ on the part of the length d closer to the j-th half line and a constant vector potential of the value $A_{(k,j)}(d) = -A_{(j,k)}(d)$ on the part of the length d closer to the k-th half line. With regard to Lemma 3.2, the impact of the added potentials consists in phase shifts by $d \cdot A_{(j,k)}(d)$ and $d \cdot A_{(k,j)}(d)$. Let us include this effect into the corresponding equations, i.e. into (19):

$$\begin{aligned} \varphi_{(j,k)}(d) &= \mathrm{e}^{\mathrm{i}dA_{(j,k)}}(\varphi_{\{j,k\}}(0) + d\,\varphi'_{(j,k)}(0)) + O(d^2)\,, \\ \varphi'_{(j,k)}(d) &= \mathrm{e}^{\mathrm{i}dA_{(j,k)}}\varphi'_{(j,k)}(0) + O(d)\,, \qquad j,k \in \hat{n}\,. \end{aligned} \tag{25}$$

The system of equations (17), (18), and (25) describes the relations between values of wave functions and their derivatives at all the vertices. Next we will eliminate the terms with the "auxiliary" functions $\varphi_{\{j,k\}}$ and express the relations between $2n$ terms $\psi_j(0)$, $\psi'_j(0)$, $j \in \hat{n}$.

We begin with the first one of the relations (25) together with the continuity requirement (18), which yields

$$d\,\varphi'_{(j,k)}(0) = \mathrm{e}^{-\mathrm{i}dA_{(j,k)}}\psi_j(0) - \varphi_{\{j,k\}}(0) + O(d^2)\,. \tag{26}$$

The same relation holds with j replaced by k, summing them together and using the second of the relations (17) we get

$$\left(2 + d\,w_{\{j,k\}}\right)\varphi_{\{j,k\}}(0) = \mathrm{e}^{-\mathrm{i}dA_{(j,k)}}\psi_j(0) + \mathrm{e}^{-\mathrm{i}dA_{(k,j)}}\psi_k(0) + O(d^2)\,.$$

We express $\varphi_{\{j,k\}}(0)$ from here and substitute into the first of the equations (25); using at the same time the first relation of (18) we get

$$\psi_j(0) = \mathrm{e}^{\mathrm{i}dA_{(j,k)}} \cdot \left(\frac{\mathrm{e}^{-\mathrm{i}dA_{(j,k)}}\psi_j(0) + \mathrm{e}^{-\mathrm{i}dA_{(k,j)}}\psi_k(0) + O(d^2)}{2 + d \cdot w_{\{j,k\}}} + d\,\varphi'_{(j,k)}(0)\right) + O(d^2)\,,$$

and considering the second of the equations (25), we have

$$\psi_j(0) = \frac{\psi_j(0) + \mathrm{e}^{\mathrm{i}d(A_{(j,k)} - A_{(k,j)})}\psi_k(0) + O(d^2)}{2 + d \cdot w_{\{j,k\}}} + d\,\varphi'_{(j,k)}(d) + O(d^2)\,.$$

Since the values of vector potentials are supposed to have the "antisymmetry" property, $A_{(k,j)}(d) = -A_{(j,k)}(d)$, we may simplify the above equation to

$$\psi_j(0) = \frac{\psi_j(0) + \mathrm{e}^{2\mathrm{i}dA_{(j,k)}}\psi_k(0) + O(d^2)}{2 + d \cdot w_{\{j,k\}}} + d\,\varphi'_{(j,k)}(d) + O(d^2)\,. \tag{27}$$

Summing the last equation over $k \in N_j$ yields

$$\#N_j \cdot \psi_j(0) = \psi_j(0) \cdot \sum_{k\in N_j} \frac{1}{2 + d \cdot w_{\{j,k\}}} + \sum_{k\in N_j} \frac{\mathrm{e}^{2\mathrm{i}dA_{(j,k)}}\psi_k(0)}{2 + d \cdot w_{\{j,k\}}} + d \cdot \sum_{k\in N_j} \varphi'_{(j,k)}(d) + \\ + \sum_{k\in N_j} \frac{O(d^2)}{2 + d \cdot w_{\{j,k\}}} + O(d^2)$$

($\#N_j$ denotes the cardinality of N_j), and with the help of the second of the relations (18) we arrive at the final expression,

$$d\psi'_j(0) = \left(dv_j + \#N_j - \sum_{k\in N_j} \frac{1}{2 + d \cdot w_{\{j,k\}}}\right)\psi_j(0) - \sum_{k\in N_j} \frac{\mathrm{e}^{\mathrm{i}d(A_{(j,k)} - A_{(k,j)})}\psi_k(0)}{2 + d \cdot w_{\{j,k\}}} \\ + \sum_{k\in N_j} \frac{O(d^2)}{2 + d \cdot w_{\{j,k\}}} + O(d^2)\,. \tag{28}$$

Our objective is to choose $v_j(d)$, $w_{\{j,k\}}(d)$ and $A_{(j,k)}(d)$ in such a way that in the limit $d \to 0$ the system of relations (28) with $j \in \hat{n}$ tends to the system of n boundary conditions (7). The lines of (7) are of two types, let us recall:

$$\psi'_j(0) + \sum_{l=m+1}^{n} T_{jl}\psi'_l(0) = \sum_{k=1}^{m} S_{jk}\psi_k(0) \qquad j \in \hat{m} \tag{29}$$

$$0 = -\sum_{k=1}^{m} \overline{T_{kj}}\psi_k(0) + \psi_j(0) \qquad j = m+1, \ldots, n\,. \tag{30}$$

We point out here with reference to (14) that these relations may be written also with the summation indices running through the restricted sets, namely

$$\psi'_j(0) + \sum_{l\in N_j\setminus\hat{m}} T_{jl}\psi'_l(0) = \sum_{k=1}^{m} S_{jk}\psi_k(0) \qquad j \in \hat{m} \tag{31}$$

$$0 = -\sum_{k\in N_j} \overline{T_{kj}}\psi_k(0) + \psi_j(0) \qquad j = m+1, \ldots, n\,, \tag{32}$$

since for any pair $j \in \hat{m}$, $l \in \{m+1, \cdots, n\}$ the implication $T_{jl} \neq 0 \Rightarrow l \in N_j$ holds, see also Eqs. (15), (16).

When looking for a suitable dependence of $v_j(d)$, $w_{\{j,k\}}(d)$ and $A_{(j,k)}(d)$ on d, we start with Eq. (28) in the case when $j \geq m+1$. Our aim is to find conditions under which (28) tends to (32) as $d \to 0$. It is obvious that the sufficient conditions are

$$\lim_{d\to 0}\left(dv_j + \#N_j - \sum_{k\in N_j} \frac{1}{2+d\cdot w_{\{j,k\}}}\right) \in \mathbb{R}\backslash\{0\}\,, \tag{33}$$

$$\lim_{d\to 0} \frac{1}{2+d\cdot w_{\{j,k\}}} \in \mathbb{R}\backslash\{0\} \quad \forall k \in N_j\,, \tag{34}$$

$$\frac{\frac{\mathrm{e}^{2\mathrm{i}dA_{(j,k)}}}{2+d\cdot w_{\{j,k\}}}}{dv_j + \#N_j - \sum_{h\in N_j}\frac{1}{2+d\cdot w_{\{j,h\}}}} = \overline{T_{kj}} \quad \forall k \in N_j\,. \tag{35}$$

Now we proceed to the case $j \in \hat{m}$. Our approach is based on substitution of (28) into the left-hand side of (31) and a subsequent comparison of the right-hand sides. The substitution is straightforward,

$$\begin{aligned}\psi_j'(0) + \sum_{l\in N_j\backslash\hat{m}} T_{jl}\cdot\psi_l'(0) = {}& \left(v_j + \frac{\#N_j}{d} - \frac{1}{d}\sum_{h\in N_j}\frac{1}{2+d\cdot w_{\{j,h\}}}\right)\psi_j(0) - \frac{1}{d}\sum_{k\in N_j}\frac{\mathrm{e}^{2\mathrm{i}dA_{(j,k)}}\psi_k(0)}{2+d\cdot w_{\{j,k\}}} \\ &+ \sum_{l\in N_j\backslash\hat{m}} T_{jl}\left[\left(v_l + \frac{\#N_l}{d} - \frac{1}{d}\sum_{h\in N_l}\frac{1}{2+d\cdot w_{\{l,h\}}}\right)\psi_l(0) - \frac{1}{d}\sum_{k\in N_l}\frac{\mathrm{e}^{2\mathrm{i}dA_{(l,k)}}\psi_k(0)}{2+d\cdot w_{\{l,k\}}}\right] \\ &+ \mathcal{O}(d) + \sum_{k\in N_j}\frac{\mathcal{O}(d)}{2+d\cdot w_{\{j,k\}}} + \sum_{l=m+1}^{n} T_{jl}\left(\mathcal{O}(d) + \sum_{h\in N_l}\frac{\mathcal{O}(d)}{2+d\cdot w_{\{l,h\}}}\right),\end{aligned} \tag{36}$$

then we apply two identities, which can be easily proven, namely

$$(i)\quad \sum_{k\in N_j}\frac{\mathrm{e}^{2\mathrm{i}dA_{(j,k)}}\psi_k(0)}{2+d\cdot w_{\{j,k\}}} = \sum_{k\in N_j\cap\hat{m}}\frac{\mathrm{e}^{2\mathrm{i}dA_{(j,k)}}\psi_k(0)}{2+d\cdot w_{\{j,k\}}} + \sum_{l\in N_j\backslash\hat{m}}\frac{\mathrm{e}^{2\mathrm{i}dA_{(j,l)}}\psi_l(0)}{2+d\cdot w_{\{j,l\}}}\,,$$

$$\begin{aligned}(ii)\quad & \sum_{l\in N_j\backslash\hat{m}} T_{jl}\sum_{k\in N_l}\frac{\mathrm{e}^{2\mathrm{i}dA_{(l,k)}}\psi_k(0)}{2+d\cdot w_{\{l,k\}}} \\ &= \left(\sum_{l\in N_j\backslash\hat{m}} T_{jl}\frac{\mathrm{e}^{2\mathrm{i}dA_{(l,j)}}}{2+d\cdot w_{\{l,j\}}}\right)\psi_j(0) + \sum_{k\in N_j\cap\hat{m}}\left(\sum_{l\in N_k\backslash\hat{m}} T_{jl}\frac{\mathrm{e}^{2\mathrm{i}dA_{(l,k)}}}{2+d\cdot w_{\{l,k\}}}\right)\psi_k(0)\end{aligned}$$

and obtain

$$\begin{aligned}
&\psi_j'(0) + \sum_{l\in N_j\setminus\hat{m}} T_{jl}\cdot\psi_l'(0)\\
&\quad= \left(v_j + \frac{\#N_j}{d} - \frac{1}{d}\sum_{h\in N_j}\frac{1}{2+d\cdot w_{\{j,h\}}} - \frac{1}{d}\sum_{l\in N_j\setminus\hat{m}} T_{jl}\frac{\mathrm{e}^{2\mathrm{i}dA_{(l,j)}}}{2+d\cdot w_{\{l,j\}}}\right)\psi_j(0)\\
&\qquad - \frac{1}{d}\sum_{k\in N_j\cap\hat{m}}\left(\frac{\mathrm{e}^{2\mathrm{i}dA_{(j,k)}}}{2+d\cdot w_{\{j,k\}}} + \sum_{l\in N_k\setminus\hat{m}} T_{jl}\frac{\mathrm{e}^{2\mathrm{i}dA_{(l,k)}}}{2+d\cdot w_{\{l,k\}}}\right)\psi_k(0)\\
&\quad + \sum_{l\in N_j\setminus\hat{m}}\left(-\frac{1}{d}\cdot\frac{\mathrm{e}^{2\mathrm{i}dA_{(j,l)}}}{2+d\cdot w_{\{j,l\}}} + T_{jl}\left(v_l + \frac{\#N_l}{d} - \frac{1}{d}\sum_{h\in N_l}\frac{1}{2+d\cdot w_{\{l,h\}}}\right)\right)\psi_l(0)\\
&\qquad + O(d) + \sum_{k\in N_j}\frac{O(d)}{2+d\cdot w_{\{j,k\}}} + \sum_{k\in N_j\cap\hat{m}}\sum_{l\in N_k\cap N_j\setminus\hat{m}}\frac{O(d)}{2+d\cdot w_{\{l,k\}}}\,. \qquad (37)
\end{aligned}$$

As we have announced above, the goal is to determine terms $v_j(d)$, $w_{\{j,k\}}(d)$ and $A_{(j,k)}(d)$ such that if $d\to 0$, the right-hand side of (37) tends to the eight-hand side of (31) for all $j\in\hat{m}$. We observe that this will be the case provided

$$v_j + \frac{\#N_j}{d} - \frac{1}{d}\sum_{h\in N_j}\frac{1}{2+d\cdot w_{\{j,h\}}} - \frac{1}{d}\sum_{l\in N_j} T_{jl}\frac{\mathrm{e}^{2\mathrm{i}dA_{(l,j)}}}{2+d\cdot w_{\{l,j\}}} = S_{jj}\,, \qquad (38)$$

$$-\frac{1}{d}\frac{\mathrm{e}^{2\mathrm{i}dA_{(j,k)}}}{2+d\cdot w_{\{j,k\}}} - \frac{1}{d}\sum_{l\in N_k\setminus\hat{m}} T_{jl}\frac{\mathrm{e}^{2\mathrm{i}dA_{(l,k)}}}{2+d\cdot w_{\{l,k\}}} = S_{jk}\quad \forall k\in N_j\cap\hat{m}\,, \qquad (39)$$

$$-\frac{1}{d}\frac{\mathrm{e}^{2\mathrm{i}dA_{(j,l)}}}{2+d\cdot w_{\{j,l\}}} + T_{jl}\left(v_l + \frac{\#N_l}{d} - \frac{1}{d}\sum_{h\in N_l}\frac{1}{2+d\cdot w_{\{l,h\}}}\right) = 0\quad \forall l\in N_j\setminus\hat{m}\,, \qquad (40)$$

$$\lim_{d\to 0}\frac{1}{2+d\cdot w_{\{j,k\}}}\in\mathbb{R}\quad \forall k\in N_j\,, \qquad (41)$$

$$\lim_{d\to 0}\frac{1}{2+d\cdot w_{\{l,k\}}}\in\mathbb{R}\quad \forall k\in N_j\cap\hat{m},\, l\in N_k\cap N_j\setminus\hat{m}\,. \qquad (42)$$

It is easy to see that the set of equations (40) for $j\in\hat{m}$, $l\in N_j\setminus\hat{m}$ is equivalent to the set (35) for $j\geq m+1$, $k\in N_j$. Similarly, Eq. (42) for $j\in\hat{m}$, $k\in N_j\cap\hat{m}$, $l\in N_k\cap N_j\setminus\hat{m}$ is a weaker set of conditions than (34) with $j\geq m+1$, $k\in N_j$. Finally, Eq. (41) reduces for $k\in N_j\setminus\hat{m}$ to (34), thus it suffices to consider (41) with $k\in N_j\cap\hat{m}$.

The procedure of determination of $v_j(d)$, $w_{\{j,k\}}(d)$ and $A_{(j,k)}(d)$ will proceed in three steps, at the end we add the fourth step involving the verification of the limit conditions (33), (34), and (41) restricted to $k\in N_j\cap\hat{m}$.

Step I. We use Eq. (40) to find an expression for $w_{\{j,l\}}(d)$ and $A_{(j,l)}(d)$ when $j\in\hat{m}$ and $l\in N_j\setminus\hat{m}$. We begin with rearranging Eq. (35) into the form

$$\frac{1}{2+d\cdot w_{\{j,l\}}} = \mathrm{e}^{-2\mathrm{i}dA_{(j,l)}}\cdot T_{jl}\left(dv_l + \#N_l - \sum_{h\in N_l}\frac{1}{2+d\cdot w_{\{l,h\}}}\right)\quad \forall l\in N_j\setminus\hat{m}\,. \qquad (43)$$

Since all the terms except $\mathrm{e}^{-2\mathrm{i}dA_{(j,l)}}$ and T_{jl} are real, we can obtain immediately a condition for $A_{(j,l)}$: We put

$$\mathrm{e}^{2\mathrm{i}dA_{(j,l)}} = \begin{cases} T_{jl}/\|T_{jl}\| & \text{if} \quad \mathrm{Re}\ T_{jl} \geq 0\,, \\ -T_{jl}/\|T_{jl}\| & \text{if} \quad \mathrm{Re}\ T_{jl} < 0\,; \end{cases}$$

it is easy to see that such a choice ensures that the expression $\mathrm{e}^{-2\mathrm{i}dA_{(j,l)}} \cdot T_{jl}$ is always real. The vector potential strength may be then chosen as follows,

$$A_{(j,l)}(d) = \begin{cases} \frac{1}{2d}\arg\, T_{jl} & \text{if} \quad \mathrm{Re}\ T_{jl} \geq 0\,, \\ \frac{1}{2d}\left(\arg\, T_{jl} - \pi\right) & \text{if} \quad \mathrm{Re}\ T_{jl} < 0 \end{cases} \tag{44}$$

for all $j \in \hat{m}$, $l \in N_j \backslash \hat{m}$. We remark that this choice is obviously not the only one possible. Note that in this situation, namely if $j \in \hat{m}$ and $l \in N_j \backslash \hat{m}$, the potentials do not depend on d. Taking (44) into account, Eq. (43) simplifies to

$$\frac{1}{2 + d \cdot w_{\{j,l\}}} = \langle T_{jl} \rangle \cdot \left(dv_l + \#N_l - \sum_{h \in N_l} \frac{1}{2 + d \cdot w_{\{l,h\}}} \right) \quad \forall l \geq m+1,\, j \in N_l\,; \tag{45}$$

note that $j \in \hat{m} \wedge l \in N_j \backslash \hat{m} \Leftrightarrow l \geq m+1 \wedge j \in N_l$. The symbol $\langle \cdot \rangle$ here has the following meaning: if $c \in \mathbb{C}$, then

$$\langle c \rangle = \begin{cases} |c| & \text{if} \quad \mathrm{Re}\ c \geq 0\,, \\ -|c| & \text{if} \quad \mathrm{Re}\ c < 0\,. \end{cases}$$

Summing (45) over $j \in N_l$ we get

$$\sum_{j \in N_l} \frac{1}{2 + d \cdot w_{\{j,l\}}} = \sum_{j \in N_l} \langle T_{jl} \rangle \cdot \left(dv_l + \#N_l - \sum_{h \in N_l} \frac{1}{2 + d \cdot w_{\{l,h\}}} \right),$$

i.e.

$$\left(1 + \sum_{h \in N_l} \langle T_{hl} \rangle \right) \sum_{j \in N_l} \frac{1}{2 + d \cdot w_{\{j,l\}}} = \sum_{j \in N_l} \langle T_{jl} \rangle \cdot (dv_l + \#N_l)\ .$$

We have to distinguish here two situations:
(i) If $1 + \sum_{h \in N_l} \langle T_{hl} \rangle \neq 0$, one obtains

$$\sum_{h \in N_l} \frac{1}{2 + d \cdot w_{\{l,h\}}} = \frac{\sum_{h \in N_l} \langle T_{hl} \rangle}{1 + \sum_{h \in N_l} \langle T_{hl} \rangle} \cdot (dv_l + \#N_l)\,,$$

and the substitution of the left-hand side into the right-hand side of (45) leads to the formula for $1/(2 + d \cdot w_{\{j,l\}})$, namely

$$\frac{1}{2 + d \cdot w_{\{j,l\}}} = \langle T_{jl} \rangle \cdot \frac{dv_l + \#N_l}{1 + \sum_{h \in N_l} \langle T_{hl} \rangle} \qquad \forall\, j \in \hat{m},\ l \in N_j \backslash \hat{m}\,.$$

We observe that the sum in the denominator may be computed over the whole set $\hat{m}$ as well, since $h \notin \mathbb{N}_l \Rightarrow T_{hl} = 0$, which slightly simplifies the formula,

$$\frac{1}{2 + d \cdot w_{\{j,l\}}} = \langle T_{jl} \rangle \cdot \frac{dv_l + \#N_l}{1 + \sum_{h=1}^{m} \langle T_{hl} \rangle} \qquad \forall\, j \in \hat{m},\ l \in N_j \backslash \hat{m}\,.$$

From here one can easily express $w_{\{j,l\}}$, if v_l is known. However, it turns out that $v_l(d)$, $l \geq m+1$ can be chosen almost arbitrarily, the only requirements are to keep the expression $dv_l + \#N_l$ nonzero and to satisfy (33), (34) and (41). The simplest choice possible is to define v_l by the expression

$$\frac{dv_l + \#N_l}{1 + \sum_{h=1}^{m} \langle T_{hl} \rangle} = 1\,,$$

which simplifies the expressions for other parameters. Here we obtain already expressions for v_l and $w_{\{j,l\}}$ if $l \geq m+1$, viz

$$v_l(d) = \frac{1 - \#N_l + \sum_{h=1}^{m} \langle T_{hl} \rangle}{d} \qquad \forall l \geq m+1\,, \tag{46}$$

$$w_{\{j,l\}}(d) = \frac{1}{d}\left(-2 + \frac{1}{\langle T_{jl} \rangle}\right) \qquad \forall j \in \hat{m},\ l \in N_j \backslash \hat{m}\,. \tag{47}$$

(ii) If $1 + \sum_{h \in N_l} \langle T_{hl} \rangle = 0$, it holds necessarily $dv_l + \#N_l = 0$, and consequently, $v_l = -\frac{\#N_l}{d}$. Note that this equation may be obtained from Eq. (46) by putting formally $1 + \sum_{h=1}^{m} \langle T_{hl} \rangle = 0$. It is easy to check that $w_{\{j,l\}}$ given by Eq. (47) satisfies (43) in the case $1 + \sum_{h \in N_l} \langle T_{hl} \rangle = 0$ as well. Summing these facts up, we conclude that Eqs. (46), (47) hold universally regardless whether $1 + \sum_{h \in N_l} \langle T_{hl} \rangle$ equals zero or not.

We would like to stress that the freedom in the choice of $v_l(d)$ is a consequence of the fact mentioned in Remark 2.2, namely that the number of parameters of a vertex coupling decreases with the decreasing value of rank(B).

Step II. Equation (39) together with the results of Step I will be used to determine $w_{\{j,k\}}(d)$ and $A_{(j,k)}(d)$ in the case when $j \in \hat{m}$ and $k \in N_j \cap \hat{m}$. From (39) we have

$$-\frac{\mathrm{e}^{2\mathrm{i}dA_{(j,k)}}}{2 + d \cdot w_{\{j,k\}}} = d \cdot S_{jk} + \sum_{l \in N_k \backslash \hat{m}} T_{jl} \frac{\mathrm{e}^{2\mathrm{i}dA_{(l,k)}}}{2 + d \cdot w_{\{l,k\}}}\,;$$

the pairs (l,k) appearing in the sum are of the type examined in Step I, i.e. $k \in \hat{m}$, $l \in N_k \backslash \hat{m}$). Thus one may substitute from (46) and (47) to obtain

$$-\frac{\mathrm{e}^{2\mathrm{i}dA_{(j,k)}}}{2 + d \cdot w_{\{j,k\}}} = d \cdot S_{jk} + \sum_{l \in N_k \backslash \hat{m}} T_{jl} \overline{T_{kl}}\,.$$

We observe that the summation index may run through the whole set $\hat{n} \backslash \hat{m}$, because $l \geq m+1 \wedge l \notin N_k \Rightarrow T_{kl} = 0$. This allows one to obtain a more elegant formula. In a similar way as above, we find the expression for $A_{(j,k)}$,

$$A_{(j,k)}(d) = \frac{1}{2d} \arg\left(d \cdot S_{jk} + \sum_{l=m+1}^{n} T_{jl} \overline{T_{kl}}\right) \qquad \text{for} \quad \mathrm{Re}\left(d \cdot S_{jk} + \sum_{l=m+1}^{n} T_{jl} \overline{T_{kl}}\right) \geq 0 \tag{48a}$$

and

$$A_{(j,k)}(d) = \frac{1}{2d}\left[\arg\left(d \cdot S_{jk} + \sum_{l=m+1}^{n} T_{jl} \overline{T_{kl}}\right) - \pi\right] \quad \text{for} \quad \mathrm{Re}\left(d \cdot S_{jk} + \sum_{l=m+1}^{n} T_{jl} \overline{T_{kl}}\right) < 0\,, \tag{48b}$$

and for S_{jk},

$$\frac{1}{2+d\cdot w_{\{j,k\}}} = -\left\langle d\cdot S_{jk} + \sum_{l=m+1}^{n} T_{jl}\overline{T_{kl}} \right\rangle . \tag{49}$$

Step III. Substitution of the results of Steps I and II into Eq. (38) provides an expression for $v_j(d)$ in the case when $j \in \hat{m}$. A simple calculation gives

$$v_j(d) = S_{jj} - \frac{\#N_j}{d} - \sum_{k=1}^{m}\left\langle S_{jk} + \frac{1}{d}\sum_{l=m+1}^{n} T_{jl}\overline{T_{kl}} \right\rangle + \frac{1}{d}\sum_{l=m+1}^{n}(1+\langle T_{jl}\rangle)\langle T_{jl}\rangle . \tag{50}$$

Since S is a self-adjoint matrix, the term S_{jj} is real, thus the whole right-hand side is a real expression.

Step IV. Finally, we verify conditions (33), (34), and (41), the last one being restricted to $k \in N_j \cap \hat{m}$. This step consists in trivial substitutions:

$$(33): \quad \lim_{d\to 0}\left(dv_j + \#N_j - \sum_{k\in N_j}\frac{1}{2+d\cdot w_{\{j,k\}}}\right) = \lim_{d\to 0} 1 = 1 \in \mathbb{R}\backslash\{0\} \quad \forall j \geq m+1 ,$$

$$(34): \quad \lim_{d\to 0}\frac{1}{2+d\cdot w_{\{j,k\}}} = \lim_{d\to 0}\langle T_{kj}\rangle = \langle T_{kj}\rangle \in \mathbb{R}\backslash\{0\} \quad \forall j \geq m+1,\ k \in N_j ,$$

$$(41): \quad \lim_{d\to 0}\frac{1}{2+d\cdot w_{\{j,k\}}} = -\lim_{d\to 0}\left\langle d\cdot S_{jk} + \sum_{l=m+1}^{n} T_{jl}\overline{T_{kl}}\right\rangle = \left\langle \sum_{l=m+1}^{n} T_{jl}\overline{T_{kl}}\right\rangle \in \mathbb{R}$$
$$\forall j \in \hat{m},\ k \in N_j \cap \hat{m} .$$

4. The norm-resolvent convergence

In the previous section we have shown that any vertex coupling in the center point of a star graph may be regarded as a limit of a certain family of graphs supporting nothing but δ couplings, δ interactions and constant vector potentials. The parameter values of all the δ's and vector potentials have been derived using a method devised originally in [CS98, SMMC99] for the case of a generalized point interaction on the line. The aim of this section is to give a clear meaning to this convergence. Specifically, we are going to show that the Hamiltonian of the approximating system converges to the Hamiltonian of the approximated system *in the norm-resolvent sense*, with the natural consequences for the convergence of eigenvalues, eigenfunctions, etc.

We denote the Hamiltonian of the star graph Γ with the coupling (6) at the vertex as H^{Ad} (referring to the *a*pproximate*d* system), and H_d^{Ag} will stand for the *a*pproximating family of graphs that has been constructed in the previous section. Symbols $R^{\mathrm{Ad}}(k^2)$ and $R_d^{\mathrm{Ag}}(k^2)$ will then denote the resolvents of H^{Ad} and H_d^{Ag} at the points k^2 from the resolvent set. Needless to say, the operators act on different spaces: $R^{\mathrm{Ad}}(k^2)$ on $L^2(G)$, where $G = (\mathbb{R}^+)^n$ corresponds to the star graph Γ, and $R_d^{\mathrm{Ag}}(k^2)$ on $L^2(G_d)$, where

$$G_d = (\mathbb{R}^+)^n \oplus (0,d)^{\sum_{j=1}^{n} N_j} . \tag{51}$$

Our goal is to compare these resolvents. In order to do that, we need to identify $R^{\mathrm{Ad}}(k^2)$ with the orthogonal sum

$$R_d^{\mathrm{Ad}}(k^2) = R^{\mathrm{Ad}}(k^2) \oplus 0 , \tag{52}$$

where 0 is a zero operator acting on the space $L^2\left((0,d)^{\sum_{j=1}^n N_j}\right)$ which is removed in the limit. Then both the operators $R_d^{\mathrm{Ad}}(k^2)$ and $R_d^{\mathrm{Ag}}(k^2)$ are defined as acting on functions from the set G_d which are vector functions with $n + \sum_{j=1}^n N_j$ components; we will index the components by the set

$$\mathcal{I} = \hat{n} \cup \{(l,h)|\ l \in \hat{n}, h \in N_l\}\ . \tag{53}$$

In this setting we are able to state now the main theorem of this section and the whole paper.

Theorem 4.1. *Let $v_j,\ j \in \hat{n},$, $w_{\{j,k\}}\ j \in \hat{n}, k \in \mathbb{N}_j$ and $A^{(j,k)}(d)$ depend on d according to* (50)*,* (46)*,* (49)*,* (47)*,* (48) *and* (44)*, respectively. Then the family $H^{\mathrm{Ag}}(d)$ converges to H_d^{Ad} in the norm-resolvent sense as $d \to 0_+$.*

Proof. We have to compare the resolvents $R_d^{\mathrm{Ad}}(k^2)$ and $R_d^{\mathrm{Ag}}(k^2)$. It is obviously sufficient to check the convergence in the Hilbert-Schmidt norm,

$$\left\| R_d^{\mathrm{Ag}}(k^2) - R_d^{\mathrm{Ad}}(k^2) \right\|_2 \to 0_+ \quad \text{as } d \longrightarrow 0_+\,,$$

in other words, to show that the difference of the corresponding resolvent kernels denoted as $\mathcal{G}_k^{\mathrm{Ag},d}$ and $\mathcal{G}_k^{\mathrm{Ad},d}$, respectively, tends to zero in $L^2(G_d \oplus G_d)$. Recall that these kernels, or Green's functions, are in our case matrix functions with $\left(n + \sum_{j=1}^n N_j\right) \times \left(n + \sum_{j=1}^n N_j\right)$ entries. We will index the entries by pairs of indices taken from the set $\mathcal{I}$ (cf. (53)).

The proof is divided into three parts. In the first and the second part we will derive the resolvent kernels $\mathcal{G}_k^{\mathrm{Ag},d}$ and $\mathcal{G}_k^{\mathrm{Ad},d}$, respectively, in the last part we compare them and demonstrate the norm-resolvent convergence.

I. Resolvent of the approximated Hamiltonian

Let us construct first $\mathcal{G}_k^{\mathrm{Ad}}$ for the star-graph Hamiltonian with the condition (1) at the vertex. We begin with n independent halflines with Dirichlet condition at its endpoints; Green's function for each of them is well-known to be

$$\mathcal{G}_{\mathrm{i}\kappa}(x,y) = \frac{\sinh \kappa x_< \, \mathrm{e}^{-\kappa x_>}}{\kappa}\,,$$

where $x_< := \min\{x,y\}$, $x_> := \max\{x,y\}$, and we put $\mathrm{i}\kappa = k$ assuming conventionally $\mathrm{Re}\,\kappa > 0$. The sought Green's function is then given by Krein's formula [AGHH05, App. A],

$$R^{\mathrm{Ad}}(k^2) = R^{Hl}(k^2) + \sum_{j,l=1}^n \lambda_{jl}(k^2)\left(\phi_l\left(\overline{k^2}\right), \cdot\right)_{L^2((\mathbb{R}^+)^n)} \phi_j(k^2)\,, \tag{54}$$

where $R^{Hl}(k^2)$ acts on each half line as an integral operator with the kernel $\mathcal{G}_{\mathrm{i}\kappa}$, and for $\phi_j(k^2)$ one can choose any elements of the deficiency subspaces of the largest common restriction; we will work with $\left(\phi_j(k^2)(\vec{x})\right)_l = \delta_{jl}\mathrm{e}^{-\kappa x_j}$ where the symbol $\vec{x}$ stands here for the vector $(x_1, \ldots, x_n) \in (\mathbb{R}^+)^n$. Then we have

$$R^{\mathrm{Ad}}(k^2)\begin{pmatrix}\psi_1\\ \vdots\\ \psi_n\end{pmatrix}\begin{pmatrix}x_1\\ \vdots\\ x_n\end{pmatrix} = \begin{pmatrix}\int_0^{+\infty}\mathcal{G}_{\mathrm{i}\kappa}(x_1,y_1)\psi_1(y_1)\mathrm{d}y_1\\ \vdots\\ \int_0^{+\infty}\mathcal{G}_{\mathrm{i}\kappa}(x_n,y_n)\psi_n(y_n)\mathrm{d}y_n\end{pmatrix} + \sum_{j,l=1}^n \lambda_{jl}(k^2)\left(\mathrm{e}^{-\bar{\kappa}y_l}, \psi_l(y_l)\right)_{L^2(\mathbb{R}^+)}\begin{pmatrix}0\\ \vdots\\ \mathrm{e}^{-\kappa x_j}\\ \vdots\\ 0\end{pmatrix},$$

which should be satisfied for any $(\psi_1,\dots,\psi_n)^T \in \bigoplus_{j=1}^n L^2(\mathbb{R}^+)$. We observe that for all $j \in \hat{n}$, the j-th component on the right hand side depends only on the variable x_j. That is why one can consider the components as functions of one variable; we denote them as $g_j(x_j)$, $j \in \hat{n}$, in other words,

$$R^{\mathrm{Ad}}(k^2)\begin{pmatrix}\psi_1\\ \vdots\\ \psi_n\end{pmatrix}\begin{pmatrix}x_1\\ \vdots\\ x_n\end{pmatrix} =: \begin{pmatrix}g_1(x_1)\\ \vdots\\ g_n(x_n)\end{pmatrix}.$$

The functions g_j are therefore given explicitly by

$$g_j(x_j) = \int_0^{+\infty} \mathcal{G}_{\mathrm{i}\kappa}(x_j,y)\psi_j(y)\mathrm{d}y + \sum_{l=1}^n \lambda_{jl}(k^2)\int_0^{+\infty} \mathrm{e}^{-\kappa y}\psi_l(y)\mathrm{d}y\cdot \mathrm{e}^{-\kappa x_j}\,.$$

Since the resolvent maps the whole Hilbert space into the domain of the operator, these functions have to satisfy the boundary conditions at the vertex,

$$\sum_{h=1}^n A_{jh}g_h(0) + \sum_{h=1}^n B_{jh}g_h'(0) = 0 \quad \text{for all} \;\; j \in \hat{n}\,, \tag{55}$$

where

$$A = \begin{pmatrix} S & 0\\ -T^* & I^{(n-m)}\end{pmatrix}, \quad -B = \begin{pmatrix} I^{(m)} & T\\ 0 & 0\end{pmatrix}.$$

Using the explicit form of $\mathcal{G}_{\mathrm{i}\kappa}(x_h,y)$ and the equality $\left.\frac{\partial\mathcal{G}_\kappa(x_h,y)}{\partial x_h}\right|_{x_h=0} = \mathrm{e}^{-\kappa y}$, we find

$$g_h(0) = \sum_{l=1}^n \lambda_{hl}(k^2)\int_0^{+\infty}\mathrm{e}^{-\kappa y}\psi_l(y)\mathrm{d}y$$

and

$$g_h'(0) = \int_0^{+\infty}\mathrm{e}^{-\kappa y}\psi_h(y)\mathrm{d}y - \kappa\sum_{l=1}^n \lambda_{hl}(k^2)\int_0^{+\infty}\mathrm{e}^{-\kappa y}\psi_l(y)\mathrm{d}y\,.$$

Substituting from these two relations into (55) we get a system of equations,

$$\sum_{l=1}^n\int_0^{+\infty}\left(\sum_{h=1}^n A_{jh}\lambda_{hl}(k^2) + B_{jl} - \kappa\sum_{h=1}^n B_{jh}\lambda_{hl}(k^2)\right)\mathrm{e}^{-\kappa y}\psi_l(y)\mathrm{d}y = 0$$

with $j \in \hat{n}$. We require that the left-hand side vanishes for any $\psi_1,\psi_2,\dots,\psi_n$; this yields the condition $A\Lambda + B - \kappa B\Lambda = 0$. From here it is easy to find the matrix $\Lambda(k^2)$: we have $(A-\kappa B)\Lambda = -B$, and therefore

$$\Lambda(k^2) = (A-\kappa B)^{-1}(-B)\,.$$

Substituting the explicit forms of A and $-B$ into the expression for Λ, we obtain

$$\Lambda(k^2) = \begin{pmatrix} S+\kappa I^{(m)} & \kappa T\\ -T^* & I^{(n-m)}\end{pmatrix}^{-1}\begin{pmatrix} I^{(m)} & T\\ 0 & 0\end{pmatrix},$$

or explicitly

$$\Lambda(k^2) = \begin{pmatrix} (S+\kappa I^{(m)}+\kappa TT^*)^{-1} & (S+\kappa I^{(m)}+\kappa TT^*)^{-1}T\\ T^*(S+\kappa I^{(m)}+\kappa TT^*)^{-1} & T^*(S+\kappa I^{(m)}+\kappa TT^*)^{-1}T\end{pmatrix}$$

provided that $(S + \kappa I^{(m)} + \kappa TT^*)^{-1}$ is well defined. To check that the matrix $S + \kappa I^{(m)} + \kappa TT^*$ is regular, we notice that

$$S + \kappa I^{(m)} + \kappa TT^* = S + \kappa(I^{(m)} + TT^*)\,, \tag{56}$$

where the matrix $I^{(m)} + TT^*$ is positive definite and thus regular, and the value κ may be chosen arbitrarily with the only restriction $\operatorname{Re}\kappa > 0$. Consequently, it suffices to choose $\operatorname{Re}\kappa$ big enough to make the matrix $\kappa(I^{(m)}+TT^*)$ dominate over S, which ensures the regularity of $S+\kappa(I^{(m)}+TT^*)$.

Having found the coefficients $\lambda_{jl}(k^2)$, we have fully determined the Green's function $\mathcal{G}^{\mathrm{Ad}}_{\mathrm{i}\kappa}$ of the approximated system. Recall that it is an $n \times n$ matrix-valued function the (j,l)-th element of which is given by

$$\mathcal{G}^{\mathrm{Ad}}_{\mathrm{i}\kappa,jl}(x,y) = \delta_{jl}\frac{\sinh\kappa x_< \,\mathrm{e}^{-\kappa x_>}}{\kappa} + \lambda_{jl}(k^2)\,\mathrm{e}^{-\kappa x}\mathrm{e}^{-\kappa y}\,; \tag{57}$$

we use the convention that x is from the j-th halfline and y from the l-th one. The kernel of the operator $R^{\mathrm{Ad}}_d(k^2)$ is according to (52) given simply by

$$\mathcal{G}^{\mathrm{Ad},d}_{\mathrm{i}\kappa} = \left(\begin{array}{c|c} \mathcal{G}^{\mathrm{Ad}}_{\mathrm{i}\kappa} & 0 \\ \hline 0 & 0 \end{array}\right), \tag{58}$$

i.e. all entries of $\mathcal{G}^{\mathrm{Ad},d}_{\mathrm{i}\kappa}$ except for those indexed by $j,l \in \hat{n}$ vanish.

II. Resolvents of the approximating family of Hamiltonians

Next we will pass to resolvent construction for the approximating family of operators H^{Ag}_d. As a starting point we consider n independent halflines and $\sum_{j=1}^n N_j$ lines of the length d with constant vector potentials $A_{(j,l)}(d)$, both halflines and lines of the finite length are supposed to have Dirichlet endpoints. We know that the Green's function is $\mathcal{G}_{\mathrm{i}\kappa}(x,y) = \kappa^{-1}\sinh\kappa x_<\mathrm{e}^{-\kappa x_>}$ in the case of the halflines. The Green's function in the case of the lines of the length d will be found in two steps. We begin with a line without vector potential and with Dirichlet endpoints; the Green's function can be easily derived being equal to

$$\tilde{\mathcal{G}}_{\mathrm{i}\kappa}(x,y) = \frac{\sinh\kappa x_< \sinh\kappa(d-x_>)}{\kappa\sinh\kappa d}\,.$$

The Hamiltonian of a free particle on a line segment acts as $-\frac{\mathrm{d}^2}{\mathrm{d}x^2}$, if a vector potential A is added it changes to $\left(-\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}x} - A\right)^2$. Using Lemma 3.3 it is easy to check that

$$\left(-\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}x} - A\right)^2 = U\left(-\frac{\mathrm{d}^2}{\mathrm{d}x^2}\right)U^*\,, \tag{59}$$

where U is the unitary operator acting as

$$(U\psi)(x) = \mathrm{e}^{\mathrm{i}Ax}\psi(x)\,.$$

If we denote $H_0 = -\frac{\mathrm{d}^2}{\mathrm{d}x^2}$ and $H_A = \left(-\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}x} - A\right)^2$, we see that

$$(H_A - \lambda)^{-1} = (UH_0U^* - \lambda)^{-1} = (U(H_0 - \lambda)\,U^*)^{-1} = U\,(H_0 - \lambda)^{-1}\,U^*\,,$$

so the corresponding resolvents are related by the relation analogous to (59). This yields

$$\left((H_A-\lambda)^{-1}\psi\right)(x) = \left(U(H_A-\lambda)^{-1}U^*\psi\right)(x) = \mathrm{e}^{\mathrm{i}Ax}\int_0^d \tilde{\mathcal{G}}_{\mathrm{i}\kappa}(x,y)\,\mathrm{e}^{-\mathrm{i}Ay}\psi(y)\mathrm{d}y$$
$$= \int_0^d \mathrm{e}^{\mathrm{i}Ax}\frac{\sinh\kappa x_<\sinh\kappa(d-x_>)}{\kappa\sinh\kappa d}\,\mathrm{e}^{-\mathrm{i}Ay}\psi(y)\mathrm{d}y\,,$$

thus the sought integral kernel is equal to

$$\tilde{\mathcal{G}}^A_{\mathrm{i}\kappa}(x,y) = \mathrm{e}^{\mathrm{i}Ax}\frac{\sinh\kappa x_<\sinh\kappa(d-x_>)}{\kappa\sinh\kappa d}\,\mathrm{e}^{-\mathrm{i}Ay}\,.$$

Now we can proceed to the derivation of the complete resolvent $R_d^{\mathrm{Ag}}(k^2)$ which will be done again by means of the Krein's formula. The situation here is more complicated than in the case of the approximated system; recall that $R_d^{\mathrm{Ag}}(k^2)$, as well as $H_d^{\mathrm{Ad}}(k^2)$, acts on the larger Hilbert space $L^2(G_d)$, where G_d has been defined in (51). Moreover, the application of Krein's formula means that we have to connect all the line segments using the appropriate boundary conditions, i.e. we must change boundary conditions at $n+2\sum_{j=1}^n N_j$ endpoints, specifically n belonging to n half lines and $2\sum_{j=1}^n N_j$ belonging to $\sum_{j=1}^n N_j$ segments of the length d. Thus the index set for the indices in the sum on the right hand side of the formula has $n+2\sum_{j=1}^n N_j$ elements; we will index them by the set

$$\hat{\mathcal{I}} = \hat{n}\cup\left\{(l,h)^0\middle|\ l\in\hat{n}, h\in N_l\right\}\cup\left\{(l,h)^d\middle|\ l\in\hat{n}, h\in N_l\right\}\,.$$

The elements of $\hat{n}$ correspond to changed boundary conditions at the endpoints of the half lines, and the elements of the type $(l,h)^0$ and $(l,h)^d$ ($h\in N_l$) correspond to changed boundary conditions at the endpoints of the segments of the length d which are connected to the endpoint of the l-th half line. If we denote by the symbol $R_d^{\mathrm{Dc}}(k^2)$ the resolvent of the system of the $n+\sum_{j=1}^n N_j$ decomposed edges with Dirichlet boundary conditions at the endpoints, Krein's formula for this pair of operators has the form

$$R_d^{\mathrm{Ag}}(k^2) = R_d^{\mathrm{Dc}}(k^2) + \sum_{J,L\in\hat{\mathcal{I}}}\lambda^d_{JL}(k^2)\left(\phi^d_L\left(\overline{k^2}\right),\cdot\right)_{L^2(G_d)}\phi^d_J(k^2)\,. \tag{60}$$

The role of the superscript d in the lambda symbols is to distinguish them from λ_{jl} that have been used in Eq. (54) for the resolvent of the approximated system. The functions ϕ^d_J ($J\in\hat{\mathcal{I}}$) may be chosen, as before in the case of the approximated system, as any elements of the corresponding deficiency subspaces of the largest common restriction. Note that each function ϕ^d_J has $n+\sum_{j=1}^n N_j$ components indexed by elements of the set $\mathcal{I} = \hat{n}\cup\{(l,h)|\ l\in\hat{n}, h\in N_l\}$. It turns out that a suitable choice is

$$\begin{aligned}
\left(\phi_j(k^2)^d(\vec{x})\right)_{\tilde{L}} &= \delta_{j\tilde{L}}\mathrm{e}^{-\kappa x_j} && \text{for}\quad j\in\hat{n}\,,\tilde{L}\in\mathcal{I}\,,\\
\left(\phi^d_{(l,h)^0}(k^2)(\vec{x})\right)_{\tilde{L}} &= \mathrm{e}^{\mathrm{i}A_{(l,h)}x_{(l,h)}}\delta_{(l,h)\tilde{L}}\sinh\kappa x_{(l,h)} && \text{for}\quad l\in\hat{n},\ h\in N_l\,,\tilde{L}\in\mathcal{I}\\
\left(\phi^d_{(l,h)^d}(k^2)(\vec{x})\right)_{\tilde{L}} &= \mathrm{e}^{\mathrm{i}A_{(l,h)}x_{(l,h)}}\delta_{(l,h)\tilde{L}}\sinh\kappa(d-x_{(l,h)}) && \text{for}\quad l\in\hat{n},\ h\in N_l\,,\tilde{L}\in\mathcal{I}\,,
\end{aligned} \tag{61}$$

where the symbol $\vec{x}$ denotes the vector from G_d with the components indexed by $\mathcal{I}$. We remark that if $J\in\hat{n}$, ϕ^d_J is independent of d and equal to the corresponding function chosen above in the case of the approximated system.

If we apply the operator (60) to an arbitrary $\Psi \in \bigoplus_{j=1}^{n} L^2(G_d)$, we obtain a vector function with $n + \sum_{j=1}^{n} N_j$ components indexed by $\mathcal{I}$, we denote them by g_j ($j \in \hat{n}$) and $g_{(l,h)}$ with $l \in \hat{n}, h \in N_l$. As in the case of the approximated system, a component g_J depends on x_J only, thus each g_J can be considered as a function of a single variable. A calculation leads to the following explicit expressions for g_j, $j \in \hat{n}$ and $g_{(l,h)}, l \in \hat{n}, h \in N_l$; for better clarity we distinguish the integral variables on $\mathbb{R}^+$ and on $(0,d)$ by a tilde, i.e. $y \in \mathbb{R}^+$, $\tilde{y} \in (0,d)$.

$$\begin{aligned} g_j(x_j) = \int_0^{+\infty} \mathcal{G}_{\mathrm{i}\kappa}(x_j, y)\psi_j(y)\,\mathrm{d}y + \sum_{j'=1}^{n} \lambda^d_{jj'}(k^2) \int_0^{+\infty} \mathrm{e}^{-\kappa y}\cdot\psi_{j'}(y)\,\mathrm{d}y\cdot\mathrm{e}^{-\kappa x_j} \\ + \sum_{l'=1}^{n}\sum_{h'\in N_{l'}} \Bigg(\lambda^d_{j(l'h')^0}(k^2) \int_0^d \mathrm{e}^{-\mathrm{i}A_{(l',h')}\tilde{y}} \sinh\kappa\tilde{y}\cdot\psi_{(l',h')}(\tilde{y})\,\mathrm{d}\tilde{y} \\ + \lambda^d_{j(l'h')^d}(k^2) \int_0^d \mathrm{e}^{-\mathrm{i}A_{(l',h')}\tilde{y}} \sinh\kappa(d-\tilde{y})\cdot\psi_{(l',h')}(\tilde{y})\,\mathrm{d}\tilde{y} \Bigg)\cdot\mathrm{e}^{-\kappa x_j}\,. \end{aligned} \tag{62a}$$

$$\begin{aligned} g_{(l,h)}(x_{(l,h)}) = \int_0^d \tilde{\mathcal{G}}^{A_{(l,h)}}_{\mathrm{i}\kappa}(x_{(l,h)}, \tilde{y})\psi_{(l,h)}(\tilde{y})\,\mathrm{d}\tilde{y} \\ + \mathrm{e}^{\mathrm{i}A_{(l,h)}x_{(l,h)}}\cdot\sinh\kappa x_{(l,h)}\cdot\Bigg[\sum_{j'=1}^{n}\lambda^d_{(l,h)^0 j'}(k^2)\int_0^{+\infty}\mathrm{e}^{-\kappa y}\cdot\psi_{j'}(y)\,\mathrm{d}y \\ + \sum_{l'=1}^{n}\sum_{h'\in N_{l'}}\Bigg(\lambda^d_{(l,h)^0(l'h')^0}(k^2)\int_0^d \mathrm{e}^{-\mathrm{i}A_{(l',h')}\tilde{y}}\sinh\kappa\tilde{y}\cdot\psi_{(l',h')}(\tilde{y})\,\mathrm{d}\tilde{y} \\ + \lambda^d_{(l,h)^0(l'h')^d}(k^2)\int_0^d \mathrm{e}^{-\mathrm{i}A_{(l',h')}\tilde{y}}\sinh\kappa(d-\tilde{y})\cdot\psi_{(l',h')}(\tilde{y})\,\mathrm{d}\tilde{y}\Bigg)\Bigg] \\ + \mathrm{e}^{\mathrm{i}A_{(l,h)}x_{(l,h)}}\cdot\sinh\kappa(d-x_{(l,h)})\cdot\Bigg[\sum_{j'=1}^{n}\lambda^d_{(l,h)^d j'}(k^2)\int_0^{+\infty}\mathrm{e}^{-\kappa y}\cdot\psi_{j'}(y)\,\mathrm{d}y \\ + \sum_{l'=1}^{n}\sum_{h'\in N_{l'}}\Bigg(\lambda^d_{(l,h)^d(l'h')^0}(k^2)\int_0^d \mathrm{e}^{-\mathrm{i}A_{(l',h')}\tilde{y}}\sinh\kappa\tilde{y}\cdot\psi_{(l',h')}(\tilde{y})\,\mathrm{d}\tilde{y} \\ + \lambda^d_{(l,h)^d(l'h')^d}(k^2)\int_0^d \mathrm{e}^{-\mathrm{i}A_{(l',h')}\tilde{y}}\sinh\kappa(d-\tilde{y})\cdot\psi_{(l',h')}(\tilde{y})\,\mathrm{d}\tilde{y}\Bigg)\Bigg]\,. \end{aligned} \tag{62b}$$

By definition the function $(g_J)_{J\in\mathcal{I}}$ belongs to the domain of the operator H_d^{Ag}, in particular, it has to satisfy the boundary conditions at the points where the edges are connected by δ interactions and δ couplings. Step by step we will write down now all these boundary conditions; this will lead to the explicit expressions for the coefficients $\lambda^d_{JL}(k^2)$.

Step 1. The continuity at the points $W_{\{j,k\}}$ means

$$g_{(l,h)}(0) = g_{(h,l)}(0) \tag{63}$$

for all $l \in \hat{n}, h \in N_l$. Since $\tilde{\mathcal{G}}^{A_{(l,h)}}_{\mathrm{i}\kappa}(0,\tilde{y}) = 0$ for all $\tilde{y} \in (0,d)$, it holds

$$g_{(l,h)}(0) = \sinh\kappa d \cdot \left[\sum_{j'=1}^{n} \lambda^d_{(l,h)^d\, j'}(k^2) \int_0^{+\infty} \mathrm{e}^{-\kappa y} \psi_{j'}(y)\,\mathrm{d}y \right.$$
$$+ \sum_{l'=1}^{n} \sum_{h' \in N_{l'}} \left(\lambda^d_{(l,h)^d (l'h')^0}(k^2) \int_0^d \mathrm{e}^{-\mathrm{i}A_{(l',h')}\tilde{y}} \sinh\kappa\tilde{y}\, \psi_{(l',h')}(\tilde{y})\,\mathrm{d}\tilde{y} \right.$$
$$\left. \left. + \lambda^d_{(l,h)^d (l'h')^d}(k^2) \int_0^d \mathrm{e}^{-\mathrm{i}A_{(l',h')}\tilde{y}} \sinh\kappa(d-\tilde{y})\, \psi_{(l',h')}(\tilde{y})\,\mathrm{d}\tilde{y} \right) \right],$$

the expression for $g_{(h,l)}(0)$ is similar, just the positions of l and h are interchanged. Since Eq. (63) must be satisfied for any choice of the function $\Psi = (\psi_J)_{J\in\mathcal{I}}$, the following equalities obviously hold for $\forall l \in \hat{n}, h \in N_l$:

$$\begin{aligned} \lambda^d_{(l,h)^d\, j'}(k^2) &= \lambda^d_{(h,l)^d\, j'}(k^2) && \forall j' \in \hat{n}\,, \\ \lambda^d_{(l,h)^d (l',h')^0}(k^2) &= \lambda^d_{(h,l)^d (l',h')^0}(k^2) && \forall l' \in \hat{n}, h' \in N_{l'}\,, \\ \lambda^d_{(l,h)^d (l',h')^d}(k^2) &= \lambda^d_{(h,l)^d (l',h')^d}(k^2) && \forall l' \in \hat{n}, h' \in N_{l'}\,. \end{aligned} \tag{64}$$

In other words, all the coefficients $\lambda^d_{(l,h)^d J}(k^2)$ with $J \in \hat{\mathcal{I}}(k^2)$ are symmetric with respect to an interchange of l and h.

Step 2. The sum of derivatives in points $W_{\{j,k\}}$ is

$$g'_{(l,h)}(0) + g'_{(h,l)}(0) = w_{\{l,h\}} \cdot g_{(l,h)}(0) \tag{65}$$

for all $l \in \hat{n}, h \in N_l$. We substitute

$$\left.\frac{\partial \tilde{\mathcal{G}}^A_{\mathrm{i}\kappa}(x,\tilde{y})}{\partial x}\right|_{x=0} = \frac{\sinh\kappa(d-\tilde{y})}{\sinh\kappa d}\,\mathrm{e}^{-\mathrm{i}A\tilde{y}}\,,$$

$$\left(\mathrm{e}^{\mathrm{i}Ax}\sinh\kappa x\right)'\Big|_{x=0} = \kappa$$

and

$$\left(\mathrm{e}^{\mathrm{i}Ax}\sinh\kappa(d-x)\right)'\Big|_{x=0} = \kappa\cosh\kappa d - \mathrm{i}A\sinh\kappa d$$

into Eq. (65) and require the equality to be satisfied for any $\Psi = (\psi_J)_{J\in\mathcal{I}}$. In the course of the calculation, the outcome of the Step 1 is also used. As a result, we find how the coefficients $\lambda^d_{(l,h)^d J}(k^2)$ ($J \in \mathcal{I}$) can be expressed in terms of $\lambda^d_{(l,h)^0 J}(k^2)$ and $\lambda^d_{(h,l)^0 J}(k^2)$:

$$\lambda^d_{(l,h)^d\, j'}(k^2) = \frac{\kappa}{2\kappa\cosh\kappa d + w_{\{l,h\}}\sinh\kappa d}\left(\lambda^d_{(l,h)^0\, j'}(k^2) + \lambda^d_{(h,l)^0\, j'}(k^2)\right) \quad \forall j' \in \hat{n}\,, \tag{66a}$$

$$\lambda^d_{(l,h)^d (l',h')^0}(k^2) = \frac{\kappa}{2\kappa\cosh\kappa d + w_{\{l,h\}}\sinh\kappa d}\left(\lambda^d_{(l,h)^0 (l',h')^0}(k^2) + \lambda^d_{(h,l)^0 (l',h')^0}(k^2)\right) \quad \forall l' \in \hat{n}, h' \in N_{l'}\,, \tag{66b}$$

$$\lambda^d_{(l,h)^d (l',h')^d}(k^2) = \frac{\kappa}{2\kappa\cosh\kappa d + w_{\{l,h\}}\sinh\kappa d}\left(\lambda^d_{(l,h)^0 (l',h')^d}(k^2) + \lambda^d_{(h,l)^0 (l',h')^d}(k^2) + \frac{\delta_{(l,h)(l',h')}}{\kappa\sinh\kappa d}\right)$$
$$\forall l' \in \hat{n}, h' \in N_{l'} \tag{66c}$$

for the indices $l \in \hat{n}, h \in N_l$.

Step 3. The continuity at the points V_j requires

$$g_j(0) = g_{(j,h)}(d) \tag{67}$$

for all $j \in \hat{n}, h \in N_j$. Since $\mathcal{G}_{\mathrm{i}\kappa}(0,y) = 0$ for all $x \in \mathbb{R}^+$ and $\tilde{\mathcal{G}}^{A_{(l,h)}}_{\mathrm{i}\kappa}(d) = 0$ for all $\tilde{y} \in (0,d)$, it holds

$$\begin{aligned} g_j(0) = \sum_{j'=1}^{n} \lambda^d_{jj'}(k^2) \int_0^{+\infty} \mathrm{e}^{-\kappa y} \psi_{j'}(y)\,\mathrm{d}y \cdot \mathrm{e}^{-\kappa x_j} \\ + \sum_{l'=1}^{n} \sum_{h' \in N_{l'}} \left(\lambda^d_{j(l'h')^0}(k^2) \int_0^d \mathrm{e}^{-\mathrm{i}A_{(l',h'),\tilde{y}}} \sinh \kappa\tilde{y} \psi_{(l',h')}(\tilde{y})\,\mathrm{d}\tilde{y} \right. \\ \left. + \lambda^d_{j(l'h')^d}(k^2) \int_0^d \mathrm{e}^{-\mathrm{i}A_{(l',h'),\tilde{y}}} \sinh \kappa(d-\tilde{y}) \psi_{(l',h')}(\tilde{y})\,\mathrm{d}\tilde{y} \right), \end{aligned} \tag{68}$$

and

$$\begin{aligned} g_{(j,h)}(d) = \mathrm{e}^{\mathrm{i}A_{(j,h)}d} \cdot \sinh \kappa d \cdot \left[\sum_{j'=1}^{n} \lambda^d_{(j,h)^0 j'}(k^2) \int_0^{+\infty} \mathrm{e}^{-\kappa y} \psi_{j'}(y)\,\mathrm{d}y \right. \\ + \sum_{l'=1}^{n} \sum_{h' \in N_{l'}} \left(\lambda^d_{(j,h)^0(l'h')^0}(k^2) \int_0^d \mathrm{e}^{-\mathrm{i}A_{(l',h'),\tilde{y}}} \sinh \kappa\tilde{y} \psi_{(l',h')}(\tilde{y})\,\mathrm{d}\tilde{y} \right. \\ \left. \left. + \lambda^d_{(j,h)^0(l'h')^d}(k^2) \int_0^d \mathrm{e}^{-\mathrm{i}A_{(l',h'),\tilde{y}}} \sinh \kappa(d-\tilde{y}) \psi_{(l',h')}(\tilde{y})\,\mathrm{d}\tilde{y} \right) \right]. \end{aligned} \tag{69}$$

The relation (67) should be satisfied for any choice of $\Psi = (\psi_J)_{J \in \mathcal{I}}$, hence we obtain the coefficients $\lambda^d_{(j,h)^0 J}(k^2)$ with $J \in \mathcal{I}$ expressed in terms of $\lambda^d_{jJ}(k^2)$ in the following way

$$\lambda^d_{(j,h)^0 j'}(k^2) = \frac{1}{\sinh \kappa d}\, \mathrm{e}^{-\mathrm{i}dA_{(j,h)}} \cdot \lambda^d_{jj'}(k^2) \qquad \forall\, j' \in \hat{n}\,, \tag{70a}$$

$$\lambda^d_{(j,h)^0(l',h')^0}(k^2) = \frac{1}{\sinh \kappa d}\, \mathrm{e}^{-\mathrm{i}dA_{(j,h)}} \cdot \lambda^d_{j(l',h')^0}(k^2) \qquad \forall l' \in \hat{n}, h' \in N_{l'}\,, \tag{70b}$$

$$\lambda^d_{(j,h)^0(l',h')^d}(k^2) = \frac{1}{\sinh \kappa d}\, \mathrm{e}^{-\mathrm{i}dA_{(j,h)}} \cdot \lambda^d_{j(l',h')^d}(k^2) \qquad \forall l' \in \hat{n}, h' \in N_{l'} \tag{70c}$$

for $j \in \hat{n}, h \in N_j$. We also return to the result of Step 2 – we substitute there for $\lambda^d_{(j,h)^0 J}(k^2)$ the expressions that we have just obtained arriving thus at

$$\lambda^d_{(l,h)^d j'}(k^2) = \frac{\kappa}{2\kappa \cosh \kappa d + w_{\{l,h\}} \sinh \kappa d} \cdot \frac{1}{\sinh \kappa d} \cdot \left(\mathrm{e}^{-\mathrm{i}dA_{(l,h)}} \lambda^d_{lj'}(k^2) + \mathrm{e}^{-\mathrm{i}dA_{(h,l)}} \lambda^d_{hj'}(k^2) \right) \quad \forall\, j' \in \hat{n}\,, \tag{71a}$$

$$\lambda^d_{(l,h)^d(l',h')^0}(k^2) = \frac{\kappa}{2\kappa \cosh \kappa d + w_{\{l,h\}} \sinh \kappa d} \cdot \frac{1}{\sinh \kappa d} \cdot \left(\mathrm{e}^{-\mathrm{i}dA_{(l,h)}} \lambda^d_{l(l',h')^0}(k^2) + \mathrm{e}^{-\mathrm{i}dA_{(h,l)}} \lambda^d_{h(l',h')^0}(k^2) \right) \quad \forall l' \in \hat{n}, h' \in N_{l'}\,, \tag{71b}$$

$$\lambda^d_{(l,h)^d(l',h')^d}(k^2) = \frac{\kappa}{2\kappa\cosh\kappa d + w_{\{l,h\}}\sinh\kappa d}\cdot\frac{1}{\sinh\kappa d}\cdot$$
$$\cdot\left(\mathrm{e}^{-\mathrm{i}dA_{(l,h)}}\cdot\lambda^d_{l(l',h')^d}(k^2) + \mathrm{e}^{-\mathrm{i}dA_{(h,l)}}\cdot\lambda^d_{h(l',h')^d}(k^2) + \frac{1}{\kappa}\delta_{(l,h)(l',h')}\right)$$
$$\forall l' \in \hat{n}, h' \in N_{l'} \quad (71c)$$

for $l \in \hat{n}, h \in N_l$.

Step 4. In this step we examine the sum of derivatives at the points V_j, i.e. at the junctions of the halflines and connecting segments. Since the connecting lines support constant vector potentials, one has to rewrite the original condition into the form derived in Corollary 3.3. Note that the variable on the connecting segments is considered in the ingoing sense, thus the sign of the potentials $A_{(j,h)}$ ($h \in N_j$) has to be taken with the minus sign. The resulting condition is

$$g'_j(0) - \sum_{h\in N_j} g'_{(j,h)}(d) = \left(v_j - \mathrm{i}\sum_{h\in N_j} A_{(j,h)}\right)\cdot g_j(0) \quad (72)$$

for all $j \in \hat{n}$.

The way how to proceed in this step is essentially the same as in previous steps, only the calculus is slightly longer. With the aid of the formulæ

$$\left.\frac{\partial\mathcal{G}_{\mathrm{i}\kappa}(x,y)}{\partial x}\right|_{x=0} = \mathrm{e}^{-\kappa y},$$
$$\left.\frac{\partial\tilde{\mathcal{G}}^A_{\mathrm{i}\kappa}(x,\tilde{y})}{\partial x}\right|_{x=d} = -\frac{\mathrm{e}^{\mathrm{i}Ad}}{\sinh\kappa d}\cdot\sinh\kappa\tilde{y}\,\mathrm{e}^{-\mathrm{i}A\tilde{y}}$$

and

$$\left(\mathrm{e}^{\mathrm{i}Ax}\sinh\kappa x\right)'\Big|_{x=d} = (\kappa\cosh\kappa d + \mathrm{i}A\sinh\kappa d)\cdot\mathrm{e}^{\mathrm{i}Ad},$$
$$\left(\mathrm{e}^{\mathrm{i}Ax}\sinh\kappa(d-x)\right)'\Big|_{x=d} = -\kappa\,\mathrm{e}^{\mathrm{i}Ad},$$

used in Eq. (72), we arrive at an expression containing $\psi_1\ldots,\psi_n$ that should be satisfied for any choice of $\Psi = (\psi_J)_{J\in\mathcal{I}}$. This yields the following three groups of conditions:

$$\delta_{jj'} - \kappa\lambda^d_{jj'}(k^2) - \sum_{h\in N_j}\left(\kappa\cosh\kappa d + \mathrm{i}A_{(j,h)}\sinh\kappa d\right)\cdot\mathrm{e}^{\mathrm{i}dA_{(j,h)}}\lambda^d_{(j,h)^0 j'}(k^2)$$
$$+\kappa\sum_{h\in N_j}\left(\mathrm{e}^{\mathrm{i}dA_{(j,h)}}\lambda^d_{(j,h)^d j'}(k^2)\right) = \left(v_j - \mathrm{i}\sum_{h\in N_j}A_{(j,h)}\right)\lambda^d_{jj'}(k^2), \quad (73a)$$

$$\delta_{jl'}\frac{\mathrm{e}^{\mathrm{i}dA_{(j,h')}}}{\sinh\kappa d} - \kappa\lambda^d_{j(l,h')^0}(k^2) - \sum_{h\in N_j}\left(\kappa\cosh\kappa d + \mathrm{i}A_{(j,h)}\sinh\kappa d\right)\cdot\mathrm{e}^{\mathrm{i}dA_{(j,h)}}\lambda^d_{(j,h)^0(l,h')^0}(k^2)$$
$$+\kappa\sum_{h\in N_j}\left(\mathrm{e}^{\mathrm{i}dA_{(j,h)}}\lambda^d_{(j,h)^d(l,h')^0}(k^2)\right) = \left(v_j - \mathrm{i}\sum_{h\in N_j}A_{(j,h)}\right)\lambda^d_{j(l,h')^0}(k^2), \quad (73b)$$

$$-\kappa\lambda^d_{j(l,h')^d}(k^2)-\sum_{h\in N_j}\left(\kappa\cosh\kappa d+\mathrm{i}A_{(j,h)}\sinh\kappa d\right)\cdot\mathrm{e}^{\mathrm{i}dA_{(j,h)}}\lambda^d_{(j,h)^0(l,h')^d}(k^2)$$
$$+\kappa\sum_{h\in N_j}\left(\mathrm{e}^{\mathrm{i}dA_{(j,h)}}\lambda^d_{(j,h)^d(l,h')^d}(k^2)\right)=\left(v_j-\mathrm{i}\sum_{h\in N_j}A_{(j,h)}\right)\lambda^d_{j(l,h')^d}(k^2)\,. \quad (73c)$$

We use the equalities (70) and (71) to eliminate all terms of the type $\lambda^d_{(j,h)^0J}(k^2)$ and $\lambda^d_{(j,h)^dJ}(k^2)$, $J\in\hat{\mathcal{I}}$. In this way we obtain three independent systems of equation for $\lambda^d_{jj'}(k^2)$ $(j,j'\in\hat{n})$, $\lambda^d_{j(l',h')^0}(k^2)$ $(j,l'\in\hat{n},h'\in N'_l)$ and $\lambda^d_{j(l',h')^d}(k^2)$ $(j,l'\in\hat{n},h'\in N'_l)$:

$$\delta_{jj'}-\kappa\lambda^d_{jj'}(k^2)-\kappa\#N_j\frac{\cosh\kappa d}{\sinh\kappa d}\lambda^d_{jj'}(k^2)+\sum_{h\in N_j}\frac{\kappa^2}{\sinh\kappa d}\cdot\frac{\lambda^d_{jj'}(k^2)+\mathrm{e}^{2\mathrm{i}dA_{(j,h)}}\lambda^d_{hj'}(k^2)}{2\kappa\cosh\kappa d+w_{\{j,h\}}\sinh\kappa d}=v_j\lambda^d_{jj'}(k^2)\,, \quad (74a)$$

$$\delta_{jl'}\frac{\mathrm{e}^{\mathrm{i}dA_{(l',h')}}}{\sinh\kappa d}-\kappa\lambda^d_{j(l,h')^0}(k^2)-\kappa\#N_j\frac{\cosh\kappa d}{\sinh\kappa d}\lambda^d_{j(l,h')^0}(k^2)$$
$$+\sum_{h\in N_j}\frac{\kappa^2}{\sinh\kappa d}\cdot\frac{\lambda^d_{j(l,h')^0}(k^2)+\mathrm{e}^{2\mathrm{i}dA_{(j,h)}}\lambda^d_{h(l,h')^0}(k^2)}{2\kappa\cosh\kappa d+w_{\{j,h\}}\sinh\kappa d}=v_j\lambda^d_{j(l,h')^0}(k^2)\,, \quad (74b)$$

$$-\kappa\lambda^d_{j(l,h')^d}(k^2)-\kappa\#N_j\frac{\cosh\kappa d}{\sinh\kappa d}\lambda^d_{j(l,h')^d}(k^2)+\sum_{h\in N_j}\frac{\kappa^2}{\sinh\kappa d}\cdot\frac{\lambda^d_{j(l,h')^d}(k^2)+\mathrm{e}^{2\mathrm{i}dA_{(j,h)}}\lambda^d_{h(l,h')^d}(k^2)}{2\kappa\cosh\kappa d+w_{\{j,h\}}\sinh\kappa d}$$
$$+\frac{\kappa}{\sinh\kappa d}\cdot\sum_{h\in N_j}\frac{\mathrm{e}^{\mathrm{i}dA_{(j,h)}}}{2\kappa\cosh\kappa d+w_{\{j,h\}}\sinh\kappa d}\delta_{jl'}\delta_{hh'}=v_j\lambda^d_{j(l,h')^d}(k^2)\,. \quad (74c)$$

Let us focus, e.g., on Eq. (74a), which can be rewritten in the form

$$\sum_{h=1}^{n}\left[\delta_{jh}\left(\kappa+\kappa\#N_j\frac{\cosh\kappa d}{\sinh\kappa d}-\frac{\kappa}{\sinh\kappa d}\sum_{\tilde{h}\in N_j}\frac{\kappa}{2\kappa\cosh\kappa d+w_{\{j,\tilde{h}\}}\sinh\kappa d}+v_j\right)\right.$$
$$\left.-\chi_{N_j}(h)\cdot\frac{\kappa}{\sinh\kappa d}\cdot\frac{\mathrm{e}^{2\mathrm{i}dA_{(j,h)}}}{2\kappa\cosh\kappa d+w_{\{j,h\}}\sinh\kappa d}\right]\lambda^d_{hj'}(k^2)=\delta_{jj'} \quad (75)$$

for all $j,j'\in\hat{n}$; the symbol $\chi_{N_j}(h)$ is equal to one if $h\in N_j$ holds and zero otherwise. As we will see within a short time, it is convenient to introduce a matrix M_d the (j,h)-th element of which is defined by

$$[M_d]_{jh}=\delta_{jh}\left(\kappa+\kappa\#N_j\frac{\cosh\kappa d}{\sinh\kappa d}-\frac{\kappa}{\sinh\kappa d}\sum_{\tilde{h}\in N_j}\frac{\kappa}{2\kappa\cosh\kappa d+w_{\{j,\tilde{h}\}}\sinh\kappa d}+v_j\right)$$
$$-\chi_{N_j}(h)\cdot\frac{\kappa}{\sinh\kappa d}\cdot\frac{\mathrm{e}^{2\mathrm{i}dA_{(j,h)}}}{2\kappa\cosh\kappa d+w_{\{j,h\}}\sinh\kappa d}\,. \quad (76)$$

We also rewrite the set $\hat{I}$ as a union,

$$\hat{I} = \hat{n} \cup \mathcal{J}^0 \cup \mathcal{J}^d\,,$$

where $\mathcal{J}^0 = \left\{(l,h)^0 \middle|\, l \in \hat{n}, h \in N_l\right\}$ and $\mathcal{J}^d = \left\{(l,h)^d \middle|\, l \in \hat{n}, h \in N_l\right\}$, and define the symbols $\Lambda^{\mathrm{Ag},d}_{XY}(k^2)$ for $X, Y \in \left\{\hat{n}, \mathcal{J}^0, \mathcal{J}^d\right\}$ by the relation

$$\Lambda^{\mathrm{Ag},d}_{XY}(k^2) = \left(\lambda^d_{JL}(k^2)\right)_{J\in X, L\in Y}\,,$$

e.g. $\Lambda^{\mathrm{Ag},d}_{\hat{n}\mathcal{J}^0}(k^2) = \left(\lambda^d_{j(l',h')^0}(k^2)\right)_{j\in\hat{n},(l',h')^0\in\mathcal{J}^0}$. Obviously, the matrix $\Lambda^{\mathrm{Ag},d}(k^2)$ has the block structure

$$\Lambda^{\mathrm{Ag},d}(k^2) = \left(\begin{array}{c|c|c} \Lambda^{\mathrm{Ag},d}_{\hat{n}\hat{n}}(k^2) & \Lambda^{\mathrm{Ag},d}_{\hat{n}\mathcal{J}^0}(k^2) & \Lambda^{\mathrm{Ag},d}_{\hat{n}\mathcal{J}^d}(k^2) \\ \hline \Lambda^{\mathrm{Ag},d}_{\mathcal{J}^0\hat{n}}(k^2) & \Lambda^{\mathrm{Ag},d}_{\mathcal{J}^0\mathcal{J}^0}(k^2) & \Lambda^{\mathrm{Ag},d}_{\mathcal{J}^0\mathcal{J}^d}(k^2) \\ \hline \Lambda^{\mathrm{Ag},d}_{\mathcal{J}^d\hat{n}}(k^2) & \Lambda^{\mathrm{Ag},d}_{\mathcal{J}^d\mathcal{J}^0}(k^2) & \Lambda^{\mathrm{Ag},d}_{\mathcal{J}^d\mathcal{J}^d}(k^2) \end{array}\right).$$

We observe that the system of equations (75) is nothing but

$$M_d \Lambda^{\mathrm{Ag},d}_{\hat{n}\hat{n}}(k^2) = I\,,$$

and therefore $\Lambda^{\mathrm{Ag},d}_{\hat{n}\hat{n}}(k^2) = (M_d)^{-1}$, or in the components

$$\lambda^d_{jj'}(k^2) = \left[(M_d)^{-1}\right]_{jj'}\,. \tag{77a}$$

The matrices $\Lambda^{\mathrm{Ag},d}_{\hat{n}\mathcal{J}^0}(k^2)$ and $\Lambda^{\mathrm{Ag},d}_{\hat{n}\mathcal{J}^d}(k^2)$ can be found in a similar way. We start from Eqs. (74b) and (74c) and arrive at

$$\lambda^d_{j(l',h')^0}(k^2) = \frac{\mathrm{e}^{\mathrm{i}dA_{(l',h')}}}{\sinh\kappa d}\left[(M_d)^{-1}\right]_{jl'} \tag{77b}$$

and

$$\lambda^d_{j(l',h')^d}(k^2) = \frac{\kappa}{\sinh\kappa d}\cdot\frac{\mathrm{e}^{\mathrm{i}dA_{(l',h')}}}{2\kappa\cosh\kappa d + w_{\{l',h'\}}\sinh\kappa d}\left[(M_d)^{-1}\right]_{jl'}\,. \tag{77c}$$

To obtain expressions for $\Lambda^{\mathrm{Ag},d}_{\mathcal{J}^0X}(k^2)$ and $\Lambda^{\mathrm{Ag},d}_{\mathcal{J}^dX}(k^2)$ ($X = \mathcal{J}^0, \mathcal{J}^d$) we substitute (77a), (77b) and (77c) into Equations (70) and (71) which gives

$$\lambda^d_{(l,h)^0\,j'}(k^2) = \frac{\mathrm{e}^{-\mathrm{i}dA_{(l,h)}}}{\sinh\kappa d}\cdot\left[(M_d)^{-1}\right]_{lj'}\,, \tag{77d}$$

$$\lambda^d_{(l,h)^0(l',h')^0}(k^2) = \frac{\mathrm{e}^{-\mathrm{i}dA_{(l,h)}}}{\sinh\kappa d}\cdot\frac{\mathrm{e}^{\mathrm{i}dA_{(l',h')}}}{\sinh\kappa d}\left[(M_d)^{-1}\right]_{ll'}\,, \tag{77e}$$

$$\lambda^d_{(l,h)^0(l',h')^d}(k^2) = \frac{\mathrm{e}^{-\mathrm{i}dA_{(l,h)}}}{\sinh^2\kappa d}\cdot\frac{\kappa\cdot\mathrm{e}^{\mathrm{i}dA_{(l',h')}}}{2\kappa\cosh\kappa d + w_{\{l',h'\}}\sinh\kappa d}\left[(M_d)^{-1}\right]_{ll'}\,, \tag{77f}$$

$$\lambda^d_{(l,h)^d\,j'}(k^2) = \frac{\kappa}{2\kappa\cosh\kappa d + w_{\{l,h\}}\sinh\kappa d}\cdot\frac{1}{\sinh\kappa d}\cdot\left(\mathrm{e}^{-\mathrm{i}dA_{(l,h)}}\left[(M_d)^{-1}\right]_{lj'} + \mathrm{e}^{-\mathrm{i}dA_{(h,l)}}\left[(M_d)^{-1}\right]_{hj'}\right), \tag{77g}$$

$$\lambda^d_{(l,h)^d(l',h')^0}(k^2) = \frac{\kappa}{2\kappa\cosh\kappa d + w_{\{l,h\}}\sinh\kappa d}\cdot\frac{\mathrm{e}^{\mathrm{i}dA_{(l',h')}}}{\sinh^2\kappa d}\cdot \cdot\left(\mathrm{e}^{-\mathrm{i}dA_{(l,h)}}\cdot\left[(M_d)^{-1}\right]_{ll'} + \mathrm{e}^{-\mathrm{i}dA_{(h,l)}}\cdot\left[(M_d)^{-1}\right]_{hl'}\right), \quad (77h)$$

$$\lambda^d_{(l,h)^d(l',h')^d}(k^2) = \frac{\kappa}{2\kappa\cosh\kappa d + w_{\{l,h\}}\sinh\kappa d}\cdot\frac{1}{\sinh\kappa d}\cdot \cdot\left[\frac{\kappa}{\sinh\kappa d}\cdot\frac{\mathrm{e}^{\mathrm{i}dA_{(l',h')}}}{2\kappa\cosh\kappa d + w_{\{l',h'\}}\sinh\kappa d}\left(\mathrm{e}^{-\mathrm{i}dA_{(l,h)}}\cdot\left[(M_d)^{-1}\right]_{ll'} + \mathrm{e}^{-\mathrm{i}dA_{(h,l)}}\cdot\left[(M_d)^{-1}\right]_{hl'}\right) + \frac{1}{\kappa}\delta_{(l,h)(l',h')}\right]. \quad (77i)$$

Once we compute the elements of $(M_d)^{-1}$ explicitly, we will have fully explicit formulae for $\Lambda^{\mathrm{Ag},d}(k^2)$ we need. We start from the matrix M_d itself. We take the formula (76), substitute there the expressions for $v_j(d)$, $w_{\{j,k\}}(d)$ and $A_{(j,k)}(d)$ that have been obtained heuristically in the previous section and apply Taylor expansions to appropriate orders. A slightly laborious calculation leads to the formulae written below; note that the structure of the expression for the (j,h)-th element of the matrix M_d depends on whether j,h belong to $\hat{m}$ or to $\hat{n}\backslash\hat{m}$:

$$[M_d]_{jh} = \delta_{jh}\left(\kappa + S_{jj} + \frac{1}{d}\sum_{l=m+1}^{n} T_{jl}\overline{T_{lj}}\right) + S_{jh} + \frac{1}{d}\sum_{l=m+1}^{n} T_{jl}\overline{T_{hl}} + O(d) \quad \text{for} \quad j,h\in\hat{m}\,, \quad (78a)$$

$$[M_d]_{jh} = -\frac{1}{d}T_{jh} + O(d) \quad \text{for} \quad j\in\hat{m}, h\geq m+1\,, \quad (78b)$$

$$[M_d]_{jh} = -\frac{1}{d}\overline{T_{hj}} + O(d) \quad \text{for} \quad j\geq m+1, h\in\hat{m}\,, \quad (78c)$$

$$[M_d]_{jh} = \delta_{jh}\left(\kappa + \frac{1}{d}\right) + O(d) \quad \text{for} \quad j,h\geq m+1\,. \quad (78d)$$

The matrix M_d has thus the form

$$M_d = \left(\begin{array}{c|c} S + \kappa I^{(m)} + \frac{1}{d}TT^* & -\frac{1}{d}T \\ \hline -\frac{1}{d}T^* & \left(\kappa+\frac{1}{d}\right)I^{(n-m)} \end{array}\right) + O(d)\,,$$

where $O(d)$ on the eight-hand side represents a matrix $n\times n$ the all entries of which are of order of $O(d)$ as $d\to 0$.

Our aim is to find the inverse of M_d. For this purpose, we denote the first term on the right-hand side, the principal one, as $M_{d,P}$ and notice that if $M_{d,P}$ is regular, then

$$[M_d]^{-1} = (M_{d,P} + O(d))^{-1} = \left[M_{d,P}(I + [M_{d,P}]^{-1}O(d))\right]^{-1} = \\ = \left[I - [M_{d,P}]^{-1}O(d)\right][M_{d,P}]^{-1} = [M_{d,P}]^{-1} - [M_{d,P}]^{-1}O(d)[M_{d,P}]^{-1}\,. \quad (79)$$

Moreover, if $[M_{d,P}]^{-1} = O(1)$ it obviously holds $[M_d]^{-1} = [M_{d,P}]^{-1} + O(d)$; in other words, under certain assumptions it suffices to find the inverse of $M_{d,P}$.

Since the matrix $M_{d,P}$ has a block structure, one can find $M_{d,P}$ in the same block structure. This in other words means that we are looking for a matrix $\left(\begin{array}{c|c} N_1 & N_2 \\ \hline N_3 & N_4 \end{array}\right)$ such that the relation

$$\left(\begin{array}{c|c} N_1 & N_2 \\ \hline N_3 & N_4 \end{array}\right) \cdot \left(\begin{array}{c|c} S + \kappa I^{(m)} + \frac{1}{d} TT^* & -\frac{1}{d} T \\ \hline -\frac{1}{d} T^* & \left(\kappa + \frac{1}{d}\right) I^{(n-m)} \end{array}\right) = \left(\begin{array}{c|c} I^{(m)} & 0 \\ \hline 0 & I^{(n-m)} \end{array}\right)$$

holds true. It turns out that

$$[M_{d,P}]^{-1} = \left(\begin{array}{cc} (S + \kappa I^{(m)} + \frac{\kappa}{1+\kappa d} TT^*)^{-1} & \frac{1}{1+\kappa d}(S + \kappa I^{(m)} + \frac{\kappa}{1+\kappa d} TT^*)^{-1} T \\ \frac{1}{1+\kappa d} T^* (S + \kappa I^{(m)} + \frac{\kappa}{1+\kappa d} TT^*)^{-1} & \frac{1}{(1+\kappa d)^2} T^* (S + \kappa I^{(m)} + \frac{\kappa}{1+\kappa d} TT^*)^{-1} T + \frac{d}{1+\kappa d} I^{(n-m)} \end{array} \right)$$

provided the matrix $S + \kappa I^{(m)} + \frac{\kappa}{1+\kappa d} TT^*$ is regular. Since $\frac{\kappa}{1+\kappa d} = \kappa + O(d)$, we may proceed in the same way as in (79), and we obtain

$$\left(S + \kappa I^{(m)} + \frac{\kappa}{1+\kappa d} TT^*\right)^{-1} = (S + \kappa I^{(m)} + \kappa TT^* + O(d))^{-1} = (S + \kappa I^{(m)} + \kappa TT^*)^{-1} + O(d)\,,$$

if the matrix $S + \kappa I^{(m)} + \kappa TT^*$ is regular. However, the regularity of this matrix has been discussed and proven for an appropriate κ at the end of the part devoted to the approximated system, see Eq. (56) and the paragraph following it. It follows that $M_{d,P}$ is regular as well, i.e. the condition on the regularity of $M_{d,P}$ in (79) is satisfied. Hence

$$[M_{d,P}]^{-1} = \left(\begin{array}{cc} (S + \kappa I^{(m)} + \kappa TT^*)^{-1} & (S + \kappa I^{(m)} + \kappa TT^*)^{-1} T \\ T^* (S + \kappa I^{(m)} + \kappa TT^*)^{-1} & T^* (S + \kappa I^{(m)} + \kappa TT^*)^{-1} T \end{array} \right) + O(d)\,,$$

and together with (79) we have

$$[M_d]^{-1} = \left(\begin{array}{cc} (S + \kappa I^{(m)} + \kappa TT^*)^{-1} & (S + \kappa I^{(m)} + \kappa TT^*)^{-1} T \\ T^* (S + \kappa I^{(m)} + \kappa TT^*)^{-1} & T^* (S + \kappa I^{(m)} + \kappa TT^*)^{-1} T \end{array} \right) + O(d)\,.$$

It is important to notice that

$$[M_d]^{-1} = O(1) \quad \text{for } d \to 0_+\,. \tag{80}$$

Combining the above result with Eq. (77a), we can conclude that

$$\Lambda^{\mathrm{Ag},d}_{\hat{n}\hat{n}}(k^2) = \left(\begin{array}{cc} (S + \kappa I^{(m)} + \kappa TT^*)^{-1} & (S + \kappa I^{(m)} + \kappa TT^*)^{-1} T \\ T^* (S + \kappa I^{(m)} + \kappa TT^*)^{-1} & T^* (S + \kappa I^{(m)} + \kappa TT^*)^{-1} T \end{array} \right) + O(d)\,,$$

hence

$$\Lambda^{\mathrm{Ag},d}_{\hat{n}\hat{n}}(k^2) = \Lambda^{\mathrm{Ad}}(k^2) + O(d)\,. \tag{81}$$

Having the coefficient matrix we can determine the resolvent kernel. First we introduce symbol $\mathcal{J} = \{(l,h)|\ l \in \hat{n}, h \in N_l\}$ (i.e. $\mathcal{I} = \hat{n} \cup \mathcal{J}$), then we employ a notation similar to the case of the matrix $\Lambda^{\mathrm{Ag},d}(k^2)$ and its submatrices. We introduce symbols $\mathcal{G}^{\mathrm{Ag},d}_{XY,k}$ for any pair $X, Y \in \{\hat{n}, \mathcal{J}\}$ to denote the blocks $\mathcal{G}^{\mathrm{Ag},d}_{k,XY} = \left(\mathcal{G}^{\mathrm{Ag},d}_{k,JL}\right)_{J\in X, L\in Y}$; then the integral kernel $\mathcal{G}^{\mathrm{Ag},d}_{k}$ of $R^{\mathrm{Ag}}_{d}(k^2)$ has the structure

$$\mathcal{G}^{\mathrm{Ag},d}_{k}(x,y) = \left(\begin{array}{c|c} \mathcal{G}^{\mathrm{Ag},d}_{k,\hat{n}\hat{n}}(x,y) & \mathcal{G}^{\mathrm{Ag},d}_{k,\hat{n}\mathcal{J}}(x,y) \\ \hline \mathcal{G}^{\mathrm{Ag},d}_{k,\mathcal{J}\hat{n}}(x,y) & \mathcal{G}^{\mathrm{Ag},d}_{k,\mathcal{J}\mathcal{J}}(x,y) \end{array}\right) \tag{82}$$

for $x, y \in G_d$. Using (58) we can write the difference in question as

$$\mathcal{G}^{\mathrm{Ag},d}_{\mathrm{i}\kappa} - \mathcal{G}^{Ad,d}_{\mathrm{i}\kappa} = \left(\begin{array}{c|c} \mathcal{G}^{\mathrm{Ag},d}_{\mathrm{i}\kappa,\hat{n}\hat{n}} - \mathcal{G}^{\mathrm{Ad}}_{\mathrm{i}\kappa} & \mathcal{G}^{\mathrm{Ag},d}_{\mathrm{i}\kappa,\hat{n}\mathcal{J}} \\ \hline \mathcal{G}^{\mathrm{Ag},d}_{\mathrm{i}\kappa,\hat{n}\mathcal{J}} & \mathcal{G}^{\mathrm{Ag},d}_{\mathrm{i}\kappa,\mathcal{J}\mathcal{J}} \end{array} \right). \tag{83}$$

III. Comparison of the resolvents

To make use of the above results we compute first explicit expressions for all the entries of $\mathcal{G}^{\mathrm{Ag},d}_{k}(x,y)$, up to the error term in the lambda coefficients indicated in (81). They may be derived from Eqs (62) together with (61):

$$\mathcal{G}^{\mathrm{Ag},d}_{\mathrm{i}\kappa,jj'}(x_j, y_{j'}) = \delta_{jj'} \frac{\sinh \kappa x_< \, \mathrm{e}^{-\kappa x_>}}{\kappa} + \lambda^d_{jj'}(k^2)\, \mathrm{e}^{-\kappa x_j} \mathrm{e}^{-\kappa y_{j'}} \quad \text{for} \quad j, j' \in \hat{n}\,, \tag{84a}$$

$$\mathcal{G}^{\mathrm{Ag},d}_{\mathrm{i}\kappa,j(l',h')}(x_j, y_{(l',h')}) = \mathrm{e}^{-\kappa x_j} \cdot \mathrm{e}^{-\mathrm{i}A_{(l',h')} y_{(l',h')}} \cdot \Big[\lambda^d_{j(l',h')^0}(k^2) \sinh \kappa y_{(l',h')} + \lambda^d_{j(l',h')^d}(k^2) \sinh \kappa (d - y_{(l',h')}) \Big]$$
$$\text{for} \quad j \in \hat{n}\,, (l',h') \in \mathcal{J}\,, \tag{84b}$$

$$\mathcal{G}^{\mathrm{Ag},d}_{\mathrm{i}\kappa,(l,h)j'}(x_{(l,h)}, y_{j'}) = \mathrm{e}^{\mathrm{i}A_{(l,h)} x_{(l,h)}} \cdot \Big[\lambda^d_{(l,h)^0 j'}(k^2) \sinh \kappa x_{(l,h)} + \lambda^d_{(l,h)^d j'}(k^2) \sinh \kappa (d - x_{(l,h)}) \Big] \cdot \mathrm{e}^{-\kappa y_{j'}}$$
$$\text{for} \quad (l,h) \in \mathcal{J}\,, j' \in \hat{n}\,, \tag{84c}$$

$$\begin{aligned} \mathcal{G}^{\mathrm{Ag},d}_{\mathrm{i}\kappa,(l,h)(l',h')}(x_{(l,h)}, y_{(l',h')}) &= \delta_{(l,h)(l',h')} \mathrm{e}^{\mathrm{i}A_{(l,h)} x_{(l,h)}} \frac{\sinh \kappa x_< \sinh \kappa (d - x_>)}{\kappa \sinh \kappa d} \, \mathrm{e}^{-\mathrm{i}A_{(l',h')} y_{(l',h')}} \\ &+ \mathrm{e}^{\mathrm{i}A_{(l,h)} x_{(l,h)}} \cdot \sinh \kappa x_{(l,h)} \cdot \mathrm{e}^{-\mathrm{i}A_{(l',h')} y_{(l',h')}} \cdot \Big[\lambda^d_{(l,h)^0 (l'h')^0} \sinh \kappa y_{(l',h')} + \lambda^d_{(l,h)^0 (l'h')^d} \sinh \kappa (d - y_{(l',h')}) \Big] \\ &+ \mathrm{e}^{\mathrm{i}A_{(l,h)} x_{(l,h)}} \cdot \sinh \kappa (d - x_{(l,h)}) \cdot \mathrm{e}^{-\mathrm{i}A_{(l',h')} y_{(l',h')}} \cdot \Big[\lambda^d_{(l,h)^d (l'h')^0} \sinh \kappa y_{(l',h')} + \lambda^d_{(l,h)^d (l'h')^d} \sinh \kappa (d - y_{(l',h')}) \Big] \end{aligned}$$
$$\text{for} \quad (l,h), (l',h') \in \mathcal{J}\,. \tag{84d}$$

Now we are able to compare the entries of $\mathcal{G}^{\mathrm{Ag},d}_{k}(x,y)$ given by (82) and $\mathcal{G}^{Ad,d}_{k}(x,y)$ as specified in (58)). We begin with the upper left submatrix $n \times n$ of (83). From the expressions for $\mathcal{G}^{\mathrm{Ad}}_{\mathrm{i}\kappa}$ and $\mathcal{G}^{\mathrm{Ag},d}_{\mathrm{i}\kappa,\hat{n}\hat{n}}$, cf. (57) and (84a), we have

$$\begin{aligned} &\Big[\mathcal{G}^{\mathrm{Ag},d}_{\mathrm{i}\kappa,\hat{n}\hat{n}} - \mathcal{G}^{\mathrm{Ad}}_{\mathrm{i}\kappa} \Big]_{jj'} (x_j, y_{j'}) \\ &\quad = \delta_{jj'} \frac{\sinh \kappa x_< \, \mathrm{e}^{-\kappa x_>}}{\kappa} + \lambda^d_{jj'}(k^2)\, \mathrm{e}^{-\kappa x_j} \mathrm{e}^{-\kappa y_{j'}} - \left[\delta_{jl} \frac{\sinh \kappa x_< \, \mathrm{e}^{-\kappa x_>}}{\kappa} + \lambda_{jj'}(k^2)\, \mathrm{e}^{-\kappa x_j} \mathrm{e}^{-\kappa y_{j'}} \right] \\ &= \Big(\lambda^d_{jj'}(k^2) - \lambda_{jj'}(k^2) \Big)\, \mathrm{e}^{-\kappa x_j} \mathrm{e}^{-\kappa y_{j'}} = \Big[\Lambda^{\mathrm{Ag},d}_{\hat{n}\hat{n}}(k^2) - \Lambda^{\mathrm{Ad}}(k^2) \Big]_{jj'}\, \mathrm{e}^{-\kappa x_j} \mathrm{e}^{-\kappa y_{j'}} = O(d)\, \mathrm{e}^{-\kappa x_j} \mathrm{e}^{-\kappa y_{j'}}\,, \end{aligned} \tag{85}$$

where the last equality holds by virtue of (81). Since such estimate is valid for all $j, j' \in \hat{n}$, there is a constant K_1 independent of j, j' and d such that

$$\Big| \mathcal{G}^{\mathrm{Ag},d}_{\mathrm{i}\kappa,jj'}(x_j, y_{j'}) - \mathcal{G}^{\mathrm{Ad}}_{\mathrm{i}\kappa,jj'}(x_j, y_{j'}) \Big| < K_1\, d\, \mathrm{e}^{-\kappa x_j} \mathrm{e}^{-\kappa y_{j'}} \tag{86}$$

holds for all $j, j' \in \hat{n}$, $x_j, y_{j'} \in \mathbb{R}^+$ and any d sufficiently small.

Then we proceed to the upper right submatrix of (83). To find a bound for the entries of $\mathcal{G}^{\mathrm{Ag},d}_{k,\hat{n}\mathcal{J}}(x,y)$, cf. (84b), we substitute values of $\lambda^d_{j(l',h')^0}(k^2)$ and $\lambda^d_{j(l',h')^d}(k^2)$ that we have obtained in (77b) and (77c):

$$\mathcal{G}^{\mathrm{Ag},d}_{\mathrm{i}\kappa,j(l',h')}(x_j, y_{(l',h')}) =$$
$$\mathrm{e}^{-\kappa x_j} \cdot \mathrm{e}^{-\mathrm{i}A_{(l',h')}y_{(l',h')}} \cdot \mathrm{e}^{\mathrm{i}dA_{(l',h')}} \cdot \left[\frac{\sinh \kappa y_{(l',h')}}{\sinh \kappa d} + \frac{\kappa}{\sinh \kappa d} \cdot \frac{\sinh \kappa(d - y_{(l',h')})}{2\kappa \cosh \kappa d + w_{\{l',h'\}} \sinh \kappa d} \right] \cdot \left[(M_d)^{-1} \right]_{jl'} .$$

It holds $\left[(M_d)^{-1} \right]_{jl'} = O(1)$ by virtue of (80) and obviously $\left| \mathrm{e}^{-\mathrm{i}A_{(l',h')}y_{(l',h')}} \right| = \left| \mathrm{e}^{\mathrm{i}dA_{(l',h')}} \right| = 1$, thus it suffices to estimate the terms in the brackets. When d is sufficiently small, it holds $\left| \frac{\sinh \kappa y_{(l',h')}}{\sinh \kappa d} \right| < 1$, because $0 < y_{(l',h')} < d$; similarly $\left| \frac{\sinh \kappa(d - y_{(l',h')})}{\sinh \kappa d} \right| < 1$. As for the denominator of the second term, we substitute for $w_{\{l',h'\}}$ from (49) or (47), depending on whether both l', h' belong to $\hat{m}$ or not, and we easily obtain the estimate

$$\frac{1}{2\kappa \cosh \kappa d + w_{\{l',h'\}} \sinh \kappa d} = O(1) .$$

Summing all this up, we get

$$\mathcal{G}^{\mathrm{Ag},d}_{\mathrm{i}\kappa,j(l',h')}(x_j, y_{(l',h')}) = \mathrm{e}^{-\kappa x_j} \left(O(1) + O(1) \right) = \mathrm{e}^{-\kappa x_j} O(1)$$

independently of j, (l', h') and x, y, thus there is a constant K_2 independent of d such that

$$\left| \mathcal{G}^{\mathrm{Ag},d}_{\mathrm{i}\kappa,j(l',h')}(x_j, y_{(l',h')}) \right| < K_2 \, \mathrm{e}^{-\kappa x_j} \tag{87}$$

for all $j \in \hat{n}$, $(l', h') \in \mathcal{J}$, $x_j \in \mathbb{R}^+$, $y_{(l',h')} \in (0, d)$ and d sufficiently small.

Similarly we proceed in the case of the left and right bottom submatrices of (83), i.e. when estimating the entries of $\mathcal{G}^{\mathrm{Ag},d}_{k,\mathcal{J}\hat{n}}(x,y)$ and $\mathcal{G}^{\mathrm{Ag},d}_{k,\mathcal{J}\mathcal{J}}(x,y)$. As for $\mathcal{G}^{\mathrm{Ag},d}_{k,\mathcal{J}\hat{n}}(x,y)$, we substitute for $\lambda^d_{(l,h)^0 j'}(k^2)$ and $\lambda^d_{(l,h)^d j'}(k^2)$ from (77d) and (77g) into (84c) and obtain

$$\begin{aligned}\mathcal{G}^{\mathrm{Ag},d}_{\mathrm{i}\kappa,(l,h)j'}(x_{(l,h)}, y_{j'}) = \mathrm{e}^{-\kappa y_{j'}} \cdot \mathrm{e}^{\mathrm{i}A_{(l,h)}x_{(l,h)}} \cdot \Bigg[& \frac{\mathrm{e}^{-\mathrm{i}dA_{(l,h)}}}{\sinh \kappa d} \cdot \left[(M_d)^{-1} \right]_{lj'} \sinh \kappa x_{(l,h)} \\ & + \frac{\kappa}{2\kappa \cosh \kappa d + w_{\{l,h\}} \sinh \kappa d} \cdot \frac{1}{\sinh \kappa d} \cdot \sinh \kappa(d - x_{(l,h)}) \cdot \\ & \cdot \left(\mathrm{e}^{-\mathrm{i}dA_{(l,h)}} \left[(M_d)^{-1} \right]_{lj'} + \mathrm{e}^{-\mathrm{i}dA_{(h,l)}} \left[(M_d)^{-1} \right]_{hj'} \right) \Bigg] .\end{aligned}$$

Using analogous estimates as in the case of $\mathcal{G}^{\mathrm{Ag},d}_{\mathrm{i}\kappa,j(l',h')}(x,y)$ above, we obtain

$$\mathcal{G}^{\mathrm{Ag},d}_{\mathrm{i}\kappa,(l,h)j'}(x_{(l,h)}, y_{j'}) = \mathrm{e}^{-\kappa y_{j'}} \left(O(1) + O(1) \right) = \mathrm{e}^{-\kappa y_{j'}} O(1) ,$$

thus there is a constant K_3 independent of d such that

$$\left| \mathcal{G}^{\mathrm{Ag},d}_{\mathrm{i}\kappa,(l,h)j'}(x_{(l,h)}, y_{j'}) \right| < K_3 \, \mathrm{e}^{-\kappa y_{j'}} \tag{88}$$

for all $(l,h) \in \mathcal{J}$, $j' \in \hat{n}$, $x_{(l,h)} \in (0,d)$, $y \in \mathbb{R}^+$ and d sufficiently small.

Finally, we substitute from (77e), (77f), (77h) and (77i) for $\lambda^d_{(l,h)^0(l'h')^0}(k^2)$, $\lambda^d_{(l,h)^0(l'h')^d}(k^2)$, $\lambda^d_{(l,h)^d(l'h')^0}(k^2)$ and $\lambda^d_{(l,h)^d(l'h')^d}(k^2)$, respectively, into Eq. (84d) and obtain

$$\begin{aligned}
\mathcal{G}^{\mathrm{Ag},d}_{\mathrm{i}\kappa,(l,h)(l',h')}(x_{(l,h)},y_{(l',h')}) &= \delta_{(l,h)(l',h')}\mathrm{e}^{\mathrm{i}A_{(l,h)}x_{(l,h)}}\frac{\sinh\kappa x_<\sinh\kappa(d-x_>)}{\kappa\sinh\kappa d}\,\mathrm{e}^{-\mathrm{i}A_{(l',h')}y_{(l',h')}}\\
&\quad+\mathrm{e}^{\mathrm{i}A_{(l,h)}x_{(l,h)}}\cdot\mathrm{e}^{-\mathrm{i}A_{(l',h')}y_{(l',h')}}\cdot\mathrm{e}^{-\mathrm{i}dA_{(l,h)}}\cdot\mathrm{e}^{\mathrm{i}dA_{(l',h')}}\cdot\frac{\sinh\kappa x_{(l,h)}}{\sinh\kappa d}\cdot\\
&\quad\cdot\left[\frac{\sinh\kappa y_{(l',h')}}{\sinh\kappa d}+\frac{\kappa}{\sinh\kappa d}\cdot\frac{\sinh\kappa(d-y_{(l',h')})}{2\kappa\cosh\kappa d+w_{\{l',h'\}}\sinh\kappa d}\right]\cdot\left[(M_d)^{-1}\right]_{ll'}\\
&\quad+\mathrm{e}^{\mathrm{i}A_{(l,h)}x_{(l,h)}}\cdot\sinh\kappa(d-x_{(l,h)})\cdot\mathrm{e}^{-\mathrm{i}A_{(l',h')}y_{(l',h')}}\cdot\frac{\kappa}{2\kappa\cosh\kappa d+w_{\{l,h\}}\sinh\kappa d}\cdot\frac{1}{\sinh\kappa d}\cdot\\
&\quad\cdot\left[\mathrm{e}^{\mathrm{i}dA_{(l',h')}}\cdot\frac{\sinh\kappa y_{(l',h')}}{\sinh\kappa d}\left(\mathrm{e}^{-\mathrm{i}dA_{(l,h)}}\cdot\left[(M_d)^{-1}\right]_{ll'}+\mathrm{e}^{-\mathrm{i}dA_{(h,l)}}\cdot\left[(M_d)^{-1}\right]_{hl'}\right)\right.\\
&\quad+\mathrm{e}^{\mathrm{i}dA_{(l',h')}}\cdot\frac{\kappa}{\sinh\kappa d}\cdot\frac{\sinh\kappa(d-y_{(l',h')})}{2\kappa\cosh\kappa d+w_{\{l',h'\}}\sinh\kappa d}\cdot\\
&\quad\left.\cdot\left(\mathrm{e}^{-\mathrm{i}dA_{(l,h)}}\cdot\left[(M_d)^{-1}\right]_{ll'}+\mathrm{e}^{-\mathrm{i}dA_{(h,l)}}\cdot\left[(M_d)^{-1}\right]_{hl'}\right)+\frac{1}{\kappa}\delta_{(l,h)(l',h')}\right]. \qquad (89)
\end{aligned}$$

It obviously holds

$$\mathcal{G}^{\mathrm{Ag},d}_{\mathrm{i}\kappa,(l,h)(l',h')}(x_{(l,h)},y_{(l',h')}) = \ = O(d)+O(1)\cdot[O(1)+O(1)]+O(1)\cdot[O(1)+O(1)] = O(1)\,,$$

thus there is a constant K_4 independent of d such that

$$\left|\mathcal{G}^{\mathrm{Ag},d}_{\mathrm{i}\kappa,(l,h)(l',h')}(x_{(l,h)},y_{(l',h')})\right| < K_4 \qquad (90)$$

for all $(l,h),(l',h') \in \mathcal{J}$, $x_{(l,h)},y_{(l',h')} \in (0,d)$ and any d sufficiently small.

With the help of (86), (87), (88) and (90), we may now estimate all the entries of (83), which will allows us to assess the Hilbert-Schmidt norm of the resolvent difference for the operators H^{Ad}_d and H^{Ag}_d. This norm can be written explicitly as follows,

$$\begin{aligned}
\left\|R^{\mathrm{Ag}}_d(k^2)-R^{\mathrm{Ad}}_d(k^2)\right\|_2^2 &= \sum_{j,j'=1}^{n}\int_0^{+\infty}\int_0^{+\infty}\left|\mathcal{G}^{\mathrm{Ag},d}_{\mathrm{i}\kappa,jj'}(x_j,y_{j'})-\mathcal{G}^{\mathrm{Ad}}_{\mathrm{i}\kappa,jj'}(x_j,y_{j'})\right|^2\mathrm{d}x_j\mathrm{d}y_{j'}\\
&\quad+\sum_{j=1}^{n}\sum_{(l',h')\in\mathcal{I}}\int_0^{+\infty}\int_0^{d}\left|\mathcal{G}^{\mathrm{Ag},d}_{\mathrm{i}\kappa,j(l',h')}(x_j,y_{(l',h')})\right|^2\mathrm{d}x_j\mathrm{d}y_{(l',h')}\\
&\quad+\sum_{(l,h)\in\mathcal{I}}\sum_{j'=1}^{n}\int_0^{d}\int_0^{+\infty}\left|\mathcal{G}^{\mathrm{Ag},d}_{\mathrm{i}\kappa,(l,h)j'}(x_{(l,h)},y_{j'})\right|^2\mathrm{d}x_{(l,h)}\mathrm{d}y_{j'}\\
&\quad+\sum_{(l,h)\in\mathcal{I}}\sum_{(l',h')\in\mathcal{I}}\int_0^{d}\int_0^{d}\left|\mathcal{G}^{\mathrm{Ag},d}_{\mathrm{i}\kappa,(l,h)(l'h')}(x_{(l,h)},y_{(l,h')})\right|^2\mathrm{d}x_{(l,h)}\mathrm{d}y_{(l',h')}\,.
\end{aligned}$$

Now we employ the estimates derived above obtaining

$$\left\|R_d^{\mathrm{Ag}}(k^2) - R_d^{\mathrm{Ad}}(k^2)\right\|_2^2 \le$$
$$\sum_{j,j'=1}^{n} \int_0^{+\infty}\int_0^{+\infty} \left|K_1\, d\, \mathrm{e}^{-\kappa x_j}\mathrm{e}^{-\kappa y_{j'}}\right|^2 \mathrm{d}x_j\mathrm{d}y_{j'} + \sum_{j=1}^{n}\sum_{(l',h')\in\mathcal{I}} \int_0^{+\infty}\int_0^{d} \left|K_2\, \mathrm{e}^{-\kappa x_j}\right|^2 \mathrm{d}x_j\mathrm{d}y_{(l',h')}$$
$$+ \sum_{(l,h)\in\mathcal{I}}\sum_{j'=1}^{n} \int_0^{d}\int_0^{+\infty} \left|K_3\, \mathrm{e}^{-\kappa y_{j'}}\right|^2 \mathrm{d}x_{(l,h)}\mathrm{d}y_{j'} + \sum_{(l,h)\in\mathcal{I}}\sum_{(l',h')\in\mathcal{I}} \int_0^{d}\int_0^{d} |K_4|^2 \,\mathrm{d}x_{(l,h)}\mathrm{d}y_{(l',h')}$$

$$\le \sum_{j,j'=1}^{n} K_1^2 d^2 \int_0^{+\infty} e^{-2(\mathrm{Re}\,\kappa)x_j}\,\mathrm{d}x_j \int_0^{+\infty} e^{-2(\mathrm{Re}\,\kappa)y_{j'}}\,\mathrm{d}y_{j'}$$
$$+ \sum_{j=1}^{n}\sum_{(l',h')\in\mathcal{I}} K_2^2 \int_0^{+\infty} e^{-2(\mathrm{Re}\,\kappa)x_j}\,\mathrm{d}x_j \cdot \int_0^{d} 1\,\mathrm{d}y_{(l',h')}$$
$$+ \sum_{(l,h)\in\mathcal{I}}\sum_{j'=1}^{n} K_3^2 \int_0^{d} 1\,\mathrm{d}x_{(l,h)} \cdot \int_0^{+\infty} e^{-2(\mathrm{Re}\,\kappa)y_{j'}}\,\mathrm{d}y_{j'}$$
$$+ \sum_{(l,h)\in\mathcal{I}}\sum_{(l',h')\in\mathcal{I}} K_4^2 \int_0^{d} 1\,\mathrm{d}x_{(l,h)} \cdot \int_0^{d} 1\,\mathrm{d}y_{(l',h')}$$

$$= \sum_{j,j'=1}^{n} K_1^2 d^2 \frac{1}{(2\mathrm{Re}\,\kappa)^2} + \sum_{j=1}^{n}\sum_{(l',h')\in\mathcal{I}} K_2^2 \frac{1}{2\mathrm{Re}\,\kappa}\cdot d + \sum_{(l,h)\in\mathcal{I}}\sum_{j'=1}^{n} K_3^2 d \cdot \frac{1}{2\mathrm{Re}\,\kappa} + \sum_{(l,h)\in\mathcal{I}}\sum_{(l',h')\in\mathcal{I}} K_4^2 d^2$$
$$= O(d)\,.$$

Hence

$$\left\|R_d^{\mathrm{Ag}}(k^2) - R_d^{\mathrm{Ad}}(k^2)\right\|_2 = O\left(\sqrt{d}\right) \qquad \text{for } d \to 0_+\,,$$

and consequently, the Hilbert-Schmidt norm of the difference $R_d^{\mathrm{Ag}}(k^2) - R_d^{\mathrm{Ad}}(k^2)$ tends to zero as $d \to 0_+$ with the explicit convergence rate. Since the HS norm dominates the operator one, it follows immediately

$$\lim_{d\to 0_+} \left\|R_d^{\mathrm{Ag}}(k^2) - R_d^{\mathrm{Ad}}(k^2)\right\| = 0\,,$$

therefore the resolvent difference tends to zero in $L^2(G_d)$ as $d \to 0_+$, which we set out to prove. □

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Appendix B

Approximations of singular vertex couplings in quantum graphs

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APPROXIMATIONS OF SINGULAR VERTEX COUPLINGS IN QUANTUM GRAPHS

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We discuss approximations of the vertex coupling on a star-shaped quantum graph of n edges in the singular case when the wave functions are not continuous at the vertex and no edge-permutation symmetry is present. It is shown that the Cheon–Shigehara technique using δ interactions with nonlinearly scaled couplings yields a $2n$-parameter family of boundary conditions in the sense of norm resolvent topology. Moreover, using graphs with additional edges, one can approximate the $\binom{n+1}{2}$-parameter family of all time-reversal invariant couplings.

Keywords: Quantum graph; vertex conditions; approximations; point interactions.

Mathematics Subject Classification 2000: 81Q10

1. Introduction

The concept of quantum mechanics on a graph is more than half a century old having roots in modeling of aromatic hydrocarbons [1]. For many years, however, it was rather a curiosity, or maybe an interesting textbook example. The situation changed two decades ago with the advent of microfabrication techniques which allow us to produce tiny graph-shaped structures of semiconductor and other materials which became a useful and versatile model. This motivated a new theoretical attention to the subject — see, e.g., [2,3]. Since then the literature on quantum graphs grew to a formidable volume, and we restrict ourselves here to mentioning recent reviews in [4–6] where an extensive bibliography can be found.

From the mathematical point of view the attractive feature of the model is that it deals with families of ordinary differential equations, the solutions of which have to be properly matched at the graph edge endpoints. Since the solutions are often explicitly known, the spectral analysis can be reduced to an algebraic problem.

The key point here are the boundary conditions through which the wave functions are matched. The Hamiltonian is typically a second-order differential operator, for instance, in the simplest case of a free spinless particle it acts on the jth edge as $H\psi_j = -\psi_j''$. Thus the boundary conditions are linear relations coupling the values of the functions and their first derivatives at graph vertices; from the physical point of view it is usually sufficient to consider only *local* couplings which involve values at a single vertex only. Another general physical restriction is the self-adjointness of the Hamiltonian; it implies that a vertex joining n graph edges may be characterized by boundary conditions involving n^2 real parameters [3].

This leaves a considerable freedom in the choice of a model to describe particular physical systems, and an understanding of the physical meaning of vertex coupling is needed to pick the appropriate operator from the class of admissible Hamiltonians. A natural way to approach this problem is through approximation, i.e. regarding the quantum graph in question as a limit of a family of more "realistic" systems with a less number of free parameters. One possibility is to approximate a graph by a family of "fat graphs" or similar manifolds equipped with the corresponding Laplace–Beltrami operators. The best studied case is the one where the approximated manifolds have Neumann boundary, or no boundary at all [7–12], where unfortunately the limit yields — of the multitude of available boundary conditions — only the most simple ones. There are also fresh results [13, 14] on the case with Dirichlet boundary but in general the approach based on squeezed manifolds did not yield so far a satisfactory answer to the question.

Another, maybe less ambitious approach is to model vertex boundary conditions through families of interactions on the graph itself. Here two cases have to be distinguished. In the n^2-parameter family mentioned above the boundary conditions with wave functions *continuous at the vertex* form just one-parameter subfamily. These boundary conditions can be approximated by families of scaled potentials in analogy is analogy with one-dimensional δ interactions [15]. The remaining, *more singular* cases require a different approach. An inspiration may be derived from the approximation of one-dimensional δ' interactions suggested, somewhat surprisingly, by Cheon and Shigehara in [16] and elaborated in a mathematically consistent way in [17, 18]. It is based on a family of δ interactions which approach each other being scaled in a particular nonlinear way. An analogous procedure for vertices of degree $n \geq 2$ was proposed in [19] in the case of the so-called δ'_s coupling; the key element here was the symmetry with respect to permutation of the edges which allowed to reduce the analysis to a one-dimensional halfline problem. The same technique was afterwards in [20] applied to the class of all permutation-symmetric boundary conditions which form a two-parameter subfamily in the n^2-parameter set.

The main goal of the present paper is to explore whether the idea of [16] can be adapted to situations without a permutation symmetry and how wide class of boundary conditions can be in this way described. As in the work mentioned above we will consider a *star graph* with a single vertex and n semi-infinite edges. For simplicity we will also assume that the motion on graphs edges is *free*; the obtained

approximations extend easily to Schrödinger operators on the graph provided the potentials involved are sufficiently regular around the vertex. We are going to show that the Cheon–Shigehara technique can produce for $n > 2$ at most a $2n$-parameter family of boundary conditions at the vertex. Furthermore, we will demonstrate that such approximations, with two δ interactions at each edge, do indeed exist and that they converge in the norm resolvent topology.

The next question is how to extend the approximation to a wider class of couplings. A natural possibility is to amend the star by extra edges supporting δ interactions which shrink to the "main" vertex with the parameter controlling the approximation. We devise such a scheme to show that it yields an $\binom{n+1}{2}$-parameter family, generically *all* couplings which are *time-reversal invariant*. In this case, however, we restrict ourselves to deriving the boundary condition formally. We are convinced that the norm resolvent convergence could be verified as in the case mentioned but the argument would be extremely cumbersome. Notice that the idea of using additional edges to model singular couplings appeared already in [21]. In contrast to that paper, however, we keep here the number of added edges fixed.

Let us review briefly the contents of the paper. In the next section we gather the needed preliminary information. We review the quantum graph concept, recall different vertex couplings and review briefly the known approximations. In Sec. 3 we analyze a CS-type approximation to the vertex in a star graph based on adding δ interactions on star edges, the following section is devoted to the proof of norm-resolvent convergence. Finally, in Sec. 5 we will describe the afore-mentioned more general approximation with extra edges added to the star graph.

2. Preliminaries

2.1. *Quantum graphs*

Let us first recall a few basic notions. A *graph* Γ is an ordered pair $\Gamma = (V, E)$, where V and E are finite or countably infinite sets of *vertices* and *edges*, respectively. Without loss of generality we may identify E with a family of two-element subsets in V, excluding thus loops and multiple edges, since in the opposite case we can simply add extra vertices. The vertex *degree* of $v \in V$ is the number of edges which have v as its endpoint. Γ is a *metric graph* if each of its edges can be equipped with a distance, i.e. identified with a finite or semi-infinite interval of length $\ell \in (0, +\infty]$; the endpoints "at infinity" are conventionally not counted as vertices. In particular a *star graph* has a finite number $n \geq 2$ of edges and a single *center* which is the only vertex where all the edges (called also *arms* in this case) meet.

The subject of our interest is quantum mechanics on graphs. Given a metric graph Γ with edges $J_1, \ldots, J_n$ we identify the orthogonal sum $\mathcal{H} = \bigoplus_{j=1}^n L^2(J_j)$ with the state Hilbert space, i.e. the wave function of a spinless particle "living" on Γ can be written as the column $\Psi = (\psi_1, \psi_2, \ldots, \psi_n)^T$ with $\psi_j \in L^2(J_j)$. In the absence of external fields the Hamiltonian H acts as $(H_\Gamma \Psi)_j = -\psi_j''$, where as usual we put $\hbar = 2m = 1$. Its domain consists of functions from

$W^{2,2}(\Gamma) := \bigoplus_{j=1}^n W^{2,2}(J_j)$; since H is required to be a self-adjoint operator they must satisfy appropriate boundary conditions at the vertices which we will recall below.

The meaning of these boundary condition is our main concern in this paper, therefore we restrict ourselves to graphs with a single vertex, namely star graphs with n semi-infinite edges $J_j \simeq \mathbb{R}^+$, $j = 1, \dots, n$; we denote them as Γ or Γ_n.

2.2. *Vertex couplings*

Since the Hamiltonian mentioned above is a second-order operator, the matching conditions involve boundary values of the functions in the vertex and of their first derivatives. Both regarded as one-sided limits, the derivatives are taken in the outward direction. We arrange them into column vectors $\Psi(0)$ and $\Psi'(0)$. The self-adjointness of H, which in the physical language means conservation of probability current at the vertex, is expressed through a linear relation between these vectors,

$$A\Psi(0) + B\Psi'(0) = 0\,, \tag{2.1}$$

by [22] the operator H is self-adjoint if and only if $A, B \in \mathbb{C}^{n,n}$ satisfy the conditions

$$\mathrm{rank}(A, B) = n\,, \quad AB^* \text{ is self-adjoint}, \tag{2.2}$$

where (A, B) denotes the $n \times 2n$ matrix with A, B forming the first and the second n columns, respectively. This parametrization is obviously non-unique, since A, B can be replaced by CA, CB with any regular $n \times n$ matrix C. This defect can be corrected by choosing the matrices in the standard form [23, 24],

$$(U - I)\Psi(0) + \mathrm{i}(U + I)\Psi'(0) = 0\,, \tag{2.3}$$

where U is an $n \times n$ unitary matrix; the Hamiltonian corresponding to this condition will be labeled as H_U. Elements of this family are labeled by n^2 real parameters which is, of course, the right number because all the H_U are self-adjoint extensions of a common symmetric restriction with deficiency indices (n, n), refer to [3].

Let us next recall a few examples of the boundary conditions (2.3). As mentioned in the introduction, the requirement of continuity at the vertex selects a one-parameter subfamily corresponding to the so-called δ *coupling*,

$$\psi_j(0) = \psi_k(0) =: \psi(0)\,, \quad j, k \in \hat{n}\,, \quad \sum_{j=1}^n \psi_j'(0) = \alpha\psi(0)\,, \tag{2.4}$$

where $\alpha \in \mathbb{R}$ and for brevity we have introduced the symbol $\hat{n} := \{1, 2, \dots, n\}$. We can add the case corresponding formally to $\alpha = \infty$, when the system decomposes into n halflines with Dirichlet endpoints, however, it is not interesting as long as we are concerned with nontrivial vertex couplings. In the particular case $\alpha = 0$ we speak about *free boundary conditions* since for the δ function on line, $n = 2$, this corresponds to a free motion (sometimes the term Kirchhoff b.c., not very

appropriate, is used). In terms of (2.3) the δ coupling corresponds to the matrix $U = \frac{2}{n+\mathrm{i}\alpha}\mathcal{J} - I$, where $\mathcal{J}$ denotes the $n \times n$ matrix where all entries equal one.

The δ' interaction on the line has two possible analogues for $n > 2$ [25,26]. One is a counterpart to (2.4) called δ'_s *coupling* with the role of $\Psi(0)$, $\Psi'(0)$ interchanged,

$$\psi'_j(0) = \psi'_k(0) =: \psi'(0)\,, \quad j,k \in \hat{n}\,, \quad \sum_{j=1}^{n} \psi_j(0) = \beta\psi'(0)\,, \tag{2.5}$$

where $\beta \in \mathbb{R} \cup \{+\infty\}$. It corresponds to $U = I - \frac{2}{n-\mathrm{i}\beta}\mathcal{J}$, in particular, the case $\beta = \infty$ refers to full Neumann decoupling. The other one, called δ' *coupling*, is

$$\sum_{j=1}^{n} \psi'_j(0) = 0\,, \quad \psi_j(0) - \psi_k(0) = \frac{\beta}{n}\big(\psi'_j(0) - \psi'_k(0)\big) \quad j,k \in \hat{n}\,, \tag{2.6}$$

with $\beta \in \mathbb{R} \cup \{+\infty\}$ which corresponds to $U = -\frac{n+\mathrm{i}\beta}{n-\mathrm{i}\beta}I + \frac{2}{n-\mathrm{i}\beta}\mathcal{J}$.

All the above examples have a common property, namely that the corresponding operators are invariant with respect to permutation of the edges, which is clear from the fact that matrices U are not changed by a simultaneous permutations of the rows and columns. The most general family of H_U with this property is characterized by two parameters, $U = aI + bJ$ with $|a| = 1$ and $|a+nb| = 1$, cf. [20], the corresponding boundary conditions being

$$\begin{aligned} &(a-1)\,(\psi_j(0) - \psi_k(0)) + \mathrm{i}(a+1)\,\big(\psi'_j(0) - \psi'_k(0)\big) = 0\,, \quad j,k \in \hat{n}\,, \\ &(a-1+nb)\sum_{k=1}^{n} \psi_k(0) + \mathrm{i}(a+1+nb)\sum_{k=1}^{n} \psi'_k(0) = 0\,. \end{aligned} \tag{2.7}$$

2.3. *Approximation of δ couplings*

Let us next recall briefly known results about approximations of vertex couplings starting from the δ coupling. The idea is the same as for δ interactions on the line.

Let $U_\delta(\alpha) := \frac{2}{n+\mathrm{i}\alpha}\mathcal{J} - I$ be the corresponding matrix of the condition (2.3). Given a family of real-valued functions $W = \{W_j : j \in \hat{n}\}$, for simplicity assumed to be compactly supported, we define scaled potentials at graph edges by

$$W_{\epsilon,j} := \frac{1}{\epsilon}\, W_j\Big(\frac{x}{\epsilon}\Big)\,, \quad j \in \hat{n}\,. \tag{2.8}$$

Starting from the free boundary conditions and choosing the family (2.8) we can approximate any nontrivial δ coupling as the following result shows.

Theorem 2.1. *Suppose that $W_j \in L^1(0,1)$ for $j \in \hat{n}$, then*

$$H_{U_\delta(0)} + W_\epsilon \longrightarrow H_{U_\delta(\alpha)} \quad \text{as} \quad \epsilon \to 0+ \tag{2.9}$$

in the norm resolvent sense, where $\alpha := \sum_{j=1}^{n} \int_0^1 W_j(x)\,dx$.

Proof. See [15] where a more general result of this type is derived, together with other extensions of the standard Sturm–Liouville theory to star graphs. □

2.4. *Approximation of singular permutation-invariant couplings*

Consider further permutation-invariant couplings with wave functions discontinuous at the vertex. Denote the operator H_U corresponding to $U = aI + bJ$ with a, b satisfying the stated conditions as $H^{a,b}$. The approximating family can be constructed as follows: we start from the operator $H_{u,0} := H_{U_\delta(u)}$ and pass to $H_{u,v}$ obtained by adding a δ interaction of strength v on each edge at a distance d from the center. We will let the δ's approach the centre scaling properly u, v.

Theorem 2.2. *Fix a pair of complex numbers $a \neq -1$ and $b \neq 0$ such that $|a| = 1$ and $|a + nb| = 1$, and set*

$$u(d) := \mathrm{i}\frac{n}{d^2}\left(\frac{a-1+nb}{a+1+nb} + \frac{a-1}{a+1}\right)^{-1}, \quad v(d) := -\frac{1}{d} - \mathrm{i}\frac{a-1}{a+1}\,. \tag{2.10}$$

Suppose that $a+1+nb \neq 0$ and $a(a+nb) \neq 1$, then the operators $H_{u(d),v(d)}$ converge to $H^{a,b}$ in the norm resolvent topology as $d \to 0_+$. Moreover, the claim remains true in the two excluded cases, provided we replace the above $u(d)$ by $-nd^{-1}$ and $\zeta d^{-\nu}$ with $\mathbb{R} \ni \zeta \neq 0$ and $\nu > 2$, respectively.

Proof. This can be found in [20], the particular case of δ'_s coupling (2.5) in which $u(d) = -\beta d^{-2}$ and $v(d) = -d^{-1}$ was discussed in [19]. □

3. CS-type Approximation of Singular Couplings

After the preliminaries let us turn to our proper task, namely approximations of singular couplings *à la* Cheon and Shigehara, i.e. by means of additional δ interactions, properly scaled, on edges of our star graph, without the requirement of permutation invariance.

3.1. *The class of approximable couplings*

The first question is how large is the class of operators H_U which can be treated in this way. We are going to answer it using the technique of [16], i.e. looking into convergence of the corresponding boundary conditions.

Proposition 3.1. *Let Γ be a star graph with n semi-infinite edges and $\Gamma(d)$ be a graph obtained from Γ by adding a finite number of vertices at each edge. Consider a family $\{\Gamma(d) : d \in \mathbb{R}^+\}$ of such graphs with the properties that the number of the added vertices at each edge is independent of d and their distances from the center are $\mathcal{O}(d)$ as $d \to 0_+$. Suppose that a family of functions $\Psi_d \in W^{2,2}(\Gamma\backslash(\{c\} \cup V_d))$, where c is the center of Γ and V_d is the set of added vertices, satisfies the conditions* (2.4) *with d-dependent parameters, and that it converges to $\Psi \in W^{2,2}(\Gamma\backslash\{c\})$ which obeys the condition* (2.1) *with some A, B satisfying the requirements* (2.2)*. The family of the conditions* (2.1) *which can be obtained in this way depends on $2n$ parameters if $n > 2$, and on three parameters for $n = 2$.*

Proof. The δ coupling in the center of Γ is expressed by the condition (2.4). Consider first δ interactions on a halfline and look how the boundary values change when we pass between different sites. Suppose that at a point x the function and its derivative have the right limits, and that $x+\epsilon$ is the site of a δ interaction, then the Taylor expansion gives

$$\psi(x+\epsilon_-) = \psi(x_+) + \epsilon\psi'(x_+) + \mathcal{O}(\epsilon^2)\,, \quad \psi'(x+\epsilon_-) = \psi'(x_+) + \mathcal{O}(\epsilon)\,,$$

and the δ interaction is according to (2.4) described by

$$\psi(x+\epsilon_+) = \psi(x+\epsilon_-) =: \psi(x+\epsilon)\,, \quad \psi'(x+\epsilon_+) - \psi'(x+\epsilon_-) = \alpha(\epsilon)\psi(x+\epsilon)\,,$$

where $\alpha(\epsilon)$ is the coupling parameter. The may be ϵ-dependent but we suppose such a dependence that the error terms can be neglected as $\epsilon \to 0_+$; then we have

$$\begin{aligned}
\psi(x+\epsilon) &= \psi(x_+) + \epsilon\psi'(x_+) + \mathcal{O}(\epsilon^2)\,,\\
\psi'(x+\epsilon_+) &= \psi'(x_+) + \mathcal{O}(\epsilon) + \alpha(\epsilon)(\psi(x_+) + \epsilon\psi'(x_+) + \mathcal{O}(\epsilon^2))\\
&= (1+\alpha(\epsilon)\epsilon)\psi'(x_+) + \alpha(\epsilon)\psi(x_+) + \mathcal{O}(\epsilon) + \alpha(\epsilon)\mathcal{O}(\epsilon^2)\,,
\end{aligned}$$

so that $\psi(x+\epsilon)$ and $\psi'(x+\epsilon_+)$ depend on $\psi(x_+)$ and $\psi'(x_+)$ linearly up to error terms. In case of a finite number of δ interactions on a halfline one can show in a similar way recursively that the function value and the right limit of the derivative at the site of the last δ depends, up to error terms, linearly on the function value and the right limit of the derivative for the first δ interaction.

Let us apply this conclusion to the edges of our star graph. We denote by d_j the distance of the last δ interaction on the jth halfline family of edges in $\Gamma(d)$; by assumption we have $d_j = \mathcal{O}(d)$. Then we have

$$\begin{aligned}
\tilde f_j^{(1)}(d)\psi_j(d_j) &= \tilde g_j^{(1)}(d)\psi(0) + \tilde h_j^{(1)}(d)\psi_j'(0) + \tilde r_j^{(1)}(d)\,,\\
\tilde f_j^{(2)}(d)\psi_j'(d_{j\,+}) &= \tilde g_j^{(2)}(d)\psi(0) + \tilde h_j^{(2)}(d)\psi_j'(0) + \tilde r_j^{(2)}(d)
\end{aligned}$$

for some $\tilde f_j^{(1)}, \tilde g_j^{(1)}, \tilde h_j^{(1)}, \tilde f_j^{(2)}, \tilde g_j^{(2)}, \tilde h_j^{(2)} : \mathbb{R}^+ \to \mathbb{R}$. The functions $\tilde r_j^{(1)}$ and $\tilde r_j^{(2)}(d)$ are error terms and we suppose that they can be neglected in the limit. We are interested in the situation when the last relations can be inverted and $\psi(0)$, $\psi_j'(0)$ can be expressed by means of $\psi_j(d_j)$ and $\psi_j'(d_{j\,+})$,

$$\psi(0) = f_j^{(1)}(d)\psi_j(d_j) + g_j^{(1)}(d)\psi_j'(d_{j\,+}) + \mathcal{R}(d)\,, \quad j \in \hat n\,, \tag{3.1}$$

$$\psi_j'(0) = \tilde f_j^{(2)}(d)\psi_j(d_j) + \tilde g_j^{(2)}(d)\psi_j'(d_{j\,+}) + \mathcal{R}(d)\,, \quad j \in \hat n\,, \tag{3.2}$$

where we have introduced $\mathcal{R}(d)$ as the symbol for a generic remainder; we still assume that it can be neglected with respect to the other terms as $d \to 0_+$. The

Eq. (3.1) yield for $j,k\in\hat n$ the conditions

$$f_j^{(1)}(d)\psi_j(d_j)-f_k^{(1)}(d)\psi_k(d_k)+g_j^{(1)}(d)\psi_j'(d_{j+})-g_k^{(1)}(d)\psi_k'(d_{k+})=\mathcal{R}(d)\,,\quad j,k\in\hat n \tag{3.3}$$

and from (3.2) together with the second one of the conditions (2.4) we get

$$\alpha\psi(0)=\sum_{k=1}^n(f_k^{(2)}(d)\psi_k(d_k)+g_k^{(2)}(d)\psi_k'(d_{k+}))+\mathcal{R}(d)\,. \tag{3.4}$$

We substitute for $\psi(0)$ from (3.1) and perform a repeated summation of (3.4) over j. After an easy rearrangement we get

$$\sum_{j=1}^n(\alpha f_j^{(1)}(d)-nf_j^{(2)}(d))\psi_j(d_j)+\sum_{j=1}^n(\alpha g_j^{(1)}(d)-ng_k^{(2)}(d))\psi_j'(d_{j+})=\mathcal{R}(d)\,. \tag{3.5}$$

Now we pass to the limit $d\to 0_+$ in the Eqs. (3.3) and (3.5). Before that we multiply both sides by a power of d such that the right-hand side tends to zero as $d\to 0_+$, while at least one coefficient at the left-hand side remains nonzero, in other words, we use the assumed existence of the limit in which the error terms can be neglected with respect to the leading ones. Equation (3.3) acquires then the form

$$c_j\psi_j(0)-c_k\psi_k(0)+t_j\psi_j'(0_+)-t_k\psi_k'(0_+)=0\,,\quad j,k\in\hat n \tag{3.6}$$

while (3.5) gives

$$\sum_{j=1}^n\gamma_j\psi_j(0)+\sum_{j=1}^n\tau_j\psi_j'(0_+)=0\,, \tag{3.7}$$

where c_j, t_j, γ_j, τ_j are the appropriate limiting values of the functions involved. The obtained conditions can also be written in a matrix form,

$$\underbrace{\begin{pmatrix} c_1 & -c_2 & 0 & \cdots & 0\\ c_1 & 0 & -c_3 & \cdots & 0\\ \vdots & & & \ddots & \\ c_1 & 0 & 0 & \cdots & -c_n\\ \gamma_1 & \gamma_2 & \gamma_3 & \cdots & \gamma_n \end{pmatrix}}_{A}\Psi(0)+\underbrace{\begin{pmatrix} t_1 & -t_2 & 0 & \cdots & 0\\ t_1 & 0 & -t_3 & \cdots & 0\\ \vdots & & & \ddots & \\ t_1 & 0 & 0 & \cdots & -t_n\\ \tau_1 & \tau_2 & \tau_3 & \cdots & \tau_n \end{pmatrix}}_{B}\Psi'(0)=0\,. \tag{3.8}$$

It is clear already now — from the fact that the coefficients $c_j,t_j,\gamma_j,\tau_j,j\in\hat n$ are real-valued — that the achievable number of parameters cannot exceed $4n$.

So far we have not brought the self-adjointness into the game. To find the true number of parameters we pass from A, B to the unitary matrix U of standard boundary conditions (2.3). This is achieved by multiplying the relation (3.8) from

the left by a regular matrix M such that $U - I = MA$ and $\mathrm{i}(U + I) = MB$. This determines U since the last relations imply

$$U = \frac{1}{2}M(A - \mathrm{i}B)\,, \quad I = -\frac{1}{2}M(A + \mathrm{i}B)\,;$$

notice that $A + \mathrm{i}B$ is regular because A and B are real and the matrix $(A|B)$ has the full rank by assumption. Hence we have $M = -2(A + \mathrm{i}B)^{-1}$, which further gives

$$U = -(A + \mathrm{i}B)^{-1} \cdot (A - \mathrm{i}B)\,.$$

We shall apply the Gauss elimination method to get the chain of equivalences

$$\big(-(A + \mathrm{i}B)|(A - \mathrm{i}B)\big) \sim \cdots \sim \big(I|\underbrace{-(A + \mathrm{i}B)^{-1} \cdot (A - \mathrm{i}B)}_{U}\big)\,;$$

the explicit form of $A \pm iB$ is obtained from (3.8). We notice that the regularity of $A + iB$ implies the following facts: (i) there is at most one $j \in \hat{n}$ such that $c_j + \mathrm{i}t_j = 0$ (and for such a j it holds that $\gamma_j + \mathrm{i}\tau_j \neq 0$), (ii) there is at least one $j \in \hat{n}$ such that $\gamma_j + \mathrm{i}\tau_j \neq 0$. The matrix $\big(-(A + \mathrm{i}B)|(A - \mathrm{i}B)\big)$ equals to

$$\left(\begin{array}{cccc|cccc}
-(c_1 + \mathrm{i}t_1) & c_2 + \mathrm{i}t_2 & \cdots & 0 & c_1 - \mathrm{i}t_1 & -(c_2 - \mathrm{i}t_2) & \cdots & 0 \\
-(c_1 + \mathrm{i}t_1) & 0 & \cdots & 0 & c_1 - \mathrm{i}t_1 & 0 & \cdots & 0 \\
\vdots & & \ddots & & \vdots & & \ddots & \\
-(c_1 + \mathrm{i}t_1) & 0 & \cdots & c_n + \mathrm{i}t_n & c_1 - \mathrm{i}t_1 & 0 & \cdots & -(c_n - \mathrm{i}t_n) \\
-(\gamma_1 + \mathrm{i}\tau_1) & -(\gamma_2 + \mathrm{i}\tau_2) & \cdots & -(\gamma_n + \mathrm{i}\tau_n) & \gamma_1 - \mathrm{i}\tau_1 & \gamma_2 - \mathrm{i}\tau_2 & \cdots & \gamma_n - \mathrm{i}\tau_n
\end{array}\right).$$

Suppose first that $c_j + \mathrm{i}t_j \neq 0$ for all $j \in \hat{n}$, then by equivalent row manipulations we pass to the matrix $(D|V)$, where

$$D = \begin{pmatrix}
-\left(\gamma_1 + \mathrm{i}\tau_1 + (c_1 + {}_1)\displaystyle\sum_{\ell=1}^{n} \frac{\gamma_\ell + \mathrm{i}\tau_\ell}{c_\ell + \mathrm{i}t_\ell}\right) & 0 & 0 & \cdots & 0 \\
0 & c_2 + \mathrm{i}t_2 & 0 & \cdots & 0 \\
0 & 0 & c_3 + \mathrm{i}t_3 & \cdots & 0 \\
\vdots & & & \ddots & \\
0 & 0 & 0 & \cdots & c_n + \mathrm{i}t_n
\end{pmatrix},$$

$$V = \begin{pmatrix}
(c_1 - \mathrm{i}t_1)S - 2\mathrm{i}\dfrac{c_1\tau_1 - \gamma_1 t_1}{c_1 + \mathrm{i}t_1} & -2\mathrm{i}\dfrac{c_2\tau_2 - \gamma_2 t_2}{c_2 + \mathrm{i}t_2} & \cdots & -2\mathrm{i}\dfrac{c_n\tau_n - \gamma_n t_n}{c_n + \mathrm{i}t_n} \\
\dfrac{2\mathrm{i}}{S}\dfrac{c_1\tau_1 - \gamma_1 t_1}{c_1 + \mathrm{i}t_1} & -c_2 + \mathrm{i}t_2 + \dfrac{2\mathrm{i}}{S}\dfrac{c_2\tau_2 - \gamma_2 t_2}{c_2 + \mathrm{i}t_2} & \cdots & \dfrac{2\mathrm{i}}{S}\dfrac{c_n\tau_n - \gamma_n t_n}{c_n + \mathrm{i}t_n} \\
\vdots & & \ddots & \\
\dfrac{2\mathrm{i}}{S}\dfrac{c_1\tau_1 - \gamma_1 t_1}{c_1 + \mathrm{i}t_1} & \dfrac{2\mathrm{i}}{S}\dfrac{c_2\tau_2 - \gamma_2 t_2}{c_2 + \mathrm{i}t_2} & \cdots & -c_n + \mathrm{i}t_n + \dfrac{2\mathrm{i}}{S}\dfrac{c_n\tau_n - \gamma_n t_n}{c_n + \mathrm{i}t_n}
\end{pmatrix},$$

where we have denoted $S = \sum_{\ell=1}^n \frac{\gamma_\ell + \mathrm{i}\tau_\ell}{c_\ell + \mathrm{i}t_\ell}$. Since we used only equivalent manipulations, the diagonal matrix D should have the same rank as $A+\mathrm{i}B$, hence it must be regular because none of its diagonal elements is zero. Consequently, we can divide each row of $(D|V)$ by the corresponding diagobal element of D. This yields $(I|U)$, where U is the sought unitary matrix and its diagonal and off-diagonal elements are given by

$$\begin{aligned} U_{jj} &= \frac{2\mathrm{i}(c_j\tau_j - t_j\gamma_j)}{(c_j+\mathrm{i}t_j)^2 \sum_{\ell=1}^n \frac{\gamma_\ell + \mathrm{i}\tau_\ell}{c_\ell + \mathrm{i}t_\ell}} - \frac{c_j - \mathrm{i}t_j}{c_j + \mathrm{i}t_j}\,, \\ U_{jk} &= \frac{2i(c_k\tau_k - t_k\gamma_k)}{(c_j+\mathrm{i}t_j)(c_k+\mathrm{i}t_k) \sum_{\ell=1}^n \frac{\gamma_\ell + \mathrm{i}\tau_\ell}{c_\ell + \mathrm{i}t_\ell}} \quad \text{if } j \neq k\,. \end{aligned} \tag{3.9}$$

The right-hand sides make sense due to the first of the conditions (2.2) and our assumptions about non-vanishing of all the expressions $c_j + it_j$.

So far we have not employed the second one of the requirements (2.2), namely the self-adjointness of the matrix AB^*. This is equivalent to unitarity of U, however, it is easier to check it in its original version. By a straightforward computation we find that the product $AB^* = AB^T$ equals

$$\begin{pmatrix} c_1t_1 + c_2t_2 & c_1t_1 & c_1t_1 & \cdots & c_1t_1 & c_1\tau_1 - c_2\tau_2 \\ c_1t_1 & c_1t_1 + c_3t_3 & c_1t_1 & \cdots & c_1t_1 & c_1\tau_1 - c_3\tau_3 \\ c_1t_1 & c_1t_1 & c_1t_1 + c_4t_4 & \cdots & c_1t_1 & c_1\tau_1 - c_4\tau_4 \\ \vdots & & & \ddots & \vdots & \\ c_1t_1 & c_1t_1 & c_1t_1 & \cdots & c_1t_1 + c_nt_n & c_1\tau_1 - c_n\tau_n \\ \gamma_1t_1 - \gamma_2t_2 & \gamma_1t_1 - \gamma_3t_3 & \gamma_1t_1 - \gamma_4t_4 & \cdots & \gamma_1t_1 - \gamma_nt_n & \gamma_1\tau_1 + \gamma_2\tau_2 + \cdots + \gamma_n\tau_n \end{pmatrix},$$

hence AB^* is self-adjoint if and only if $c_1\tau_1 - c_j\tau_j = \gamma_1t_1 - \gamma_jt_j$ holds for all $j = 2, \ldots, n$, and therefore

$$c_1\tau_1 - \gamma_1t_1 = c_2\tau_2 - \gamma_2t_2 = c_3\tau_3 - \gamma_3t_3 = \cdots = c_n\tau_n - \gamma_nt_n\,. \tag{3.10}$$

We denote the common value $c_j\tau_j - \gamma_jt_j$ as κ and recall that we have denoted $S = \sum_{\ell=1}^n \frac{\gamma_\ell + \mathrm{i}\tau_\ell}{c_\ell + \mathrm{i}t_\ell}$, then the matrix U given by (3.9) can be simplified,

$$U = \begin{pmatrix} \frac{2\mathrm{i}\kappa}{(c_1+\mathrm{i}t_1)^2S} - \frac{c_1-\mathrm{i}t_1}{c_1+\mathrm{i}t_1} & \frac{2\mathrm{i}\kappa}{(c_1+\mathrm{i}t_1)(c_2+\mathrm{i}t_2)S} & \cdots & \frac{2\mathrm{i}\kappa}{(c_1+\mathrm{i}t_1)(c_n+\mathrm{i}t_n)S} \\ \frac{2\mathrm{i}\kappa}{(c_2+\mathrm{i}t_2)(c_1+\mathrm{i}t_1)S} & \frac{2\mathrm{i}\kappa}{(c_2+\mathrm{i}t_2)^2S} - \frac{c_2-\mathrm{i}t_2}{c_2+\mathrm{i}t_2} & \cdots & \frac{2\mathrm{i}\kappa}{(c_2+\mathrm{i}t_2)(c_n+\mathrm{i}t_n)S} \\ \vdots & & \ddots & \\ \frac{2\mathrm{i}\kappa}{(c_n+\mathrm{i}t_n)(c_1+\mathrm{i}t_1)S} & \frac{2\mathrm{i}\kappa}{(c_n+\mathrm{i}t_n)(c_2+\mathrm{i}t_2)S} & \cdots & \frac{2\mathrm{i}\kappa}{(c_n+\mathrm{i}t_n)(c_n+\mathrm{i}t_n)S} - \frac{c_n-\mathrm{i}t_n}{c_n+\mathrm{i}t_n} \end{pmatrix}.$$

Let us show that the matrix (3.9) can be parametrized by $2n$ real numbers. We rewrite the quantity S introduced above in the following way,

$$S = \sum_{\ell=1}^{n} \frac{(\gamma_\ell + \mathrm{i}\tau_\ell)(c_\ell - \mathrm{i}t_\ell)}{c_\ell^2 + t_\ell^2} = \sum_{\ell=1}^{n} \frac{c_\ell\gamma_\ell + t_\ell\tau_\ell}{c_\ell^2 + t_\ell^2} + \mathrm{i}\kappa \sum_{\ell=1}^{n} \frac{1}{c_\ell^2 + t_\ell^2}\,,$$

and make first several observations: (i) regarding (3.8) as a system of linear equations its solvability is not affected if the last one is multiplied by a nonzero number. At the same time, the value of κ is directly proportional to γ_j, τ_j, and consequently, one can suppose without loss of generality that $\kappa = 1$ (the case $\kappa = 0$ gives rise to the same situation as $c_1 + \mathrm{i}t_1 = 0$ which we shall discuss below), (ii) if $\kappa = 1$ the imaginary part of S is determined only by the values of c_j, t_j, $j \in \hat{n}$, (iii) and finally, one can also suppose without loss of generality that $|c_1 + \mathrm{i}t_1| = 1$, since in the opposite case we can divide all but the last of the equations in the system (3.8) by $|c_1 + \mathrm{i}t_1|$ which is nonzero by assumption.

With the above convention we can denote $c_1 + \mathrm{i}t_1 =: \mathrm{e}^{\mathrm{i}\theta}$ and $\operatorname{Re} S =: \rho$ so that

$$S = \rho + \mathrm{i}\left(1 + \sum_{\ell=2}^{n} \frac{1}{c_\ell^2 + t_\ell^2}\right)$$

and U can be written explicitly as

$$U = \begin{pmatrix} \frac{2\mathrm{i}}{S}\mathrm{e}^{-2\mathrm{i}\theta} - \mathrm{e}^{-2\mathrm{i}\theta} & \frac{2\mathrm{i}}{(c_2+\mathrm{i}t_2)S}\mathrm{e}^{-\mathrm{i}\theta} & \cdots & \frac{2\mathrm{i}}{(c_n+\mathrm{i}t_n)S}\mathrm{e}^{-\mathrm{i}\theta} \\ \frac{2\mathrm{i}}{(c_2+\mathrm{i}t_2)S}\mathrm{e}^{-\mathrm{i}\theta} & \frac{2\mathrm{i}}{(c_2+\mathrm{i}t_2)^2 S} - \frac{c_2-\mathrm{i}t_2}{c_2+\mathrm{i}t_2} & \cdots & \frac{2\mathrm{i}}{(c_2+\mathrm{i}t_2)(c_n+\mathrm{i}t_n)S} \\ \vdots & & \ddots & \\ \frac{2\mathrm{i}}{(c_n+\mathrm{i}t_n)S}\mathrm{e}^{-\mathrm{i}\theta} & \frac{2\mathrm{i}}{(c_n+\mathrm{i}t_n)(c_2+\mathrm{i}t_2)S} & \cdots & \frac{2\mathrm{i}}{(c_n+\mathrm{i}t_n)(c_n+\mathrm{i}t_n)S} - \frac{c_n-\mathrm{i}t_n}{c_n+\mathrm{i}t_n} \end{pmatrix} \tag{3.11}$$

being dependent on $2n$ real parameters $\theta, c_2, c_3, \ldots, c_n, t_2, t_3, \ldots, t_n, \rho$.

The above argument applies to any $n > 2$. In the case $n = 2$ the situation is somewhat different, because we have $n^2 = 2n = 4$ but (3.11) does not give the whole family of unitary 2×2 matrices; notice that the off-diagonal elements coincide. It is easy to show that the admissible U can be for $n = 2$ characterized by three real parameters. Indeed, writing $U = \left(\begin{smallmatrix} a & b \\ b & c \end{smallmatrix}\right)$ the unitarity requirement reads

$$|a|^2 + |b|^2 = 1, \quad |b|^2 + |c|^2 = 1, \quad a\bar{b} + b\bar{c} = 0\,.$$

Knowing the modulus and phase of a, the modulus of b is determined so one has to choose its phase. Furthermore, since we assume $b \neq 0$ the element c is uniquely determined. Hence the matrix U of (3.11) is described by three parameters which can be chosen, e.g., as the real parts of U_{jj} and the phase of U_{12}.

Returning to the general case one can also write the conditions (2.1) explicitly in terms of the parameters. A straightforward way is to put $\tilde{A} = U - I$, $\tilde{B} = \mathrm{i}(U + I)$

with U given by (3.11). To get a simpler expression one can pass from the system $\tilde{A}\Psi(0)+\tilde{B}\Psi'(0)=0$ to an equivalent one multiplying it from the left by the matrix

$$\frac{1}{2}\begin{pmatrix} -\mathrm{e}^{\mathrm{i}\theta} & c_2+\mathrm{i}t_2 & 0 & \cdots & 0 \\ -\mathrm{e}^{\mathrm{i}\theta} & 0 & c_3+\mathrm{i}t_3 & \cdots & 0 \\ \vdots & & & \ddots & \\ -\mathrm{e}^{\mathrm{i}\theta} & 0 & 0 & \cdots & c_n+\mathrm{i}t_n \\ \mathrm{e}^{\mathrm{i}\theta} & c_2+\mathrm{i}t_2 & c_3+\mathrm{i}t_3 & \cdots & c_n+\mathrm{i}t_n \end{pmatrix};$$

this yields an explicit parametrization of the conditions (2.1) with

$$A=\begin{pmatrix} \cos\theta & -c_2 & 0 & \cdots & 0 \\ \cos\theta & 0 & -c_3 & \cdots & 0 \\ \vdots & & & \ddots & \\ \cos\theta & 0 & 0 & \cdots & -c_n \\ S\cos\theta-\frac{\mathrm{i}}{c_1+\mathrm{i}t_1} & Sc_2-\frac{\mathrm{i}}{c_2+\mathrm{i}t_2} & Sc_3-\frac{\mathrm{i}}{c_3+\mathrm{i}t_3} & \cdots & Sc_n-\frac{\mathrm{i}}{c_n+\mathrm{i}t_n} \end{pmatrix},$$

$$B=\begin{pmatrix} \sin\theta & -t_2 & 0 & \cdots & 0 \\ \sin\theta & 0 & -t_3 & \cdots & 0 \\ \vdots & & & \ddots & \\ \sin\theta & 0 & 0 & \cdots & -t_n \\ S\sin\theta+\frac{1}{c_1+\mathrm{i}t_1} & St_2+\frac{1}{c_2+\mathrm{i}t_2} & St_3+\frac{1}{c_3+\mathrm{i}t_3} & \cdots & St_n+\frac{1}{c_n+\mathrm{i}t_n} \end{pmatrix} \tag{3.12}$$

and concludes the argument in the generic case when $c_j+\mathrm{i}t_j\neq 0$ for all $j\in\hat{n}$.

It remains to deal with the case when the last mentioned requirement is violated; without loss of generality we may suppose that $c_1+\mathrm{i}t_1=0$. The corresponding matrix $\big(-(A+\mathrm{i}B)|(A-\mathrm{i}B)\big)$ has the form

$$\left(\begin{array}{cccc|cccc} 0 & c_2+\mathrm{i}t_2 & \cdots & 0 & 0 & -(c_2-\mathrm{i}t_2) & \cdots & 0 \\ \vdots & & \ddots & & \vdots & & \ddots & \\ 0 & 0 & \cdots & c_n+\mathrm{i}t_n & 0 & 0 & \cdots & -(c_n-\mathrm{i}t_n) \\ -(\gamma_1+\mathrm{i}\tau_1) & -(\gamma_2+\mathrm{i}\tau_2) & \cdots & -(\gamma_n+\mathrm{i}\tau_n) & \gamma_1-\mathrm{i}\tau_1 & \gamma_2-\mathrm{i}\tau_2 & \cdots & \gamma_n-\mathrm{i}\tau_n \end{array}\right).$$

Using the Gauss elimination scheme we arrive at $(D|V)$ with a diagonal D and upper-triangular V, and from here in the same way as above to $(I|U)$ with

$$U=\begin{pmatrix} -\frac{\gamma_1-\mathrm{i}\tau_1}{\gamma_1+\mathrm{i}\tau_1} & \frac{2\mathrm{i}}{\gamma_1+\mathrm{i}\tau_1}\frac{c_2\tau_2-\gamma_2t_2}{c_2+\mathrm{i}t_2} & \frac{2\mathrm{i}}{\gamma_1+\mathrm{i}\tau_1}\frac{c_3\tau_3-\gamma_3t_3}{c_3+\mathrm{i}t_3} & \cdots & \frac{2\mathrm{i}}{\gamma_1+\mathrm{i}\tau_1}\frac{c_n\tau_n-\gamma_nt_n}{c_n+\mathrm{i}t_n} \\ 0 & -\frac{c_2-\mathrm{i}t_2}{c_2+\mathrm{i}t_2} & 0 & \cdots & 0 \\ 0 & 0 & -\frac{c_3-\mathrm{i}t_3}{c_3+\mathrm{i}t_3} & \cdots & 0 \\ \vdots & & & \ddots & \\ 0 & 0 & 0 & \cdots & -\frac{c_n-\mathrm{i}t_n}{c_n+\mathrm{i}t_n} \end{pmatrix}.$$

Furthermore, it follows from the condition (3.10) with $c_1 = t_1 = 0$ that

$$c_2\tau_2 - \gamma_2 t_2 = c_3\tau_3 - \gamma_3 t_3 = \cdots = c_n\tau_n - \gamma_n t_n = 0$$

hence all the off-diagonal elements in the above matrix U vanish which means that it is characterized by n real parameters,

$$U = \mathrm{diag}\{\mathrm{e}^{\mathrm{i}\theta_1}, \ldots, \mathrm{e}^{\mathrm{i}\theta_n}\}.$$

It is easy to rewrite the boundary conditions in the form (2.1) and check that they correspond to the fully separated case,

$$\sin\frac{\theta_j}{2}\cdot\psi_j(0) + \cos\frac{\theta_j}{2}\cdot\psi_j'(0) = 0\,, \quad j \in \hat{n}\,, \tag{3.13}$$

which is, of course, trivial for the viewpoint of quantum mechanics on Γ. □

3.2. *A concrete 2n-parameter approximation*

Knowing the maximum number of parameters in the boundary conditions (2.1) which can be achieved in this way, we are naturally led to the idea of placing two δ interactions at each of the n halflines. In this section we are going to concretize this proposal. We will concentrate at the matrix (3.11) in the generic case leaving out the trivial situation (3.13) mentioned at the end of the previous proof. We will also leave out the case $n = 2$ which was discussed in the paper [27].

Let us specify the approximation arrangement. The δ's are placed as sketched in Fig. 1, all dependent on a parameter d in terms of which the limit is performed:

- there is a δ coupling with parameter $u(d)$ in the star center;
- on each halfline there is a δ interaction with parameter $v_j(d)$, where j is the halfline index, at a distance $D(d)$ from the center (it will turn out in the following that we may choose $D(d) = d^3$);
- furthermore, each halfline supports another δ interaction with parameter $w_j(d)$ at the distance $D(d) + d$ from the center.

For the sake of brevity we will not indicate the d-dependence of the parameters u, v_j, w_j and the distance D unless necessary. The boundary conditions which the functions $\psi_1, \ldots, \psi_n$ on Γ have to satisfy are

$$\psi_1(0) = \psi_2(0) = \cdots = \psi_n(0) =: \psi(0)\,, \quad \sum_{j=1}^{n}\psi_j'(0_+) = u\psi(0), \tag{3.14}$$

$$\psi_j(D_+) = \psi_j(D_-) =: \psi_j(D)\,, \quad \psi_j'(D_+) - \psi_j'(D_-) = v_j\psi_j(D), \tag{3.15}$$

$$\psi_j(D+d_\pm) =: \psi_j(D+d)\,, \quad \psi_j'(D+d_+) - \psi_j'(D+d_-) = w_j\psi_j(D+d)\,. \tag{3.16}$$

Further relations which will in the following serve to determine the parameter dependence on d are obtained from Taylor expansion of the respective wave functions,

$$\psi_j(D) = \psi_j(0) + D\psi_j'(0_+) + \mathcal{O}(D^2)\,, \qquad \psi_j'(D_-) = \psi_j'(0_+) + \mathcal{O}(D)\,, \tag{3.17}$$

$$\psi_j(D+d) = \psi_j(D) + d\psi_j'(D_+) + \mathcal{O}(d^2)\,, \quad \psi_j'(D+d_-) = \psi_j'(D_+) + \mathcal{O}(d) \tag{3.18}$$

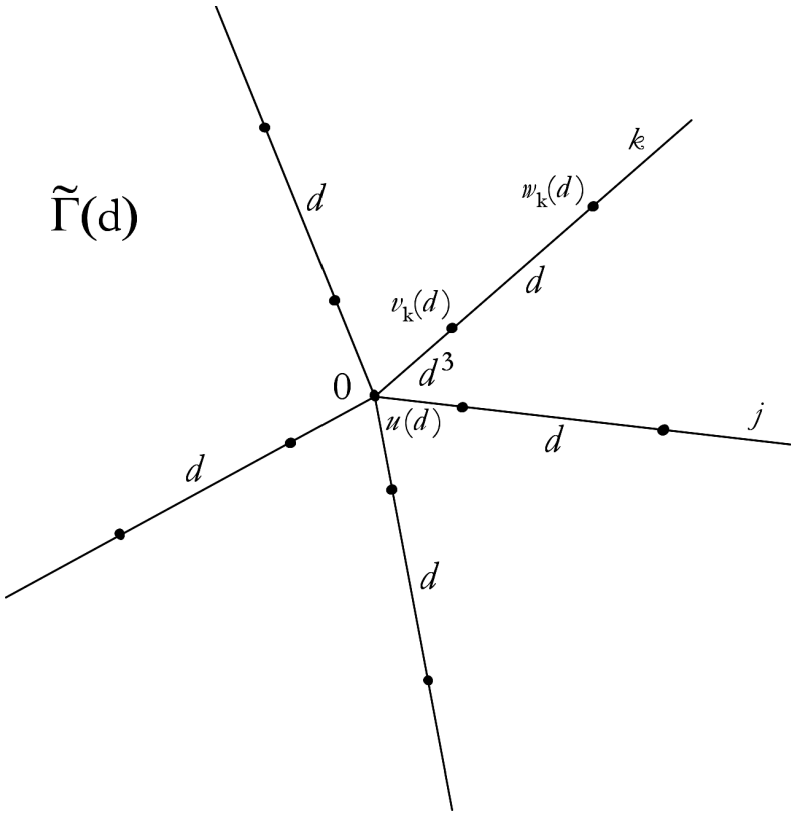

Fig. 1. Scheme of a $2n$-parameter approximation.

for $j \in \hat{n}$. We need to find relations between the values $\psi_1(D+d), \dots, \psi_n(D+d)$ and $\psi_1'(D+d_+), \dots, \psi_n'(D+d_+)$. To this aim we express them first in terms of $\psi(0)$ and $\psi_j'(0_+)$. Using the relations (3.15) and (3.17) we get

$$\begin{aligned}\psi_j'(D_+) &= \psi_j'(0_+) + \mathcal{O}(D) + v_j(\psi_j(0) + D\psi_j'(0_+) + \mathcal{O}(D^2)) \\ &= v_j\psi(0) + (1+v_jD)\psi_j'(0_+) + \mathcal{O}(D) + v_j\mathcal{O}(D^2)\,.\end{aligned}$$

Substituting into the first one of the relations (3.18) and using (3.15) again we find

$$\begin{aligned}\psi_j(D+d) = (1+dv_j)\psi(0) + (D + d(1+v_jD))\,\psi_j'(0_+) \\ + \mathcal{O}(D^2) + d\mathcal{O}(D) + dv_j\mathcal{O}(D^2) + \mathcal{O}(d^2)\,. \qquad (3.19)\end{aligned}$$

The already obtained expression for $\psi_j'(D_+)$ together with the second one of the relations (3.18) give

$$\psi_j'(D+d_-) = v_j\psi(0) + (1+v_jD)\psi_j'(0_+) + \mathcal{O}(D) + v_j\mathcal{O}(D^2) + \mathcal{O}(d)\,.$$

Substituting from here and (3.19) into the second one of the relations (3.16) we get after a simple rearrangement

$$\begin{aligned}\psi_j'(D+d_+) = (v_j + w_j(1+dv_j))\psi(0) + (1 + v_jD + w_j(D + d(1+v_jD)))\psi_j'(0_+) \\ + \mathcal{O}(D) + v_j\mathcal{O}(D^2) + \mathcal{O}(d) + w_j(\mathcal{O}(D^2) + d\mathcal{O}(D) \\ + dv_j\mathcal{O}(D^2) + \mathcal{O}(d^2)). \qquad (3.20)\end{aligned}$$

Next we eliminate $\psi_j'(0_+)$ (for simplicity we write $\psi_j'(0)$) from the obtained relations (3.19) and (3.20), multiplying them by $1 + v_jD + w_j(D + d(1 + v_jD))$ and $D + d(1 + v_jD)$, respectively, and subtracting. In the resulting expression the coefficient at $\psi(0)$ equals one,

$$\begin{aligned}(1 + v_jD + w_j(D + d(1 + v_jD)))\psi_j(D + d)\\ = \psi(0) + (D + d(1 + v_jD))\psi_j'(D + d_+) + \mathcal{R}_j\,,\end{aligned} \tag{3.21}$$

with the remainder term

$$\begin{aligned}\mathcal{R}_j := (1 + v_jD + w_j(D + d(1 + v_jD)))(\mathcal{O}(D^2) + d\mathcal{O}(D) + dv_j\mathcal{O}(D^2) + \mathcal{O}(d^2))\\ - (D + d(1 + v_jD))(\mathcal{O}(D) + v_j\mathcal{O}(D^2) + \mathcal{O}(d)\\ + w_j(\mathcal{O}(D^2) + d\mathcal{O}(D) + dv_j\mathcal{O}(D^2) + \mathcal{O}(d^2)))\,.\end{aligned}$$

So far the edge index has been kept fixed. Subtracting mutually the relations (3.21) for different values of $j, k \in \mathbb{N}$, we can eliminate $\psi(0)$,

$$\begin{aligned}(1 + v_jD + w_j(D + d(1 + v_jD)))\psi_j(D + d)\\ - (1 + v_kD + w_k(D + d(1 + v_kD)))\psi_k(D + d)\\ = (D + d(1 + v_jD))\psi_j'(D + d_+) - (D + d(1 + v_kD))\psi_k'(D + d_+) + \mathcal{R}_j - \mathcal{R}_k.\end{aligned} \tag{3.22}$$

Returning to the relations (3.19) and (3.20) we can eliminate from them $\psi(0)$ in a similar way as above arriving at the relation

$$(1 + dv_j)\psi_j'(D + d_+) - (v_j + w_j(1 + dv_j))\,\psi_j(D + d) = \psi_j'(0) - \tilde{\mathcal{R}}_j \tag{3.23}$$

with the remainder term

$$\begin{aligned}\tilde{\mathcal{R}}_j := (v_j + w_j(1 + dv_j))(\mathcal{O}(D^2) + d\mathcal{O}(D) + dv_j\mathcal{O}(D^2) + \mathcal{O}(d^2))\\ - (1 + dv_j)((\mathcal{O}(D) + v_j\mathcal{O}(D^2) + \mathcal{O}(d) + w_j(\mathcal{O}(D^2)\\ + d\mathcal{O}(D) + dv_j\mathcal{O}(D^2) + \mathcal{O}(d^2)))\,.\end{aligned}$$

Summing the above relations over $j \in \mathbb{N}$ and using (3.14) we get

$$\sum_{j=1}^{n}(1+dv_j)\psi_j'(D+d_+) - \sum_{j=1}^{n}(v_j + w_j(1 + dv_j))\,\psi_j(D+d) = u\psi(0) - \sum_{j=1}^{n}\tilde{\mathcal{R}}_j\,. \tag{3.24}$$

The right-hand side can rewritten using the continuity condition (3.14) in combination with the relation (3.21),

$$\begin{aligned}u\psi(0) = \frac{u}{n}\sum_{j=1}^{n}\psi_j(0) = \frac{u}{n}\sum_{j=1}^{n}\big((1 + v_jD + w_j(D + d(1 + v_jD)))\psi_j(D + d)\\ - (D + d(1 + v_jD))\psi_j'(D + d_+) + \mathcal{R}_j\big)\,.\end{aligned}$$

This allows us to cast (3.24) into a form which contains neither $\psi(0)$ nor $\psi'_j(0)$,

$$\sum_{j=1}^{n}\left(v_j + w_j(1+dv_j) + \frac{u}{n}\left(1 + v_jD + w_j\left(D + d(1+v_jD)\right)\right)\right)\psi_j(D+d) \\ = \sum_{j=1}^{n}\left(1 + dv_j + \frac{u}{n}\left(D + d(1+v_jD)\right)\right)\psi'_j(D+d_+) + \sum_{j=1}^{n}\left(\tilde{\mathcal{R}}_j - \frac{u}{n}\mathcal{R}_j\right). \tag{3.25}$$

The Eqs. (3.22) and (3.25) are the sought relations between the function values and derivatives at the sites of the "outer" δ's with $\psi(0)$ and $\psi'_j(0)$ eliminated.

In the next step we are going to choose the dependences $D = D(d)$, $u = u(d)$, $v_j = v_j(d)$ and $w_j = w_j(d)$ for $j \in \hat{n}$ in such a way that the limit $d \to 0_+$ will yield the ($2n$-parameter family of) boundary conditions (2.1) satisfying the requirement (2.2). It appears that a suitable choice is the following one,

$$\begin{aligned} D(d) &:= d^3 \\ 1 + v_jD &= \alpha_j d\,, \quad \text{i.e.} \quad v_j(d) := -\frac{1}{d^3} + \frac{\alpha_j}{d^2}, \\ 1 + w_jd &= \beta_j d\,, \quad \text{i.e.} \quad w_j(d) := -\frac{1}{d} + \beta_j, \\ u(d) &:= \frac{\omega}{d^4}. \end{aligned} \tag{3.26}$$

Indeed, in such a case the coefficients in (3.22) acquire the form

$$(1 + v_jD)(1 + w_jd) + w_jD = (\alpha_j\beta_j - 1)d^2 + \beta_jd^3\,, \\ D + d(1 + v_jD) = \alpha_jd^2 + d^3 \tag{3.27}$$

and a straightforward computation shows that the remainders are $\mathcal{R}_j = d^2\mathcal{O}(d)$, hence dividing (3.22) by d^2 we arrive at

$$(\alpha_j\beta_j - 1 + \beta_jd)\psi_j(d^3+d) - (\alpha_k\beta_k - 1 + \beta_kd)\psi_k(d^3+d) \\ = (\alpha_j + d)\psi'_j(d^3+d_+) - (\alpha_k + d)\psi'_k(d^3+d_+) + \mathcal{O}(d)\,.$$

Taking the limit $d \to 0_+$ we have to realize that the condition $\psi_j \in W^{2,2}(\mathbb{R}^+)$, $j \in \hat{n}$, requires that $\psi_j(d) = o(d^{-1/2})$ holds at the halfline endpoint, hence we have

$$(\alpha_j\beta_j - 1)\psi_j(0) - (\alpha_k\beta_k - 1)\psi_k(0) = \alpha_j\psi'_j(0) - \alpha_k\psi'_k(0)\,, \quad j,k \in \hat{n}\,. \tag{3.28}$$

In a similar way we proceed with Eq. (3.25). We employ (3.27), then a straightforward computation gives for the coefficients at $\psi_j(D+d)$ and $\psi'_j(D+d_+)$ the

following expressions

$$v_j + w_j(1+dv_j) + \frac{u}{n}\left(1 + v_jD + w_j\left(D + d(1+v_jD)\right)\right)$$

$$= \left(-\beta_j + \frac{\omega}{n}(\alpha_j\beta_j - 1)\right)\frac{1}{d^2} + \left(\alpha_j\beta_j - 1 + \frac{\omega}{n}\beta_j\right)\frac{1}{d} + \beta_j\,,$$

$$1 + dv_j + \frac{u}{n}(D + d(1+v_jD)) = \left(-1 + \frac{\omega}{n}\alpha_j\right)\frac{1}{d^2} + \left(\alpha_j + \frac{\omega}{n}\right)\frac{1}{d} + 1\,,$$

and the remainder terms $\tilde{\mathcal{R}}_j$ and $\frac{u}{n}\mathcal{R}_j$ are both $d^{-2}\mathcal{O}(d)$. We substitute from here to (3.25), multiply the result by d^2 and pass to the limit $d \to 0_+$; this yields

$$\sum_{j=1}^{n}\left(-\beta_j + \frac{\omega}{n}(\alpha_j\beta_j - 1)\right)\psi_j(0) = \sum_{j=1}^{n}\left(-1 + \frac{\omega}{n}\alpha_j\right)\psi_j'(0)\,, \quad j \in \hat{n}\,. \tag{3.29}$$

The relations (3.28) and (3.29) are the sought boundary conditions. It remains to express them as (2.1) and to find relations between the parameters contained in them to those of (3.11). The matrix forms of (3.28) and (3.29) looks as follows,

$$\begin{pmatrix} \alpha_1\beta_1 - 1 & -(\alpha_2\beta_2 - 1) & \cdots & 0 \\ \vdots & & \ddots & \\ \alpha_1\beta_1 - 1 & 0 & \cdots & -(\alpha_n\beta_n - 1) \\ \tilde{\gamma}_1 & \tilde{\gamma}_2 & \cdots & \tilde{\gamma}_n \end{pmatrix}\Psi(0)$$
$$+ \begin{pmatrix} -\alpha_1 & \alpha_2 & \cdots & 0 \\ \vdots & & \ddots & \\ -\alpha_1 & 0 & \cdots & \alpha_n \\ \tilde{\tau}_1 & \tilde{\tau}_2 & \cdots & \tilde{\tau}_n \end{pmatrix}\Psi'(0) = 0, \tag{3.30}$$

where $\tilde{\gamma}_j := \frac{\omega}{n}(\alpha_j\beta_j - 1) - \beta_j$ and $\tilde{\tau}_j := 1 - \frac{\omega}{n}\alpha_j$. We know that the corresponding matrix of (2.3) is given by $U = -(A + \mathrm{i}B)^{-1}\cdot(A - \mathrm{i}B)$, its matrix element being

$$U_{jj} = \frac{2\mathrm{i}}{(\alpha_j\beta_j - 1 - \mathrm{i}\alpha_j)^2\left(\sum_{l=1}^{n}\frac{\beta_l(\alpha_l\beta_l - 1) + \alpha_l}{(\alpha_l\beta_l - 1)^2 + \alpha_l^2} - \omega + \mathrm{i}\sum_{l=1}^{n}\frac{1}{(\alpha_l\beta_l - 1)^2 + \alpha_l^2}\right)} - \frac{\alpha_j\beta_j - 1 + \mathrm{i}\alpha_j}{\alpha_j\beta_j - 1 - \mathrm{i}\alpha_j}$$

and

$$U_{jk} = \frac{2\mathrm{i}}{(\alpha_j\beta_j - 1 - \mathrm{i}\alpha_j)(\alpha_k\beta_k - 1 - \mathrm{i}\alpha_k)} \times \left(\sum_{l=1}^{n}\frac{\beta_l(\alpha_l\beta_l - 1) + \alpha_l}{(\alpha_l\beta_l - 1)^2 + \alpha_l^2} - \omega + \mathrm{i}\sum_{l=1}^{n}\frac{1}{(\alpha_l\beta_l - 1)^2 + \alpha_l^2}\right)$$

for $j \neq k$. If the latter should correspond to (3.11), it is sufficient to require

$$|\alpha_1\beta_1 - 1 - \mathrm{i}\alpha_1| = 1 \tag{3.31}$$

and to set

$$\sum_{l=1}^{n} \frac{\beta_l(\alpha_l\beta_l - 1) + \alpha_l}{(\alpha_l\beta_l - 1)^2 + \alpha_l^2} - \omega = \rho\,, \tag{3.32}$$

$$\alpha_j\beta_j - 1 = c_j\,, \quad -\alpha_j = t_j\,. \tag{3.33}$$

For $\alpha_1 = 0$ the condition (3.31) is satified trivially, while for a nonzero value it is equivalent to $\alpha_1(\alpha_1(\beta_1^2 + 1) - 2\beta_1) = 0$, in other words we have to put

$$\alpha_1 = \frac{2\beta_1}{\beta_1^2 + 1}\,.$$

In this way we have eliminated the parameter α_1, and just $2n$ of them is left. The correspondence between the $2n$-tuples $\beta_1, \beta_2, \beta_3, \ldots, \beta_n, \alpha_2, \alpha_3, \ldots, \alpha_n, \omega$ and $\theta, c_2, c_3, \ldots, c_n, t_2, t_3, \ldots, t_n, \rho$ looks as follows:

- $\beta_1 \leftrightarrow \theta$: they are related by $\frac{\beta_1 - \mathrm{i}}{\beta_1 + \mathrm{i}} = \mathrm{e}^{\mathrm{i}\theta}$
- $\alpha_j, \beta_j \leftrightarrow c_j, t_j$, $j \in \{2, \ldots, n\}$: see (3.33),
- $\omega \leftrightarrow \rho$: see (3.32).

In what follows we will work with $\beta_1, \beta_2, \beta_3, \ldots, \beta_n, \alpha_2, \alpha_3, \ldots, \alpha_n, \omega$, for simplicity we will use also α_1 remembering that it is determined by β_1 and the relation (3.31).

4. Norm-Resolvent Convergence

The approximation worked out in the previous section was in the spirit of [16, 27] being expressed in terms of boundary conditions. One asks naturally what can be said about the relation between the corresponding operators. We denote the Hamiltonian with the coupling (3.30) in center of the star as $H^{\omega,\vec{\alpha},\vec{\beta}}$, and $H^{u,\vec{v},\vec{w}}(d)$ will be the approximating family constructed above, with a pair of δ interactions added at each halfline. Our aim here is to demonstrate the following claim.

Theorem 4.1. *Let $u, v_j, w_j, j \in \hat{n}$, depend on d according to* (3.26)*, i.e.*

$$u(d) = \frac{\omega}{d^4}\,, \quad v_j(d) = -\frac{1}{d^3} + \frac{\alpha_j}{d^2}\,, \quad w_j(d) = -\frac{1}{d} + \beta_j\,.$$

Then $H^{u,\vec{v},\vec{w}}(d)$ converges to $H^{\omega,\vec{\alpha},\vec{\beta}}$ in the norm-resolvent sense as $d \to 0_+$.

Proof. We have to compare the resolvents $R_{H^{u,\vec{v},\vec{w}}(d)}(k^2)$ and $R_{H^{\omega,\vec{\alpha},\vec{\beta}}}(k^2)$ of the two operators for k^2 in the resolvent set. It is clearly sufficient to check the convergence in the Hilbert–Schmidt norm,

$$\left\| R_{H^{u,\vec{v},\vec{w}}(d)}(k^2) - R_{H^{\omega,\vec{\alpha},\vec{\beta}}}(k^2) \right\|_2 \to 0_+ \quad \text{as } d \longrightarrow 0_+\,,$$

in other words, to show that the difference of the corresponding resolvent kernels denoted as $\mathcal{G}_k^{u,\vec{v},\vec{w}}$ and $\mathcal{G}_k^{\omega,\vec{\alpha},\vec{\beta}}$, respectively, tends to zero in $L^2((\mathbb{R}^+)^{2n})$. Recall that these jernels, or Green functions, are in our case $n \times n$ matrix functions.

Let us construct first $\mathcal{G}_k^{\omega,\vec{\alpha},\vec{\beta}}$ for the star-graph Hamiltonian referring to the condition (2.1) in the center. We begin with n independent halflines with Dirichlet condition at its endpoints; Green's function for each of them is well known to be

$$\mathcal{G}_{\mathrm{i}\kappa}(x,y) = \frac{\sinh \kappa x_< \, \mathrm{e}^{-\kappa x_>}}{\kappa}\,,$$

where $x_< := \min\{x,y\}$, $x_> := \max\{x,y\}$, and we put $\mathrm{i}\kappa = k$ assuming $\mathrm{Re}\,\kappa > 0$. The sought Green's function is then given by Krein's formula [4, App. A],

$$R_{H^{A,B}}(k^2) = R_H(k^2) + \sum_{j,l=1}^{n} \lambda_{jl}(k^2)(\phi_l(\bar{k}^2),\cdot)_{L^2((\mathbb{R}^+)^n)}\phi_j(k^2)\,, \tag{4.1}$$

where $R_H(k^2)$ acts on each halfline as an integral operator with the kernel $\mathcal{G}_\kappa$ and for $\phi_j(k^2)$ one can choose any elements of the deficiency subspaces of the largest common restriction; we will work with $\big(\phi_j(k^2)(x)\big)_m = \delta_{jm}\mathrm{e}^{-\kappa x}$.

To find the coefficients $\lambda_{jl}(k^2)$ we apply (4.1) to an arbitrary $\Psi \in \bigoplus_{j=1}^n L^2(\mathbb{R}^+)$ and denote the components of the resulting vector as h_j; it yields

$$h_j(x_j) = \int_0^{+\infty} \mathcal{G}_{\mathrm{i}\kappa}(x,y_j)\psi_j(y_j)\mathrm{d}y_j + \sum_{l=1}^{n} \lambda_{jl}(k^2) \int_0^{+\infty} e^{-\kappa y_l}\psi_l(y_l)\mathrm{d}y_l \cdot \mathrm{e}^{-\kappa x_j}\,.$$

These functions have to satisfy the boundary conditions in the center,

$$\sum_{m=1}^{n} A_{jm}h_m(0) + \sum_{m=1}^{n} B_{jm}h'_m(0) = 0 \quad \text{for all } j \in \hat{n}\,. \tag{4.2}$$

Using the explicit form of $\mathcal{G}_{\mathrm{i}\kappa}(x,y)$ and $\frac{\partial \mathcal{G}_\kappa(x_m,y_m)}{\partial x_m}|_{x_m=0} = \mathrm{e}^{-\kappa y_m}$ we find

$$h_m(0) = \sum_{l=1}^{n} \lambda_{ml}(k^2) \int_0^{+\infty} \mathrm{e}^{-\kappa y_l}\psi_l(y_l)\mathrm{d}y_l \tag{4.3}$$

and

$$h'_m(0) = \int_0^{+\infty} \mathrm{e}^{-\kappa y_m}\psi_m(y_m)\mathrm{d}y_m - \kappa \sum_{l=1}^{n} \lambda_{ml}(k^2) \int_0^{+\infty} \mathrm{e}^{-\kappa y_l}\psi_l(y_l)\mathrm{d}y_l\,. \tag{4.4}$$

Substituting from these relations into (4.2) we get a system of equations,

$$\sum_{l=1}^{n} \int_0^{+\infty} \left(\sum_{m=1}^{n} A_{jm}\lambda_{ml}(k^2) + B_{jl} - \kappa \sum_{m=1}^{n} B_{jm}\lambda_{ml}(k^2) \right) \mathrm{e}^{-\kappa y_l}\psi_l(y_l)\mathrm{d}y_l = 0\,,$$

with $j \in \hat{n}$. We require that the left-hand side vanishes for any $\psi_1, \psi_2, \ldots, \psi_n$; this yields the condition $A\Lambda + B - \kappa B\Lambda = 0$. From here it is easy to find the coefficients $\lambda_{jl}(k^2)$: we have $(A - \kappa B)\Lambda = -B$, and therefore

$$\lambda_{jl}(k^2) = -\left[(A - \kappa B)^{-1}B\right]_{jl}\,.$$

Notice that the matrix $A - \kappa B$ is regular in view of the first conditions in (2.2); since A, B are real and $\mathrm{Im}\,\kappa \neq 0$, the requirement $\mathrm{rank}(A,B) = n$ implies that we have also $\mathrm{rank}(A - \kappa B) = n$.

Let us now concentrate on the class of couplings for which we established in the previous section the boundary condition convergence. In this case $A-\kappa B$ equals

$$\begin{pmatrix} \alpha_1(\beta_1+\kappa)-1 & -(\alpha_2(\beta_2+\kappa)-1) & \cdots & 0 \\ \vdots & & \ddots & \\ \alpha_1(\beta_1+\kappa)-1 & 0 & \cdots & -(\alpha_n(\beta_n+\kappa)-1) \\ (\beta_1+\kappa)\left(\frac{\omega}{n}\alpha_1-1\right)-\frac{\omega}{n} & (\beta_2+\kappa)\left(\frac{\omega}{n}\alpha_2-1\right)-\frac{\omega}{n} & \cdots & (\beta_n+\kappa)\left(\frac{\omega}{n}\alpha_n-1\right)-\frac{\omega}{n} \end{pmatrix},$$

and a tedious by straightforward computation yields an explicit form of the matrix $-(A-\kappa B)^{-1}B$, namely

$$[-(A-\kappa B)^{-1}B]_{jl} = \frac{1}{\omega-\sum_{m=1}^{n}\frac{\beta_m+\kappa}{\alpha_m(\beta_m+\kappa)-1}}\cdot\frac{1}{(\alpha_j(\beta_j+\kappa)-1)(\alpha_l(\beta_l+\kappa)-1)} \quad \text{for } j\neq l\,,$$

$$[-(A-\kappa B)^{-1}B]_{jj} = \frac{1}{\omega-\sum_{m=1}^{n}\frac{\beta_m+\kappa}{\alpha_m(\beta_m+\kappa)-1}}\cdot\frac{1}{(\alpha_j(\beta_j+\kappa)-1)^2}+\frac{\alpha_j}{\alpha_j(\beta_j+\kappa)-1}\,.$$

In this way we get the Green function $\mathcal{G}_{\mathrm{i}\kappa}^{\omega,\vec{\alpha},\vec{\beta}}$. As we have mentioned above, it is an $n\times n$ matrix-valued function the (j,l)th element of which is given by

$$\mathcal{G}_{\mathrm{i}\kappa,jl}^{\omega,\vec{\alpha},\vec{\beta}}(x,y) = \delta_{jl}\left(\frac{\sinh\kappa x_<\,\mathrm{e}^{-\kappa x_>}}{\kappa}+\mathrm{e}^{-\kappa(x+y)}\frac{\alpha_j}{\alpha_j(\beta_j+\kappa)-1}\right) + \frac{1}{\omega-\sum_{m=1}^{n}\frac{\beta_m+\kappa}{\alpha_m(\beta_m+\kappa)-1}}\cdot\frac{1}{(\alpha_j(\beta_j+\kappa)-1)(\alpha_l(\beta_l+\kappa)-1)}\;\mathrm{e}^{-\kappa x}\mathrm{e}^{-\kappa y};$$

we use the convention that x is from the jth halfline and y from the lth one.

Next we will pass to resolvent construction for the approximating family of operators $H^{u,\vec{v},\vec{w}}(d)$. As a starting point we consider n independent halflines with Dirichlet endpoints; we know that the appropriate Green's function is $\mathcal{G}_{\mathrm{i}\kappa}(x,y)=\kappa^{-1}\sinh\kappa x_<\mathrm{e}^{-\kappa x_>}$. The sought resolvent kernel will be then found in several steps. Each of them represents an application of Krein's formula. First we add the δ interaction with the parameter v at the distance d^3 from the endpoint, then another one with the parameter w at the distance $d+d^3$, again from the endpoint. This is done on each halfline separately. In the final step we find Green's function for the star in which the Dirichlet ends are replaced by the δ coupling with

the parameter u. That will require, of course, to distinguish the halflines by their indices.

The first step is rather standard [19] and resulting Green function is

$$\mathcal{G}^v_{\mathrm{i}\kappa}(x,y) = \mathcal{G}_{\mathrm{i}\kappa}(x,y) - \frac{v}{1+v\cdot\mathcal{G}_{\mathrm{i}\kappa}(d^3,d^3)}\,\mathcal{G}_{\mathrm{i}\kappa}(y,d^3)\,\mathcal{G}_{\mathrm{i}\kappa}(x,d^3)\,. \tag{4.5}$$

Adding another δ interaction at the distance d from the previous one we seek the kernel in the form $R^{v,w}(k^2) = R^v(k^2) + \lambda(k^2)\big(\phi(\bar{k}^2),\cdot\big)\phi(k^2)$ where the first term is $R^v(k^2) := \mathcal{G}^v_{\mathrm{i}\kappa}$ and the deficiency-subspace element $\phi(k^2)$ is chosen as

$$\phi(k^2)(x) := \mathcal{G}^v_{\mathrm{i}\kappa}(x, d+d^3)\,.$$

We apply this Ansatz to any $\psi\in L^2(\mathbb{R}^+)$ and denote $h := R^{v,w}(k^2)\psi$. It is easy to check that $\overline{\mathcal{G}^v_{\mathrm{i}\bar\kappa}(x,y)} = \mathcal{G}^v_{\mathrm{i}\kappa}(x,y)$, hence we can write h explicitly as

$$h(x) = \int_0^{+\infty}\mathcal{G}^v_{\mathrm{i}\kappa}(x,y)\psi(y)\,\mathrm{d}y + \lambda(k^2)\int_0^{+\infty}\mathcal{G}^v_{\mathrm{i}\kappa}(y,d+d^3)\psi(y)\,\mathrm{d}y\cdot\mathcal{G}^v_{\mathrm{i}\kappa}(x,d+d^3)\,.$$

By definition this function this function belongs to the domain of the operator with two δ interactions, in particular, it has to satisfy the boundary conditions

$$h(d+d^3{}_+) = h(d+d^3{}_-) =: h(d+d^3)\,, \tag{4.6}$$

$$h'(d+d^3{}_+) - h'(d+d^3{}_-) \;=\; w\cdot h(d+d^3)\,. \tag{4.7}$$

Green's function continuity implies (4.6). Furthermore, we have

$$h'(x) = \int_0^{+\infty}\frac{\partial\mathcal{G}^v_{\mathrm{i}\kappa}(x,y)}{\partial x}\psi(y)\,\mathrm{d}y + \lambda(k^2)\int_0^{+\infty}\mathcal{G}^v_{\mathrm{i}\kappa}(y,d+d^3)\psi(y)\,\mathrm{d}y\cdot\frac{\partial\mathcal{G}^v_{\mathrm{i}\kappa}(x,d+d^3)}{\partial x}\,,$$

which allows us to express $h'(d+d^3_+) - h'(d+d^3_-)$. The first term obviously does not contribute to the difference, while the contribution of the second one simplifies in view of $\frac{\partial\mathcal{G}(x,y)}{\partial x}\Big|_{y_+} - \frac{\partial\mathcal{G}(x,y)}{\partial x}\Big|_{y_-} = -1$ to the form

$$h'(d+d^3_+) - h'(d+d^3_-) = -\lambda(k^2)\int_0^{+\infty}\mathcal{G}^v_{\mathrm{i}\kappa}(y,d+d^3)\psi(y)\,\mathrm{d}y\,.$$

To satisfy (4.7) the coefficient $\lambda(k^2)$ must obey the condition

$$\int_0^{+\infty}\big[\lambda(k^2) + w + w\lambda(k^2)\mathcal{G}^v_{\mathrm{i}\kappa}(d+d^3,d+d^3)\big]\mathcal{G}^v_{\mathrm{i}\kappa}(y,d+d^3)\psi(y)\,\mathrm{d}y = 0$$

for any $\psi\in L^2(\mathbb{R}^+)$, where we have taken Green's function symmetry with respect to the argument interchange into account. Consequently, the square bracket has to vanish and we get the formula for the kernel with two δ interactions,

$$\mathcal{G}^{v,w}_{\mathrm{i}\kappa}(x,y) = \mathcal{G}^v_{\mathrm{i}\kappa}(x,y) - \frac{w}{1+w\cdot\mathcal{G}^v_{\mathrm{i}\kappa}(d+d^3,d+d^3)}\mathcal{G}^v_{\mathrm{i}\kappa}(y,d+d^3)\mathcal{G}^v_{\mathrm{i}\kappa}(x,d+d^3)\,. \tag{4.8}$$

The remaining step will be more complicated because we are going to introduce a coupling between different halflines working this with matrix-valued functions.

Our tool will be again Krein's formula which now takes the form

$$R_{H^{u,\vec{v},\vec{w}}}(k^2) = R_{H^{\vec{v},\vec{w}}}(k^2) + \sum_{j,l=1}^{n} \lambda_{jl}(k^2)(\phi_l(\bar{k}^2),\cdot)_{L^2((\mathbb{R}^+)^n)} \cdot \phi_j(k^2)\,,$$

where the functions $\phi_j(k^2)$ will be chosen as

$$\big(\phi_j(k^2)(x)\big)_m = \delta_{jm} \cdot \left.\frac{\partial \mathcal{G}_{\mathrm{i}\kappa}^{v_m,w_m}(x,y)}{\partial y}\right|_{y=0}.$$

We apply this Ansatz to an arbitrary $\Psi = \{\psi_1,\dots,\psi_n\}^T$ and denote the elements of the resulting vector as h_j, explicitly

$$\begin{aligned} h_j(x) = &\int_0^{+\infty} \mathcal{G}_{\mathrm{i}\kappa}^{v_j,w_j}(x,y)\psi_j(y)\,\mathrm{d}y \\ &+ \sum_{l=1}^{n} \lambda_{jl}(k^2) \int_0^{+\infty} \left.\frac{\partial \mathcal{G}_{\mathrm{i}\kappa}^{v_l,w_l}(x,y)}{\partial x}\right|_{x=0} \psi_l(y)\,\mathrm{d}y \cdot \left.\frac{\partial \mathcal{G}_{\mathrm{i}\kappa}^{v_j,w_j}(x,y)}{\partial y}\right|_{y=0}, \end{aligned} \tag{4.9}$$

where we have used Green's function symmetry and the fact that its complex conjugation is equivalent to switching from κ to $\bar{\kappa}$. As before the functions $h_1, h_2, \dots, h_n$ have to satisfy the boundary conditions expressing the δ coupling in the star centre,

$$h_1(0) = h_2(0) = \cdots = h_n(0) =: h(0)\,, \tag{4.10}$$

$$h_1'(0) + h_2'(0) + \cdots + h_n'(0) = u \cdot h(0)\,, \tag{4.11}$$

for any $\psi_1,\dots,\psi_n \in L^2(\mathbb{R}^+)$. Let us first express $h_j(0)$. The first term in the above expression does not contribute since $\mathcal{G}_{\mathrm{i}\kappa}^{v_j,w_j}(0,y) = \mathcal{G}_{\mathrm{i}\kappa}^{v}(0,y) = 0$. The second one contains the value of Green's function derivative which can be expressed using (4.8),

$$\begin{aligned} \left.\frac{\partial \mathcal{G}_{\mathrm{i}\kappa}^{v_j,w_j}(x,y)}{\partial y}\right|_{y=0} = &\left.\frac{\partial \mathcal{G}_{\mathrm{i}\kappa}^{v}(x,y)}{\partial y}\right|_{y=0} - \frac{w}{1 + w \cdot \mathcal{G}_{\mathrm{i}\kappa}^{v}(d+d^3, d+d^3)} \\ &\cdot \left.\frac{\partial \mathcal{G}_{\mathrm{i}\kappa}^{v}(y, d+d^3)}{\partial y}\right|_{y=0} \cdot \mathcal{G}_{\mathrm{i}\kappa}^{v}(x, d+d^3)\,. \end{aligned}$$

The first term is obtained from (4.5) together with the explicit form of the "free" kernel $\mathcal{G}_{\mathrm{i}\kappa}(x,y)$: we have

$$\left.\frac{\partial \mathcal{G}_{\mathrm{i}\kappa}^{v}(x,y)}{\partial y}\right|_{y=0} = \mathrm{e}^{-\kappa x} - \frac{v}{1 + v \cdot \mathcal{G}_{\mathrm{i}\kappa}(d^3,d^3)}\ \mathrm{e}^{-\kappa d^3}\ \cdot \mathcal{G}_{\mathrm{i}\kappa}(x,d^3)\,,$$

in particular, $\frac{\partial \mathcal{G}_{\mathrm{i}\kappa}^{v}(x,y)}{\partial y}|_{x=y=0} = 1$. This further implies

$$\begin{aligned} \left.\frac{\partial \mathcal{G}_{\mathrm{i}\kappa}^{v_j,w_j}(x,y)}{\partial y}\right|_{y=0} = &\mathrm{e}^{-\kappa x} - \frac{v_j}{1 + v_j \cdot \mathcal{G}_{\mathrm{i}\kappa}(d^3,d^3)} \mathrm{e}^{-\kappa d^3} \mathcal{G}_{\mathrm{i}\kappa}(x,d^3) \\ &- \frac{w_j}{1 + w_j \cdot \mathcal{G}_{\mathrm{i}\kappa}^{v_j}(d+d^3, d+d^3)} \\ &\cdot \left(\mathrm{e}^{-\kappa(d+d^3)} - \frac{v_j}{1 + v_j \cdot \mathcal{G}_{\mathrm{i}\kappa}(d^3,d^3)} \mathrm{e}^{-\kappa d^3} \mathcal{G}_{\mathrm{i}\kappa}(d+d^3, d^3) \right) \\ &\cdot \mathcal{G}_{\mathrm{i}\kappa}^{v_j}(x, d+d^3)\,, \end{aligned} \tag{4.12}$$

in particular, $\frac{\partial \mathcal{G}_{\mathrm{i}\kappa}^{v_j,w_j}(x,y)}{\partial y}|_{x=y=0} = 1$. Putting these results together, we can simplify the expression for the boundary values $h_j(0)$ as follows,

$$h_j(0) = \sum_{l=1}^{n} \lambda_{jl}(k^2) \int_0^{+\infty} \left. \frac{\partial \mathcal{G}_{\mathrm{i}\kappa}^{v_l,w_l}(x,y)}{\partial x} \right|_{x=0} \psi_l(y)\,\mathrm{d}y\,.$$

Now we can find what is required to fulfill the conditions (4.10), i.e. $h_j(0) = h_m(0)$ for all $j, m \in \hat{n}$. This is true provided

$$\sum_{l=1}^{n} \big(\lambda_{jl}(k^2) - \lambda_{ml}(k^2)\big) \int_0^{+\infty} \left. \frac{\partial \mathcal{G}_{\mathrm{i}\kappa}^{v_l,w_l}(x,y)}{\partial x} \right|_{x=0} \psi_l(y)\,\mathrm{d}y = 0\,,$$

holds for any n-tuple of functions $\psi_1, \ldots, \psi_n \in L^2(\mathbb{R}^+)$ which is possible if

$$\lambda_{jl}(k^2) = \lambda_{ml}(k^2) \quad \text{for all } j, m \in \hat{n},\ l \in \hat{n}\,,$$

thus we can simplify notation writing $\lambda_l := \lambda_{jl}(k^2)$ for a fixed $l \in \hat{n}$.

Values of the coefficients $\lambda_1, \ldots, \lambda_n$ can be found from the remaining condition (4.11). To this aim we have to find explicit form of $h_j'(0)$. It follows from the expression (4.9) for $h_j(x)$ that

$$\begin{aligned} h_j'(0) = &\int_0^{+\infty} \left. \frac{\partial \mathcal{G}_{\mathrm{i}\kappa}^{v_j,w_j}(x,y)}{\partial x} \right|_{x=0} \psi_j(y)\,\mathrm{d}y \\ &+ \sum_{l=1}^{n} \lambda_l \int_0^{+\infty} \left. \frac{\partial \mathcal{G}_{\mathrm{i}\kappa}^{v_l,w_l}(x,y)}{\partial x} \right|_{x=0} \psi_l(y)\,\mathrm{d}y \cdot \left. \frac{\mathrm{d}}{\mathrm{d}x} \left(\left. \frac{\partial \mathcal{G}_{\mathrm{i}\kappa}^{v_j,w_j}(x,y)}{\partial y} \right|_{y=0} \right) \right|_{x=0}. \end{aligned}$$

The boundary condition (4.11) then requires that the expression

$$\begin{aligned} \sum_{l=1}^{n} \int_0^{+\infty} &\left(1 + \lambda_l \sum_{j=1}^{n} \frac{\mathrm{d}}{\mathrm{d}x} \left(\left. \frac{\partial \mathcal{G}_{\mathrm{i}\kappa}^{v_j,w_j}(x,y)}{\partial y} \right|_{y=0} \right) \right|_{x=0} - u \cdot \lambda_l \right) \\ &\cdot \left. \frac{\partial \mathcal{G}_{\mathrm{i}\kappa}^{v_l,w_l}(x,y)}{\partial x} \right|_{x=0} \psi_l(y)\,\mathrm{d}y \end{aligned}$$

vanishes for any $\psi_1, \ldots, \psi_n$, and this in turn yields

$$\lambda_l = \left[u - \sum_{j=1}^{n} \frac{\mathrm{d}}{\mathrm{d}x} \left(\left. \frac{\partial \mathcal{G}_{\mathrm{i}\kappa}^{v_j,w_j}(x,y)}{\partial y} \right|_{y=0} \right) \right|_{x=0} \Bigg]^{-1} \quad \text{for all } l \in \hat{n}$$

showing, in particular, that λ_l does not depend on l, which means that all the coefficients $\lambda_{jl}(k^2)$ are the same and equal to the right-hand side of the last relation.

Before specifying the expression in the square bracket let us write down the formula for the (j,l)th component of the sought Green function: we have

$$\begin{aligned}
&\mathcal{G}^{u,\vec{v},\vec{w}}_{\mathrm{i}\kappa,jl}(x,y) \\
&\quad = \delta_{jl}\cdot\mathcal{G}^{v_j,w_j}_{\mathrm{i}\kappa}(x,y) + \frac{\left.\dfrac{\partial\mathcal{G}^{v_j,w_j}_{\mathrm{i}\kappa}(x,y)}{\partial y}\right|_{y=0}\cdot\left.\dfrac{\partial\mathcal{G}^{v_l,w_l}_{\mathrm{i}\kappa}(x,y)}{\partial x}\right|_{x=0}}{u-\displaystyle\sum_{m=1}^{n}\frac{\mathrm{d}}{\mathrm{d}x}\left(\left.\frac{\partial\mathcal{G}^{v_m,w_m}_{\mathrm{i}\kappa}(x,y)}{\partial y}\right|_{y=0}\right)\Bigg|_{x=0}}\,. \qquad (4.13)
\end{aligned}$$

The first derivative in the numerator was found in (4.12) and by Green's function symmetry the other one is given by the same expression, with y replaced by x. The same relation allows us to compute $\frac{\mathrm{d}}{\mathrm{d}x}(\frac{\partial\mathcal{G}^{v_m,w_m}_{\mathrm{i}\kappa}(x,y)}{\partial y}|_{y=0})$, in particular, to evaluate the quantity appearing in the square bracket above,

$$\begin{aligned}
&\frac{\mathrm{d}}{\mathrm{d}x}\left(\left.\frac{\partial\mathcal{G}^{v_m,w_m}_{\mathrm{i}\kappa}(x,y)}{\partial y}\right|_{y=0}\right)\Bigg|_{x=0} \\
&\quad = -\kappa - \frac{v_m}{1+v_m\cdot\mathcal{G}_{\mathrm{i}\kappa}(d^3,d^3)}\mathrm{e}^{-\kappa d^3}\cdot\mathrm{e}^{-\kappa d^3} - \frac{w_m}{1+w_m\cdot\mathcal{G}^{v_m}_{\mathrm{i}\kappa}(d+d^3,d+d^3)} \\
&\qquad \cdot\left(\mathrm{e}^{-\kappa(d+d^3)} - \frac{v_m}{1+v_m\cdot\mathcal{G}_{\mathrm{i}\kappa}(d^3,d^3)}\mathrm{e}^{-\kappa d^3}\mathcal{G}_{\mathrm{i}\kappa}(d+d^3,d^3)\right)^2. \qquad (4.14)
\end{aligned}$$

The relations (4.13) and (4.14) together with (4.12) and its mirror counterpart describe completely Green's function $\mathcal{G}^{u,\vec{v},\vec{w}}_{\mathrm{i}\kappa}$ of the approximating operators.

After deriving explicit expressions for the resolvent we can pass to our proper goal which is to prove that the matrix-valued kernel $\mathcal{G}^{u,\vec{v},\vec{w}}_{\mathrm{i}\kappa}$ converges to $\mathcal{G}^{\omega,\vec{\alpha},\vec{\beta}}_{\mathrm{i}\kappa}$ as $d\to 0_+$ which in terms of their components can be written as

$$\lim_{d\to 0+}\left\|\mathcal{G}^{u,\vec{v},\vec{w}}_{\mathrm{i}\kappa,jl}-\mathcal{G}^{\omega,\vec{\alpha},\vec{\beta}}_{\mathrm{i}\kappa,jl}\right\|_{L^2(\mathbb{R}^+\times\mathbb{R}^+)}=0\,.$$

Depending on the values x, y the difference $\mathcal{G}^{u,\vec{v},\vec{w}}_{\mathrm{i}\kappa,jl}(x,y)-\mathcal{G}^{\omega,\vec{\alpha},\vec{\beta}}_{\mathrm{i}\kappa,jl}(x,y)$ takes different forms. Notice that one can suppose without loss of generality that $x\le y$, and therefore there are six different situations to inspect, namely

- $d+d^3\le x\le y$,
- $d\le x\le d+d^3\le y$,
- $0<x\le d^3$, $d+d^3\le y$,

- $d^3 \le x \le y \le d + d^3$,
- $0 < x \le d^3 \le y \le d + d^3$,
- $0 < x \le y \le d^3$.

To express the kernel difference we employ Taylor expansion of $\mathcal{G}^{u,\vec{v},\vec{w}}_{\mathrm{i}\kappa,jl}(x,y)$. Let us start with expressions which appear in the formulae repeatedly. The first one is

$$\frac{v_m}{1 + v_m \cdot \mathcal{G}_{\mathrm{i}\kappa}(d^3, d^3)} = \frac{-\dfrac{1}{d^3} + \dfrac{\alpha_m}{d^2}}{1 + \left(-\dfrac{1}{d^3} + \dfrac{\alpha_m}{d^2}\right) \cdot \dfrac{\sinh \kappa d^3 \, \mathrm{e}^{-\kappa d^3}}{\kappa}} = (*).$$

Using $\sinh(x) = x + \mathcal{O}(x^2)$ and $\mathrm{e}^x = 1 + \mathcal{O}(x)$ we get

$$\frac{\sinh \kappa d^3 \, \mathrm{e}^{-\kappa d^3}}{\kappa} = \frac{(\kappa d^3 + \mathcal{O}(d^6))(1 + \mathcal{O}(d^3))}{\kappa} = d^3(1 + \mathcal{O}(d^3)) \,,$$

and this in turn allows us to express (*) as follows,

$$(*) = -\frac{1}{d^3} \cdot \frac{1 - \alpha_m d}{1 + \left(-\dfrac{1}{d^3} + \dfrac{\alpha_m}{d^2}\right) \cdot (d^3(1 + \mathcal{O}(d^3)))} = -\frac{1}{d^4} \cdot \left(\frac{1}{\alpha_m} + \mathcal{O}(d)\right) .$$

The next frequent expression is $w_m \left(1 + w_m \cdot \mathcal{G}^{v_m}_{\mathrm{i}\kappa}(d + d^3, d + d^3)\right)^{-1}$. We employ relation (4.5) with $v = v_m$ and the expansion $\mathrm{e}^x = 1 + x + \mathcal{O}(x^2)$ together with the explicit form of $\mathcal{G}_{\mathrm{i}\kappa}$; this yields after a straightforward computation

$$\mathcal{G}^{v_m}_{\mathrm{i}\kappa}(d+d^3, d+d^3) = d\left(1 - \kappa d - \frac{d}{\alpha_m} + \mathcal{O}(d^2)\right) = \mathcal{G}_{\mathrm{i}\kappa}(d+d^3, d+d^3) - \frac{d^2}{\alpha_m} + \mathcal{O}(d^3) \,,$$

and therefore

$$\frac{w_m}{1 + w_m \cdot \mathcal{G}^{v_m}_{\mathrm{i}\kappa}(d + d^3, d + d^3)} = -\frac{1}{d^2}\left(\frac{1}{\beta_m + \kappa - \dfrac{1}{\alpha_m}} + \mathcal{O}(d)\right) .$$

Now we can expand the first term in $\mathcal{G}^{u,\vec{v},\vec{w}}_{\mathrm{i}\kappa,jl}(x,y)$. Using (4.8) for the parameters $v = v_j$, $w = w_j$ together with the previous result we get

$$\begin{aligned}
\mathcal{G}^{v_j,w_j}_{\mathrm{i}\kappa}(x,y) &= \frac{\sinh \kappa x \, \mathrm{e}^{-\kappa y}}{\kappa} + \frac{1}{d^2}\left(\frac{1}{\beta_m + \kappa - \frac{1}{\alpha_m}} + \mathcal{O}(d)\right) \\
&\qquad \times \frac{\sinh \kappa(d + d^3)\mathrm{e}^{-\kappa y}}{\kappa} \frac{\sinh \kappa(d + d^3)\mathrm{e}^{-\kappa x}}{\kappa} \\
&= \frac{\sinh \kappa x \mathrm{e}^{-\kappa y}}{\kappa} + \frac{1}{\beta_m + \kappa - \dfrac{1}{\alpha_m}} \mathrm{e}^{-\kappa x} \mathrm{e}^{-\kappa y}(1 + \mathcal{O}(d)).
\end{aligned}$$

As for the second term in ((4.13)), we first expand the derivative in the denominator using $\mathcal{G}_{\mathrm{i}\kappa}(d+d^3,d^3) = d^3(1+\mathcal{O}(d))$ and (4.14). A direct computation yields

$$\frac{\mathrm{d}}{\mathrm{d}x}\left(\left.\frac{\partial\mathcal{G}_{\mathrm{i}\kappa}^{v_m,w_m}(x,y)}{\partial y}\right|_{y=0}\right)\Bigg|_{x=0} = \frac{1}{d^4}\cdot\left(\frac{\beta_m+\kappa}{\alpha_m(\beta_m+\kappa)-1}+\mathcal{O}(d)\right),$$

and therefore

$$\left(u-\sum_{m=1}^{n}\frac{\mathrm{d}}{\mathrm{d}x}\left(\left.\frac{\partial\mathcal{G}_{\mathrm{i}\kappa}^{v_m,w_m}(x,y)}{\partial y}\right|_{y=0}\right)\Bigg|_{x=0}\right)^{-1}$$
$$= d^4\left(\frac{1}{\omega-\sum_{m=1}^{n}\dfrac{\beta_m+\kappa}{\alpha_m(\beta_m+\kappa)-1}}+\mathcal{O}(d)\right).$$

Next we expand the derivatives which appear in the numerator using the relation $\mathcal{G}_{\mathrm{i}\kappa}^{v_m}(x,d+d^3) = d(1+\mathcal{O}(d))\,\mathrm{e}^{-\kappa x}$; it gives

$$\begin{aligned}\left.\frac{\partial\mathcal{G}_{\mathrm{i}\kappa}^{v_m,w_m}(x,y)}{\partial y}\right|_{y=0} &= \mathrm{e}^{-\kappa x} - \frac{v_m}{1+v_m\cdot\mathcal{G}_{\mathrm{i}\kappa}(d^3,d^3)}\mathrm{e}^{-\kappa d^3}\mathcal{G}_{\mathrm{i}\kappa}(x,d^3)\\ &\quad - \frac{w_m}{1+w_m\cdot\mathcal{G}_{\mathrm{i}\kappa}^{v_m}(d+d^3,d+d^3)}\\ &= \frac{1}{d^2}\left(\frac{1}{\alpha_m(\beta_m+\kappa)-1}+\mathcal{O}(d)\right)\mathrm{e}^{-\kappa x}\end{aligned}$$

and the analogous expression for $\left.\frac{\partial\mathcal{G}_{\mathrm{i}\kappa}^{v_m,w_m}(x,y)}{\partial x}\right|_{x=0}$ with x replaced by y. This determines the behavior of the second term at the right-hand side of (4.13) as $d\to 0_+$, and for the full kernel $\mathcal{G}_{\mathrm{i}\kappa,jl}^{u,\vec{v},\vec{w}}(x,y)$ we consequently have

$$\begin{aligned}\mathcal{G}_{\mathrm{i}\kappa,jl}^{u,\vec{v},\vec{w}}(x,y) &= \delta_{jl}\left(\frac{\sinh\kappa x\mathrm{e}^{-\kappa y}}{\kappa}+\frac{1+\mathcal{O}(d)}{\beta_j+\kappa-\frac{1}{\alpha_j}}\mathrm{e}^{-\kappa x}\mathrm{e}^{-\kappa y}\right)\\ &\quad+\left(\frac{1}{\omega-\sum_{m=1}^{n}\dfrac{\beta_m+\kappa}{\alpha_m(\beta_m+\kappa)-1}}\cdot\frac{1}{\alpha_j(\beta_j+\kappa)-1}\right.\\ &\quad\left.\cdot\ \frac{1}{\alpha_l(\beta_l+\kappa)-1}+\mathcal{O}(d)\right)\mathrm{e}^{-\kappa x}\mathrm{e}^{-\kappa y}.\end{aligned}$$

On the other hand, for $x \le y$ we have

$$\begin{aligned}\mathcal{G}^{\omega,\vec{\alpha},\vec{\beta}}_{\mathrm{i}\kappa,jl}(x,y) = \delta_{jl}\bigg(&\frac{\sinh\kappa x\ \mathrm{e}^{-\kappa y}}{\kappa} + \mathrm{e}^{-\kappa(x+y)}\frac{\alpha_j}{\alpha_j(\beta_j+\kappa)-1}\bigg)\\ &+\frac{1}{\omega - \sum_{m=1}^{n}\dfrac{\beta_m+\kappa}{\alpha_m(\beta_m+\kappa)-1}}\\ &\cdot\frac{1}{(\alpha_j(\beta_j+\kappa)-1)(\alpha_l(\beta_l+\kappa)-1)}\ \mathrm{e}^{-\kappa x}\mathrm{e}^{-\kappa y}\,,\end{aligned}$$

hence the Green function difference satisfies

$$\mathcal{G}^{u,\vec{v},\vec{w}}_{\mathrm{i}\kappa,jl}(x,y) - \mathcal{G}^{\omega,\vec{\alpha},\vec{\beta}}_{\mathrm{i}\kappa,jl}(x,y) = \mathcal{O}(d)\mathrm{e}^{-\kappa x}\mathrm{e}^{-\kappa y} \quad \text{as } d \to 0_+\,.$$

The same estimate is obviously valid also for $d < y < x$, hence there is a constant K independent of d, x and y such that

$$\left|\mathcal{G}^{u,\vec{v},\vec{w}}_{\mathrm{i}\kappa,jl}(x,y) - \mathcal{G}^{\omega,\vec{\alpha},\vec{\beta}}_{\mathrm{i}\kappa,jl}(x,y)\right| < Kd\mathrm{e}^{-\kappa x}\mathrm{e}^{-\kappa y} \tag{4.15}$$

holds for all $d < 1, x \ge d + d^3$ and $y \ge d + d^3$. Now we are in position to estimate the Hilbert–Schmidt norm of the resolvent difference for the operators $H^{\omega,\vec{\alpha},\vec{\beta}}$ and $H^{u,\vec{v},\vec{w}}(d)$ which can be written explicitly as follows,

$$\begin{aligned}&\left\|R_{H^{u,\vec{v},\vec{w}}(d)}(k^2) - R_{H^{\omega,\vec{\alpha},\vec{\beta}}}\right\|_2^2\\ &\quad= \sum_{j,l=1}^{n}\int_0^{+\infty}\int_0^{+\infty}\left|\mathcal{G}^{u,\vec{v},\vec{w}}_{\mathrm{i}\kappa,jl}(x,y) - \mathcal{G}^{\omega,\vec{\alpha},\vec{\beta}}_{\mathrm{i}\kappa,jl}(x,y)\right|^2\mathrm{d}x\mathrm{d}y\\ &\quad= \sum_{j,l=1}^{n}\bigg(\int_{d+d^3}^{+\infty}\int_{d+d^3}^{+\infty}\left|\mathcal{G}^{u,\vec{v},\vec{w}}_{\mathrm{i}\kappa,jl}(x,y) - \mathcal{G}^{\omega,\vec{\alpha},\vec{\beta}}_{\mathrm{i}\kappa,jl}(x,y)\right|^2\mathrm{d}x\mathrm{d}y\\ &\qquad+\int_{d^3}^{d+d^3}\int_{d+d^3}^{+\infty}\left|\mathcal{G}^{u,\vec{v},\vec{w}}_{\mathrm{i}\kappa,jl}(x,y) - \mathcal{G}^{\omega,\vec{\alpha},\vec{\beta}}_{\mathrm{i}\kappa,jl}(x,y)\right|^2\mathrm{d}x\mathrm{d}y\\ &\qquad+\int_{d+d^3}^{+\infty}\int_{d^3}^{d+d^3}\left|\mathcal{G}^{u,\vec{v},\vec{w}}_{\mathrm{i}\kappa,jl}(x,y) - \mathcal{G}^{\omega,\vec{\alpha},\vec{\beta}}_{\mathrm{i}\kappa,jl}(x,y)\right|^2\mathrm{d}x\mathrm{d}y\\ &\qquad+\int_{0}^{d^3}\int_{d+d^3}^{+\infty}\left|\mathcal{G}^{u,\vec{v},\vec{w}}_{\mathrm{i}\kappa,jl}(x,y) - \mathcal{G}^{\omega,\vec{\alpha},\vec{\beta}}_{\mathrm{i}\kappa,jl}(x,y)\right|^2\mathrm{d}x\mathrm{d}y\\ &\qquad+\int_{d+d^3}^{+\infty}\int_{0}^{d^3}\left|\mathcal{G}^{u,\vec{v},\vec{w}}_{\mathrm{i}\kappa,jl}(x,y) - \mathcal{G}^{\omega,\vec{\alpha},\vec{\beta}}_{\mathrm{i}\kappa,jl}(x,y)\right|^2\mathrm{d}x\mathrm{d}y\\ &\qquad+\int_{d^3}^{d+d^3}\int_{d^3}^{d+d^3}\left|\mathcal{G}^{u,\vec{v},\vec{w}}_{\mathrm{i}\kappa,jl}(x,y) - \mathcal{G}^{\omega,\vec{\alpha},\vec{\beta}}_{\mathrm{i}\kappa,jl}(x,y)\right|^2\mathrm{d}x\mathrm{d}y\end{aligned}$$

$$+\int_0^{d^3}\int_{d^3}^{d+d^3}\left|\mathcal{G}^{u,\vec{v},\vec{w}}_{\mathrm{i}\kappa,jl}(x,y)-\mathcal{G}^{\omega,\vec{\alpha},\vec{\beta}}_{\mathrm{i}\kappa,jl}(x,y)\right|^2\mathrm{d}x\mathrm{d}y$$
$$+\int_{d^3}^{d+d^3}\int_0^{d^3}\left|\mathcal{G}^{u,\vec{v},\vec{w}}_{\mathrm{i}\kappa,jl}(x,y)-\mathcal{G}^{\omega,\vec{\alpha},\vec{\beta}}_{\mathrm{i}\kappa,jl}(x,y)\right|^2\mathrm{d}x\mathrm{d}y$$
$$+\int_0^{d^3}\int_0^{d^3}\left|\mathcal{G}^{u,\vec{v},\vec{w}}_{\mathrm{i}\kappa,jl}(x,y)-\mathcal{G}^{\omega,\vec{\alpha},\vec{\beta}}_{\mathrm{i}\kappa,jl}(x,y)\right|^2\mathrm{d}x\mathrm{d}y\Bigg)\,.$$

The inequality (4.15) makes it possible to estimate the first one of the integrals,

$$\int_{d+d^3}^{+\infty}\int_{d+d^3}^{+\infty}\left|\mathcal{G}^{u,\vec{v},\vec{w}}_{\mathrm{i}\kappa,jl}(x,y)-\mathcal{G}^{\omega,\vec{\alpha},\vec{\beta}}_{\mathrm{i}\kappa,jl}(x,y)\right|^2\mathrm{d}x\mathrm{d}y$$
$$\le K^2d^2\left(\int_{d+d^3}^{+\infty}e^{-2(\mathrm{Re}\,\kappa)x}\,\mathrm{d}x\right)^2=K^2d^2\,\frac{e^{-2(\mathrm{Re}\,\kappa)(d+d^3)}}{2\mathrm{Re}\,\kappa}\le\frac{K^2}{2\mathrm{Re}\,\kappa}\,d^2\,,$$

and it is obvious from this inequality that for $d\to 0_+$ the integral tends to zero for any $j,l\in\hat{n}$. In a similar way one can estimate each of the remaining eight integrals: using Taylor expansions of $\mathcal{G}^{u,\vec{v},\vec{w}}_{\mathrm{i}\kappa,jl}$ we get a bound for the integrand which shows that the integral vanishes as $d\to 0_+$. Since the argument repeats the procedure described above, we skip the details. Putting all this together, we conclude that

$$\lim_{d\to 0_+}\left\|R_{H^{u,\vec{v},\vec{w}}(d)}(k^2)-R_{H^{\omega,\vec{\alpha},\vec{\beta}}}\right\|_2^2=0\,,$$

and therefore the resolvent difference tends to zero in Hilbert–Schmidt norm as $d\to 0_+$ which is what we set up to demonstrate. □

5. Approximations with Added Edges

We have seen that a CS-type scheme can produce a $2n$-parameter family of (self-adjoint) couplings out of the whole set depending on n^2 real numbers. To get a wider class we have to add to the star graph Γ not only vertices but edges as well.

5.1. *Admissible couplings*

The first question naturally is how many parameters can be achieved in this way. An upper bound on this number is given by the following statement.

Proposition 5.1. *Let Γ be a star graph with n semi-infinite edges and denote by $\{\tilde{\Gamma}(d):d\in\mathbb{R}^+\}$ a family of graphs obtained from Γ by adding finite edges connecting pairwise the halflines; their number may be arbitrary finite but independent of d. Suppose that $\tilde{\Gamma}(d)$ supports only δ couplings and δ interactions, their number again independent of d, and that the distances between all their sites are $\mathcal{O}(d)$ as $d\to 0_+$. Suppose that a family of functions $\Psi_d\in W^{2,2}(\Gamma\backslash(\{c\}\cup V_d))$, where c is the center of Γ, and V_d is the set of the vertices added on the halflines, satisfies the conditions* (2.4) *with d-dependent parameters, and that it converges to $\Psi\in W^{2,2}(\Gamma\backslash\{c\})$ which obeys the condition* (2.1) *with some A,B satisfying the requirements* (2.2)*. The*

family of the conditions (2.1) *which can be obtained in this way has real-valued coefficients,* $A, B \in \mathbb{R}^{n,n}$*, depending thus on at most* $\binom{n+1}{2}$ *parameters.*

Proof. The δ coupling in the center of $\tilde{\Gamma}(d)$, identified with center of Γ, is expressed by the conditions (2.4). For any $j \in \hat{n}$ we denote by d_j the coordinate of the most distant point on the jth halfline which supports either a δ interaction or a δ coupling at the endpoint of an added edge. We arrange the function values at these points into the n-tuple $\Psi(d)$, and similarly $\Psi'(d_+)$ is the n-tuple of right derivatives. Let us stress that this a symbolic notation; the elements are $\psi_j(d_j)$ and $\psi_j'(d_{j+})$, respectively.

As in the proof of Proposition 3.1 we can use (2.4) to express these quantities through the common value $\psi(0)$ and the right derivatives $\Psi'(0_+)$ at the origin

$$\begin{aligned} M_1(d)\Psi(d) &= \psi(0)\cdot m_2(d) + M_3(d)\Psi'(0) + \mathcal{R}(d)\,, \\ N_1(d)\Psi'(d_+) &= \psi(0)\cdot n_2(d) + N_3(d)\Psi'(0) + \tilde{\mathcal{R}}(d) \end{aligned}$$

for some $M_1, M_3, N_1, N_3 : \mathbb{R}^+ \to \mathbb{R}^{n,n}$, $m_2, n_2 : \mathbb{R}^+ \to \mathbb{R}^n$ and error terms $\mathcal{R}, \tilde{\mathcal{R}} : \mathbb{R}^+ \to \mathbb{R}^n$ supposed to be negligible as $d \to 0_+$; we may assume that $\mathcal{R}$, $\tilde{\mathcal{R}} = o(1)$. The above system can be also written in a matrix form,

$$\begin{pmatrix} M_1(d) & 0 & -m_2(d) & -M_3(d) \\ 0 & N_1(d) & -n_2(d) & -N_3(d) \\ 0 & 0 & -\alpha & 1\ \ 1\ \cdots\ 1 \end{pmatrix} \begin{pmatrix} \Psi(d) \\ \Psi'(d_+) \\ \psi(0) \\ \Psi'(0) \end{pmatrix} = \begin{pmatrix} o(1) \\ o(1) \\ 0 \end{pmatrix}.$$

To find an approximation in the described sense one has to find a relation between $\Psi(d)$ and $\Psi'(d_+)$ eliminating $\psi(0)$, $\Psi'(0)$. Since the former are determined by the latter we may suppose that the matrices $M_1(d)$ a $N_1(d)$ are regular; the elimination then leads to a system

$$A(d)\Psi(d) + B(d)\Psi'(d_+) = \breve{\mathcal{R}}(d)\,,$$

where the matrices $A(d)$, $B(d)$ are real for all $d \in \mathbb{R}^+$ and the right-hand side consists of an error term $\breve{\mathcal{R}} : \mathbb{R}^+ \to \mathbb{R}^n$. We multiply the last equation by a power of d such that the right-hand side is $o(1)$ as $d \to 0_+$ while the left-hand side one has a nontrivial limit. It is clear that we can get in this way the condition (2.3) with real-valued coefficients, $A, B \in \mathbb{R}^{n,n}$. □

5.2. *A concrete approximation arrangement*

The above discussion leaves open the question how such an approximation can be constructed to cover the mentioned $\binom{n+1}{2}$-parameter family. Our aim here is to demonstrate a specific way to do that. We consider the coupling (2.3) with real A, B, and for simplicity we restrict our attention only to the generic case assuming

that B is regular so that the boundary conditions acquire the form

$$\Psi'(0) = -B^{-1}A\Psi(0)$$

with a symmetric matrix $-B^{-1}A$. We can also write them as

$$\Psi'(0) = (D+S)\Psi(0)\,, \tag{5.1}$$

where the real matrix D is diagonal while S is real symmetric with a vanishing diagonal; it is clear that D and S depend on n and $\binom{n}{2}$ real parameters, respectively.

To construct approximation of the corresponding operator $H^{A,B}$ we have find suitable family of graphs $\tilde{\Gamma}(d)$. The decomposition of the matrix in (5.1) into the diagonal and off-diagonal part inspires the following scheme:

- the center of Γ supports a δ coupling with the parameter $u(d)$ the dependence of which on d will be specified below;
- at each edge of Γ we place a δ coupling at the distance d from the center; the corresponding parameter $v_j(d)$, to be again specified, will be related to the diagonal element D_{jj} of the matrix D;
- the pairs of edges whose indices j,k correspond to nonzero elements of the matrix S we join by an additional edge, whose endpoints are the δ coupling sites mentioned above, and in the middle of this edge we place the δ interaction with a parameter $w_{\{j,k\}}(d)$ related to the value of S_{jk}.

The metric on Γ and $\tilde{\Gamma}(d)$ is intrinsic, nevertheless, it is useful to think of it as of induced by embedding of the graphs into a Euclidean space. Without loss of generality we may consider the original star Γ as a planar graph and to construct as embedded into $\mathbb{R}^3$. In such a case, of course, we have to make sure that the added edges do not intersect. This can be achieved in the way sketched in Fig. 2. A possible way is to employ the bijection b from the family of two-element subsets of $\{1,2,\dots,n\}$ to the set $\{1,2,\dots,\frac{n(n-1)}{2}\}$. The edge connecting the jth and kth halfline is formed by two segments connected in a V-shape. Its endpoints are at the jth and kth halfline, both at the distance d from the center. The tip of this V-graph is placed on the halfline starting from the center of Γ in the perpendicular direction to its plane — see Fig. 3 — at the distance $b_{jk}\cdot d^2$, so that the length of the connecting V-graph is $d\sqrt{1+(b_{jk}d)^2}$.

As before we denote by ψ_j the wave function on the jth halfline assuming that all the coordinates have zero in the center of Γ. Furthermore, we denote by $\varphi_j^{\{j,k\}}$ and $\varphi_k^{\{j,k\}}$ the wave function on the line segment part of the connection between the jth and kth halfline which is attached by one of its endpoints to the jth and kth halfline, respectively; notice that the order of the upper indices is irrelevant. Such a connecting link is regarded as a star with two edges of the same length. For

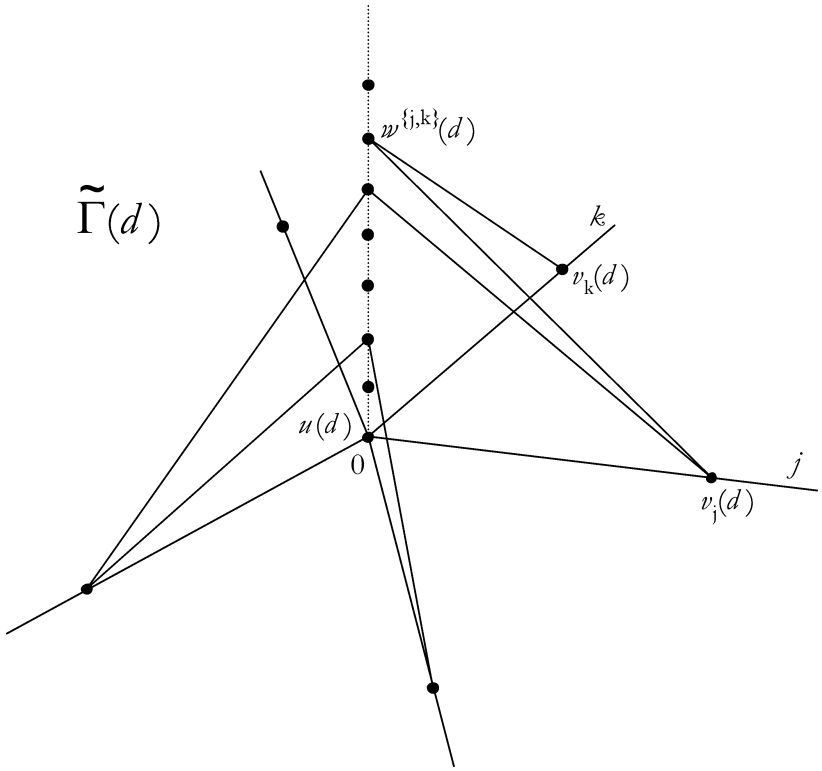

Fig. 2. Approximating graph: A star amended by connections of the edges, with a δ coupling in the center, one δ coupling at each edge and one δ interaction at each (broken) connection segment.

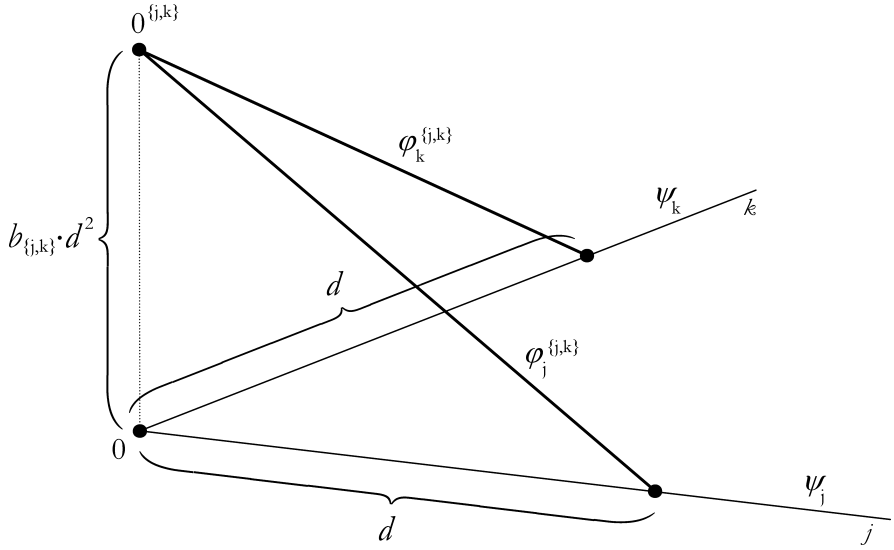

Fig. 3. The connecting edge between the jth and kth halfline.

the sake of brevity we introduce also the set N_j defined as

$$N_j = \{k \in \hat{n} : \ S_{jk} \neq 0\} ;$$

its cardinality $\#N_j$ tells us how many nonzero elements are in the jth row of the matrix S, in other words, how many V-shaped connecting edges sprout from the point $x_j = d$ on the jth halfline.

Next we will write down the boundary conditions describing the involved δ couplings; for simplicity we will not indicate the dependence of the parameters $u, v_j, w_{\{j,k\}}$ on the distance d. The δ coupling in the centre of Γ means

$$\psi_1(0) = \psi_2(0) = \cdots = \psi_n(0) =: \psi(0)\,, \quad \sum_{j=1}^{n} \psi_j'(0_+) = u\psi(0)\,, \tag{5.2}$$

the δ interaction at the "tip" of the broken edge connecting the jth and kth halfline between the vertices added at the distance d from the center (of course, for $j,k \in \hat{n}$ such that $S_{jk} \neq 0$ only) is expressed through the conditions

$$\begin{aligned} \varphi_j^{\{j,k\}}(0) = \varphi_k^{\{j,k\}}(0) =: \varphi^{\{j,k\}}(0)\,, \\ (\varphi^{\{j,k\}})_j'(0_+) + (\varphi^{\{j,k\}})_k'(0_+) = w_{\{j,k\}}\varphi^{\{j,k\}}(0)\,, \end{aligned} \tag{5.3}$$

and finally, the δ coupling at the mentioned added vertices added requires

$$\begin{aligned} \psi_j(d_+) = \psi_j(d_-) = \varphi_j^{\{j,k\}}\big(d\sqrt{1+(b_{jk}d)^2}\big) =: \psi_j(d)\,, \quad j \in \hat{n}\,, \quad k \in N_j \\ \psi_j'(d_+) - \psi_j'(d_-) - \sum_{k\in N_j} (\varphi_j^{\{j,k\}})'\big(d\sqrt{1+(b_{jk}d)^2}\,{}_-\big) \;=\; v_j\psi_j(d)\,, \quad j \in \hat{n}\,. \end{aligned} \tag{5.4}$$

Further relations which will help us to find the parameter dependence on d come from Taylor expansion,

$$\psi_j(d) = \psi_j(0) + d\psi_j'(0) + \mathcal{O})(d^2)\,, \quad \psi_j'(d_-) = \psi_j'(0_+) + \mathcal{O}(d)\,, \quad j \in \hat{n}\,, \tag{5.5}$$

$$\begin{aligned} \varphi_j^{\{j,k\}}\big(d\sqrt{1+(b_{jk}d)^2}\big) = \varphi^{\{j,k\}}(0) + d\sqrt{1+(b_{jk}d)^2}\,(\varphi_j^{\{j,k\}})'(0_+) + \mathcal{O}(d^2)\,, \\ (\varphi_j^{\{j,k\}})'\big(d\sqrt{1+(b_{jk}d)^2}\,{}_-\big) = (\varphi_j^{\{j,k\}})'(0_+) + \mathcal{O}(d)\,, \quad j,k \in \hat{n}\,, \end{aligned} \tag{5.6}$$

where we have used the fact that $\sqrt{1+(b_{jk}d)^2} = 1 + \mathcal{O}(d^2)$. Now we employ the first of the relations (5.6) together with the continuity (5.4), which yields

$$d\sqrt{1+(b_{jk}d)^2}\,(\varphi_j^{\{j,k\}})'(0_+) = \psi_j(d) - \varphi^{\{j,k\}}(0) + \mathcal{O}(d^2)\,. \tag{5.7}$$

The same relation holds with j replaced by k, summing them together and using the second of the relations (5.3) we get

$$\big(2 + d\sqrt{1+(b_{jk}d)^2}\,w_{\{j,k\}}\big)\varphi^{\{j,k\}}(0) = \psi_j(d) + \psi_k(d) + \mathcal{O}(d^2)\,.$$

We express $\varphi^{\{j,k\}}(0)$ from here and substitute into (5.7) obtaining

$$d\sqrt{1+(b_{jk}d)^2}\,(\varphi_j^{\{j,k\}})'(0_+) = \psi_j(d) - \frac{\psi_j(d) + \psi_k(d) + \mathcal{O}(d^2)}{2 + d\sqrt{1+(b_{jk}d)^2}\cdot w_{\{j,k\}}} + \mathcal{O}(d^2)\,. \tag{5.8}$$

The relations (5.5) and (5.2) give

$$d\psi_j'(0_+) = \psi_j(d) - \psi(0) + \mathcal{O}(d^2)\,, \tag{5.9}$$

and summing this over $j \in \hat{n}$ we arrive at the identity

$$d\sum_{j=1}^{n} \psi_j'(0_+) = \sum_{j=1}^{n} \psi_j(d) - n\psi(0) + \mathcal{O}(d^2)\,.$$

The right-hand side of it can be rewritten using (5.2). This makes it possible to express $\psi(0)$; substituting it into (5.9) we get

$$d\psi_j'(0_+) = \psi_j(d) - \frac{\sum_{k=1}^{n} \psi_k(d) + \mathcal{O}(d^2)}{n + du} + \mathcal{O}(d^2)\,. \tag{5.10}$$

Next we use consecutively the second relations of (5.4), (5.5) and (5.6) to infer

$$\begin{aligned}\psi_j'(d_+) &= v_j\psi_j(d) + \sum_{k\in N_j} (\varphi^{\{j,k\}})_k'\big(d\sqrt{1+(b_{jk}d)^2}\,\_\big) + \psi_j'(d_-) \\ &= v_j\psi_j(d) + \sum_{k\in N_j} (\varphi^{\{j,k\}})_k'(0_+) + \psi_j'(0_+) + \mathcal{O}(d)\,.\end{aligned}$$

Substituting into the last relation from (5.8) and (5.10) we get

$$\begin{aligned}\psi_j'(d_+) = {} & \left(v_j + \frac{1}{d}\left(\sum_{k\in N_j} \frac{1}{\sqrt{1+(b_{jk}d)^2}} + 1\right)\right)\psi_j(d) \\ & - \frac{1}{d}\sum_{k\in N_j} \frac{1}{\sqrt{1+(b_{jk}d)^2}} \cdot \frac{\psi_j(d) + \psi_k(d)}{2 + d\sqrt{1+(b_{jk}d)^2}\cdot w_{\{j,k\}}} \\ & - \frac{1}{d(n+du)}\left(\sum_{k=1}^{n} \psi_k(d) + \mathcal{O}(d^2)\right) + \mathcal{O}(d)\,,\end{aligned}$$

where we have also employed the fact that $\mathcal{O}(d)\,[1+(b_{jk}d)^2]^{-1/2} = \mathcal{O}(d)$ holds as $d \to 0_+$ for all $j \neq k$, $j, k \in \hat{n}$.

Now we can finally ask about the parameter dependence on d. Since the last relation is supposed to yield in the limit $d \to 0_+$ the jth row of the matrix condition

(5.1), it would be sufficient to have the following requirements satisfied:

$$\lim_{d\to 0_+}\left(v_j+\frac{1}{d}\left(\sum_{k\in N_j}\frac{1}{\sqrt{1+(b_{jk}d)^2}}+1-\sum_{k\in N_j}\frac{1}{2+d\sqrt{1+(b_{jk}d)^2}w_{\{j,k\}}}\right)\right)=D_j \tag{5.11}$$

for all $j\in\hat{n}$,

$$\lim_{d\to 0_+}\frac{1}{d}\cdot\frac{1}{\sqrt{1+(b_{jk}d)^2}}\cdot\frac{-1}{2+d\sqrt{1+(b_{jk}d)^2}w_{\{j,k\}}}=S_{jk} \tag{5.12}$$

for all $j\neq k$, $j,k\in\hat{n}$, and finally

$$\frac{1}{d(n+du)}=\mathcal{O}(d) \tag{5.13}$$

as $d\to 0_+$. To fulfil (5.12) one can choose

$$w_{\{j,k\}}(d):=-\frac{1}{S_{jk}}\cdot\frac{1}{d^2}-\frac{2}{d}\,, \tag{5.14}$$

which makes sense because $S_{jk}\neq 0$ by assumption, since then the limit equals

$$\lim_{d\to 0_+}\frac{1}{1+\mathcal{O}(d^2)}\cdot\frac{-1}{2d+(1+\mathcal{O}(d^2))\left(-\dfrac{1}{S_{jk}}-2d\right)}=S_{jk}\,.$$

With the choice (5.14) taken into account the condition (5.11) will be satisfied provided $v_j+\frac{1}{d}(\#N_j+1)-\sum_{k\in N_j}S_{jk}=D_j$, i.e.

$$v_j(d):=D_j-\frac{\#N_j+1}{d}-\sum_{k\in N_j}S_{jk}\,. \tag{5.15}$$

Finally, the last requirement will be satisfied, e.g., if the expression equals d which is true if

$$u(d):=\frac{1}{d^3}-\frac{n}{d^2}\,. \tag{5.16}$$

Summarizing the argument we conclude that choosing the parameters in the described approximation according to (5.14)–(5.16) we get in the limit the generic boundary conditions (5.1). We conjecture that such an approximation would again converge in the norm-resolvent topology.

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Appendix C

Spectral filtering in quantum Y-junction

Spectral filtering in quantum Y-junction

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We examine scattering properties of singular vertex of degree $n = 2$ and $n = 3$, taking advantage of a new form of representing the vertex boundary condition, which has been devised to approximate a singular vertex with finite potentials. We show that proper identification of δ and δ' components in the connection condition between outgoing lines enables the designing of quantum spectral branch-filters.

KEYWORDS: quantum graph, singular vertex, quantum wire, spectral filtering

1. Introduction

The quantum graph is an abstract mathematical model of single-electron quantum device made up of interconnected one-dimensional lines, in which quantum particles propagate.[1)] Fundamental element of quantum graph is the star graph, or the singular vertex of degree n, which is a single node where n outgoing half-lines are connected. Although the general mathematical characterization of a singular vertex in terms of parameter space of unitary group $U(n)$ has been there for some time,[2–6)] the analysis of its physical contents other than the simplest case of $n = 2$ is still missing. In this article, we address the problem of making sense of $U(n)$ parameter space by examining the basic and simplest example of $n = 3$ singular vertex, or Y-junction, in detail. We show that the recent work on the approximation of singular vertex by finite potentials supplies the basis for our analysis. Central to the physical understanding of singular vertex is the realization that a connection between each pair of outgoing lines can be classified by its δ and δ' contents supplemented by "magnetic" phase change.[7)] We show that this classification leads directly to the spectral filtering property between the pair of lines, enabling us to design the spectral branching filter using quantum Y-junction.

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2. Reduction of boundary matrices

Consider a quantum particle on a star graph with a single node and n half lines. The system is specified by boundary conditions that have in general the following structure,

$$A\Psi + B\Psi' = 0, \tag{2.1}$$

where A and B are matrices $n \times n$ which must satisfy certain conditions, and Ψ, Ψ' are the state vectors given by

$$\Psi = \begin{pmatrix} \varphi_1 \\ \vdots \\ \varphi_n \end{pmatrix}, \quad \Psi' = \begin{pmatrix} \varphi'_1 \\ \vdots \\ \varphi'_n \end{pmatrix}. \tag{2.2}$$

For simplicity of the notation, we have dropped the x location when it is $x = 0$, i.e. we use φ_i, φ'_i in place of $\varphi_i(0)$, $\varphi'_i(0)$. In this paper we start from the form of A, B that we have devised in our previous work[7] and where the crucial numbers are the ranks of the matrices A and B which we denote here $r_A = \mathrm{rank}(A)$ and $r_B = \mathrm{rank}(B)$. We can transform the $n \times n$ matrices A and B to the following *ST form*;

$$A = -\begin{pmatrix} S & 0 \\ -T^\dagger & I \end{pmatrix}, \quad B = \begin{pmatrix} I & T \\ 0 & 0 \end{pmatrix}, \tag{2.3}$$

with $r_B \times r_B$ Hermitian matrix S and $r_B \times (n - r_B)$ complex matrix T. The identity submatrix I is understood as having proper dimensions, namely $r_B \times r_B$ in B and $(n - r_B) \times (n - r_B)$ in A. If we denote the rank of S as r_S, we obviously have $0 \le r_S \le r_B$, and moreover,

$$r_A + r_B = n + r_S, \tag{2.4}$$

which comes in handy to us later on.

Let us consider the scattering solution for incoming wave entering from j-th line with the wave number k;

$$\begin{aligned} \varphi_i^{(j)}(x_i) &= e^{-\mathrm{i}kx_i} + \mathcal{R}_i e^{\mathrm{i}kx_i} \quad (i = j), \\ &= \mathcal{T}_{ij}\, e^{\mathrm{i}kx_i} \qquad\qquad (i \neq j), \end{aligned} \tag{2.5}$$

where $\mathcal{R}_i$ represents the reflection amplitude for i-th line, and $\mathcal{T}_{ij}$ the transmission amplitude from j-th to i-th line. From the vectors $\Psi^{(j)}$ and $\Psi'^{(j)}$ made from $\varphi_i^{(j)}$ and $\varphi_i'^{(j)}$ respectively, we can construct matrices

$$\begin{aligned} (\Psi^{(1)} \dots \Psi^{(n)}) &= \mathcal{S}(k) + I, \\ (\Psi'^{(1)} \dots \Psi'^{(n)}) &= \mathrm{i}k(\mathcal{S}(k) - I). \end{aligned} \tag{2.6}$$

where the scattering matrix $\mathcal{S}(k)$ (which is not to be confused with the sub-matrix S appearing

in (2.3)) is given by

$$\mathcal{S}(k) = \begin{pmatrix} \mathcal{R}_1(k) & \mathcal{T}_{12}(k) & \cdots & \mathcal{T}_{1n}(k) \\ \mathcal{T}_{21}(k) & \mathcal{R}_2(k) & \cdots & \mathcal{T}_{2n}(k) \\ \vdots & & & \vdots \\ \mathcal{T}_{n1}(k) & \mathcal{T}_{n2}(k) & \cdots & \mathcal{R}_n(k) \end{pmatrix}. \tag{2.7}$$

From (2.1), we obtain

$$\mathcal{S}(k) = -\frac{1}{A + \mathrm{i}kB}(A - \mathrm{i}kB), \tag{2.8}$$

where $\frac{1}{M}$ represents the inverse matrix of M.

A vertex coupling can be also described by boundary conditions formulated as $\bar{A}\Psi + \bar{B}\Psi' = 0$ for

$$\bar{A} = \begin{pmatrix} I & \bar{T} \\ 0 & 0 \end{pmatrix}, \quad \bar{B} = -\begin{pmatrix} \bar{S} & 0 \\ -\bar{T}^\dagger & I \end{pmatrix}; \tag{2.9}$$

this will be called a *reverse ST form*. It is obvious that for a given vertex coupling the matrices A and $\bar{A}$ differ, as well as B, $\bar{B}$. And conversely, a simple interchange of A and B in (2.2), namely $B\Psi + A\Psi' = 0$, leads to boundary conditions that correspond to a different system; this system may be considered as a counterpart of the original one. Let us examine how the scattering matrices are related in this case:

$$\begin{aligned} \mathcal{S}_d(k) &= -\frac{1}{B + \mathrm{i}kA}(B - \mathrm{i}kA) \\ &= \frac{1}{A + \frac{\mathrm{i}}{-k}B}(A - \frac{\mathrm{i}}{-k}B) = -\mathcal{S}(-1/k). \end{aligned} \tag{2.10}$$

This formula signifies a *high-low wave number duality* $k \leftrightarrow -1/k$ between the scattering matrix $\mathcal{S}(k)$ of system described by the ST form and $\mathcal{S}_d(k)$ of its counterpart.

We now consider a single system and two its characterizations: one by the ST form $A\Psi + B\Psi' = 0$ with (2.3), one by the reverse ST form $\bar{A}\Psi + \bar{B}\Psi' = 0$ with (2.9). Although the matrices A and $\bar{A}$ are very different, as well as B, $\bar{B}$, it naturally holds $\mathrm{rank}(A) = \mathrm{rank}(\bar{A})$ and $\mathrm{rank}(B) = \mathrm{rank}(\bar{B})$, which, because of (2.4), further leads to $\mathrm{rank}(S) = \mathrm{rank}(\bar{S})$. In other words, the quantity $r_S = r_A + r_B - n$ is a characteristic number of a system, that is independent of the representation.

3. Scattering matrices and boundary conditions: n=2 case

We start by examining the known case of $n = 2$, namely, the *point interaction on a line*, in order to see the effectiveness of our ST form in identifying the physical content of the singular vertex.

3.1 **rank(B)=0, rank(A)=2**

For this case, the first condition $\mathrm{rank}(B) = 0$ automatically guarantees the second condition $\mathrm{rank}(A) = 2$. We have the equation

$$\Psi = 0, \tag{3.11}$$

which determines disjoint Dirichlet boundaries $\varphi_1 = \varphi_2 = 0$.

3.2 rank(B)=1

Suppose we now have $\mathrm{rank}(B) = 1$. The relation (2.4) reads $\mathrm{rank}(A) = \mathrm{rank}(S) + 1$. There are two possibilities.

3.2.1 **rank(B)=1, rank(A)=1**

This corresponds to $\mathrm{rank}(S) = 0$. We have the equation

$$\begin{pmatrix} 1 & t \\ 0 & 0 \end{pmatrix} \begin{pmatrix} \varphi_1' \\ \varphi_2' \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ -t^* & 1 \end{pmatrix} \begin{pmatrix} \varphi_1 \\ \varphi_2 \end{pmatrix}, \tag{3.12}$$

which is the pure Fülöp-Tsutsui scale invariant boundary condition,[5] $t^*\varphi_1 = \varphi_2$ and $\varphi_1' = -t\varphi_2'$.

3.2.2 **rank(B)=1, rank(A)=2**

This corresponds to $\mathrm{rank}(S) = 1$. We have, in this case, the form

$$\begin{pmatrix} 1 & t \\ 0 & 0 \end{pmatrix} \begin{pmatrix} \varphi_1' \\ \varphi_2' \end{pmatrix} = \begin{pmatrix} s & 0 \\ -t^* & 1 \end{pmatrix} \begin{pmatrix} \varphi_1 \\ \varphi_2 \end{pmatrix}, \tag{3.13}$$

with a non-zero real number s and a complex number t. With $t = 1$, we have $\varphi_1' + \varphi_2' = s\varphi_1 = s\varphi_2$, which is nothing but the δ interaction with strength s. (Note the outgoing directions for all x_is.)

In general, the case $\mathrm{rank}(B) = 1$ is understood as the combination of δ and Fülöp-Tsutsui interactions. This is evident from the transmission amplitude

$$\mathcal{T}_{12}(k) = \frac{2kt}{k(1 + t^*t) + \mathrm{i}s}, \tag{3.14}$$

whose characteristic length scale is $(1 + t^*t)/s$. Inverse of this length scale divides the wave number into two regions. We find the low wave number blockade $\mathcal{T}_{12}(0) = 0$ and high wave number transparency $\mathcal{T}_{12}(\infty) = \frac{2t}{1+t^*t}$ which becomes the perfect transparency $\mathcal{T}_{12}(\infty) = 1$ for $t = 1$.

3.3 rank(B)=2

We have the form

$$\begin{pmatrix} \varphi_1' \\ \varphi_2' \end{pmatrix} = \begin{pmatrix} s_{11} & s_{12} \\ s_{12}^* & s_{22} \end{pmatrix} \begin{pmatrix} \varphi_1 \\ \varphi_2 \end{pmatrix}. \tag{3.15}$$

From the relation (2.4), we obtain $\mathrm{rank}(A) = \mathrm{rank}(S)$, which leaves us with three possibilities $\mathrm{rank}(A) = 0$, 1 and 2.

3.3.1 rank(B)=2, rank(A)=0

This corresponds to $\mathrm{rank}(S) = 0$, and we have the equation

$$\Psi' = 0, \tag{3.16}$$

representing disjoint Neumann boundaries $\varphi_1' = \varphi_2' = 0$.

3.3.2 rank(B)=2, rank(A)=1

When the rank of the matrix A is one, we can re-parametrize the above equation as

$$\begin{pmatrix} \varphi_1' \\ \varphi_2' \end{pmatrix} = \begin{pmatrix} s & cs \\ c^* s & c^* cs \end{pmatrix} \begin{pmatrix} \varphi_1 \\ \varphi_2 \end{pmatrix} \tag{3.17}$$

with a real number s and a complex number c. Multiplying the both sides by

$$\begin{pmatrix} 1/s & 0 \\ -c^* & 1 \end{pmatrix}, \tag{3.18}$$

we obtain the reverse ST form,

$$\begin{pmatrix} \bar{s} & 0 \\ -\bar{t}^* & 1 \end{pmatrix} \begin{pmatrix} \varphi_1' \\ \varphi_2' \end{pmatrix} = \begin{pmatrix} 1 & \bar{t} \\ 0 & 0 \end{pmatrix} \begin{pmatrix} \varphi_1 \\ \varphi_2 \end{pmatrix}, \tag{3.19}$$

with $\bar{s} = 1/s$ and $\bar{t} = c$, signifying the *pure* δ' *interaction* amended by the Fülöp-Tsutsui scaling. The transmission amplitude,

$$\mathcal{T}_{12}(k) = \frac{-2\bar{t}}{(1 + \bar{t}^*\bar{t}) - \mathrm{i}k\bar{s}}, \tag{3.20}$$

shows both the high-wave number blockade, $\mathcal{T}_{12}(\infty) = 0$, and low-wave number pass filtering behavior, $\mathcal{T}_{12}(0) = \frac{-2\bar{t}}{1+t^*t}$. Obviously, this is a dual partner of previous example of pure δ connection.

3.3.3 rank(B)=2, rank(A)=2

When the rank of the matrix A is two, we have the generic connection condition for a quantum particle residing on two joint lines, namely the combinations of δ and δ' interactions. This can be seen from the low-wave number and high-wave number blockade behavior

$$\mathcal{T}_{12}(k) = \frac{2ks_{12}}{ik^2 - k\,\mathrm{tr}[S] - \mathrm{i}\det[S]}. \tag{3.21}$$

In summary, for the case of $n = 2$, the rank of the matrices A and B, and resultantly, that of S, are the determining factors of physical contents of point interactions.

4. Scattering matrices and boundary conditions: n=3 case

We now examine the quantum Y-junction, namely, the singular vertex of $n = 3$. We shall show that the concept of "δ-like" and "δ'-like" couplings can be established between each pair

of lines outgoing from the singular vertex.

In idealized limit, two lines i and j are identified as having "pure δ-like" connections when we have

$$\mathcal{T}_{ij}(0) = 0, \quad \text{and} \quad \mathcal{T}_{ij}(k) = Const. \ (k \to \infty). \tag{4.22}$$

Conversely, i and j are identified as " pure δ'-like" if we have

$$\mathcal{T}_{ij}(0) = Const. \ (k \to 0), \quad \text{and} \quad \mathcal{T}_{ij}(\infty) = 0. \tag{4.23}$$

Since the quantum flux can circumvent direct blocking between i and j through indirect path $i \to k \to j$, strict conditions $\mathcal{T}_{ij}(0) = 0$ for δ-like and $\mathcal{T}_{ij}(\infty) = 0$ for δ'-like connection are to be breached when other types of connections are present among other lines, and therefore, zeros for $\mathcal{T}_{ij}$ need to be replaced by *small* number, $\mathcal{T}_{ij} \approx 0$ in above conditions. General characterization of pure δ-like connection as high-pass frequency filter, and pure δ'-like connection low-pass filter is still valid.

As in the case of $n = 2$, we classify the boundary condition according to the ranks of matrices A and B.

4.1 **rank(B)=0, rank(A)=3**

The first condition automatically ensures the second. We again have disjoint condition

$$\Psi = 0, \tag{4.24}$$

which is disconnected Dirichlet boundaries $\varphi_1 = \varphi_2 = \varphi_3 = 0$.

4.2 rank(B)=1

With this condition, the relation (2.4) now reads $\mathrm{rank}(A) = \mathrm{rank}(S) + 2$. There are two possibilities, $\mathrm{rank}(A) = 2$ and 3.

4.2.1 **rank(B)=1, rank(A)=2**

This corresponds to $\mathrm{rank}(S) = 0$, and we have the equation

$$\begin{pmatrix} 1 & t_2 & t_3 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \varphi_1' \\ \varphi_2' \\ \varphi_3' \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 \\ -t_2^* & 1 & 0 \\ -t_3^* & 0 & 1 \end{pmatrix} \begin{pmatrix} \varphi_1 \\ \varphi_2 \\ \varphi_3 \end{pmatrix}, \tag{4.25}$$

which is $n = 3$ version of pure scale invariant Fülöp-Tsutsui boundary condition, given by $t_2^* t_3^* \varphi_1 = t_3^* \varphi_2 = t_2^* \varphi_3$ and $\varphi_1' + t_2 \varphi_2' + t_3 \varphi_3' = 0$.

4.2.2 rank(B)=1, rank(A)=3

This case corresponds to rank(S) = 1. We have

$$\begin{pmatrix} 1 & t_2 & t_3 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \varphi_1' \\ \varphi_2' \\ \varphi_3' \end{pmatrix} = \begin{pmatrix} s & 0 & 0 \\ -t_2^* & 1 & 0 \\ -t_3^* & 0 & 1 \end{pmatrix} \begin{pmatrix} \varphi_1 \\ \varphi_2 \\ \varphi_3 \end{pmatrix}, \tag{4.26}$$

with non-zero real number s. With $t_2 = t_3 = 1$, we have $\varphi_1' + \varphi_2' + \varphi_3' = s\varphi_1 = s\varphi_2 = s\varphi_3$, which is the $n = 3$ generalization of *pure δ potential connection conditions*[8] between all half lines. With general t_2 and t_3, Fülöp-Tsutsui scalings t_2^*, t_3^* and t_2^*/t_3^* are introduced on φ_2/φ_1, φ_3/φ_1 and on φ_2/φ_3, respectively. The transmission amplitudes for this case are given by

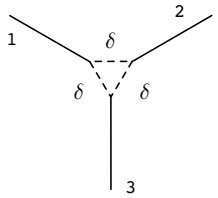

Fig. 1. Pure δ type connection between all lines, obtained from ST form with rank(B) = 1 and rank(A) = 3.

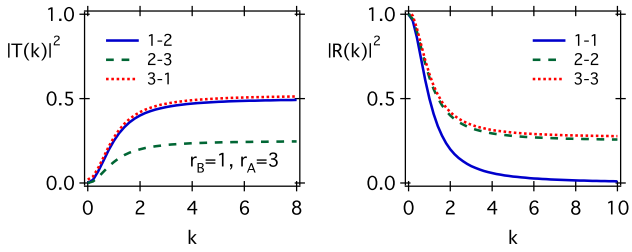

Fig. 2. Transmission and reflection probabilities for Y-junction with pure δ type connection between all lines. In the left side, solid line represents $|\mathcal{T}_{12}(k)|^2$, dashed line $|\mathcal{T}_{23}(k)|^2$, and dotted line $|\mathcal{T}_{31}(k)|^2$. In the right, solid line represents $|\mathcal{R}_1(k)|^2$, dashed line $|\mathcal{R}_2(k)|^2$, and dotted lin $|\mathcal{R}_3(k)|^2$. Parameter values $t_2 = t_3 = 1/\sqrt{2}$, $s = 2$ are used in (4.27). Two identical lines are drawn with slight offsets for better viewing.

$$\begin{aligned} \mathcal{T}_{31}(k) &= \frac{2t_3^* k}{\mathrm{i}s + (1 + t_2^* t_2 + t_3^* t_3)k}, \\ \mathcal{T}_{12}(k) &= \frac{2t_2 k}{\mathrm{i}s + (1 + t_2^* t_2 + t_3^* t_3)k}, \\ \mathcal{T}_{23}(k) &= \frac{2t_2^* t_3 k}{\mathrm{i}s + (1 + t_2^* t_2 + t_3^* t_3)k}. \end{aligned} \tag{4.27}$$

which has the length scale $(1+t_2^*t_2+t_3^*t_3)/s$. Below this length scale, the transmission coefficients show the high-wave number pass filtering behavior

$$\mathcal{T}_{ij}(0)=0, \quad \mathcal{T}_{ij}(k)=Const. \text{ as } k\to 0, \tag{4.28}$$

which is a hallmark of pure δ connections between all branches (See Figs. 1 and 2).

4.3 rank(B)=2

The ST form $B\Psi'=-A\Psi$ now reads

$$\begin{pmatrix}1&0&t_1\\0&1&t_2\\0&0&0\end{pmatrix}\begin{pmatrix}\varphi_1'\\\varphi_2'\\\varphi_3'\end{pmatrix}=\begin{pmatrix}s_{11}&s_{12}&0\\s_{12}^*&s_{22}&0\\-t_1^*&-t_2^*&1\end{pmatrix}\begin{pmatrix}\varphi_1\\\varphi_2\\\varphi_3\end{pmatrix}. \tag{4.29}$$

The relation (2.4) becomes $\mathrm{rank}(A)=1+\mathrm{rank}(S)$. We have three possibilities:

4.3.1 **rank(B)=2, rank(A)=1**

This corresponds to $\mathrm{rank}(S)=0$. We have $s_{11}=s_{12}=s_{22}=0$ in (4.29). This situation represents a scale invariant interaction between lines 1–3, described by $\varphi_1'=-t_3\varphi_3'$, and a scale invariant interaction between lines 2–3, described by $\varphi_2'=-t_3\varphi_3'$.

4.3.2 **rank(B)=2, rank(A)=2**

Suppose that the rank of the sub-matrix S is one, namely top two raws of the RHS are linearly dependent to each other. We can write (4.29) in the form

$$\begin{pmatrix}1&0&t_1\\0&1&t_2\\0&0&0\end{pmatrix}\begin{pmatrix}\varphi_1'\\\varphi_2'\\\varphi_3'\end{pmatrix}=\begin{pmatrix}s&cs&0\\c^*s&c^*cs&0\\-t_1^*&-t_2^*&1\end{pmatrix}\begin{pmatrix}\varphi_1\\\varphi_2\\\varphi_3\end{pmatrix}. \tag{4.30}$$

Interestingly, we can reverse the role of A and B in the following manner. We now write (4.30) in the form

$$\begin{pmatrix}1&t_1&0\\0&0&0\\0&t_2&1\end{pmatrix}\begin{pmatrix}\varphi_1'\\\varphi_3'\\\varphi_2'\end{pmatrix}=\begin{pmatrix}s&0&cs\\-t_1^*&1&-t_2^*\\c^*s&0&c^*cs\end{pmatrix}\begin{pmatrix}\varphi_1\\\varphi_3\\\varphi_2\end{pmatrix}. \tag{4.31}$$

Multiplying the both sides by

$$\begin{pmatrix}1/s&0&0\\t_1^*/s&1&0\\-c^*&0&1\end{pmatrix}, \tag{4.32}$$

we obtain a reverse ST form $-B\Psi'=A\Psi$ as

$$\begin{pmatrix}\bar{s}&\bar{c}\bar{s}&0\\\bar{c}^*\bar{s}&\bar{c}^*\bar{c}s&0\\-\bar{t}_1^*&-\bar{t}_3^*&1\end{pmatrix}\begin{pmatrix}\varphi_1'\\\varphi_3'\\\varphi_2'\end{pmatrix}=\begin{pmatrix}1&0&\bar{t}_1\\0&1&\bar{t}_3\\0&0&0\end{pmatrix}\begin{pmatrix}\varphi_1\\\varphi_3\\\varphi_2\end{pmatrix}, \tag{4.33}$$

with $\bar{s} = 1/s$, $\bar{c} = t_1$, $\bar{t}_1 = c$, and $\bar{t}_3 = ct_1^* - t_2^*$. Note that two forms (4.30) and (4.33) are dual to each other, and that this case can be also viewed as having $\mathrm{rank}(A) = 2$ and $\mathrm{rank}(\bar{S}) = 1$, as well as $\mathrm{rank}(B) = 2$ and $\mathrm{rank}(S) = 1$.

It is instructive to look at the transmission amplitudes, which, for this case, are given by

$$\begin{aligned}
\mathcal{T}_{31}(k) &= \frac{2t_1^* k + 2\mathrm{i}c^* s(ct_1^* - t_2^*)}{D_1 k + \mathrm{i}sD_0}, \\
\mathcal{T}_{12}(k) &= \frac{-2t_2^* t_1 k - 2\mathrm{i}cs}{D_1 k + \mathrm{i}sD_0}, \\
\mathcal{T}_{23}(k) &= \frac{2t_2 k - 2\mathrm{i}s(c^* t_1 - t_2)}{D_1 k + \mathrm{i}sD_0}.
\end{aligned} \tag{4.34}$$

where we set

$$\begin{aligned}
D_0 &= 1 + c^* c + (ct_1^* - t_2^*)(c^* t_1 - t_2), \\
D_1 &= 1 + t_1^* t_1 + t_2^* t_2.
\end{aligned} \tag{4.35}$$

Two special cases are noteworthy, at which we shall look in detail.

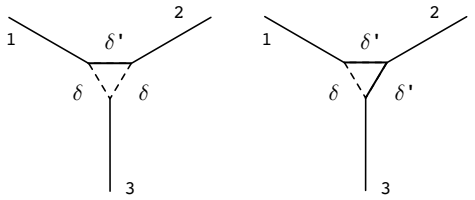

Fig. 3. Mixed type vertex coupling obtained from ST form with $\mathrm{rank}(B) = 2$ and $\mathrm{rank}(A) = 2$. The δ–δ–δ' (left) and δ'–δ'–δ (right) type connection are obtained from conditions $\bar{t}_3 = 0$ and $t_2 = 0$, respectively.

4.3.2.1 δ-δ-δ' type

Let us suppose for now, that we have $ct_1^* - t_2^* (= \bar{t}_3^*) = 0$. This results in $\mathcal{T}_{31}(0) = \mathcal{T}_{23}(0) = 0$, indicating the presence of two pure δ-like connections between lines $3-1$, and between $2-3$. When further condition $s \gg t_1^* t_1$ and $c \neq 0$ are met, we have $T_{12}(k) = Const.$ as $k \to 0$ and $T_{12}(\infty) \approx 0$, signifying the pure δ'-like connection between lines $1-2$. The same conclusion is drawn from the consideration of connection conditions which reads

$$\begin{aligned}
\frac{1}{t_1}\varphi_1' + \varphi_3' = \frac{1}{t_2}\varphi_2' + \varphi_3' &= \frac{s}{t_1^* t_1}\varphi_3 \\
\varphi_3 &= t_1^*\varphi_1 + t_2^*\varphi_2 \\
\frac{1}{t_1}\varphi_1' &= \frac{1}{t_2}\varphi_2'.
\end{aligned} \tag{4.36}$$

The last equation, which is not independent of the first three, is shown to display the pure δ'-like interaction between the half lines 1 and 2, ammended by the Fülöp-Tsutsui scaling by

factor t_1/t_2. The first two equations clearly show the fact that the connections between the half lines 2 and 3, and between 3 and 1 are pure δ-like (See Fig. 3, left, and Fig. 4).

4.3.2.2 δ'-δ'-δ type

Let us now suppose, in place of previous conditions, that we have $t_2 = 0$ and $t_1 \neq 0$. We then have $\mathcal{T}_{12}(\infty) = \mathcal{T}_{23}(\infty) = 0$, $\mathcal{T}_{12}(k) = Const. \neq 0$ and $\mathcal{T}_{23}(k) = Const. \neq 0$ as we let $k \to 0$, indicating the presence of two pure δ'-like connections between lines $1-2$ and between $2-3$. With further assumption $c \ll 1$, we have $\mathcal{T}_{31}(0) \approx 0$, signifying the pure δ-like connection between lines $3-1$ (See Fig. 3, right, and Fig. 5). These facts are again clearly visible in the following expressions for the boundary condition;

$$\begin{aligned} \frac{1}{c}\varphi_1 + \varphi_2 = \frac{1}{ct_1^*}\varphi_3 + \varphi_2 = \frac{1}{sc^*c}\varphi_2', \\ \varphi_2' = c^*\varphi_1' + c^*t_1\varphi_3', \\ t_1^*\varphi_1 = \varphi_3. \end{aligned} \tag{4.37}$$

Thus we have shown that this case corresponds to a mixture of δ and δ' connections including two pure connections $\delta - \delta - \delta'$ and $\delta' - \delta' - \delta$ as two limiting cases.

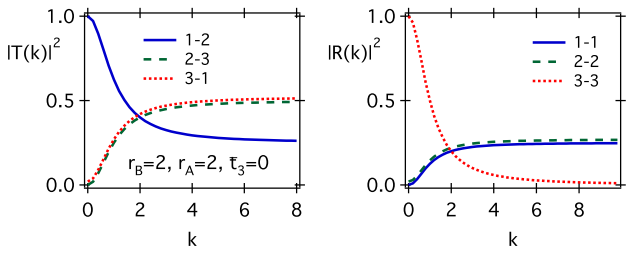

Fig. 4. Transmission and reflection probabilities for Y-junction with δ–δ–δ' type connection. In the left side, solid line represents $|\mathcal{T}_{12}(k)|^2$, dashed line $|\mathcal{T}_{23}(k)|^2$, and dotted line $|\mathcal{T}_{31}(k)|^2$. In the right, solid line represents $|\mathcal{R}_1(k)|^2$, dashed line $|\mathcal{R}_2(k)|^2$, and dotted lin $|\mathcal{R}_3(k)|^2$. Parameter values $t_1 = t_2 = 1/\sqrt{2}$, $s_{11} = s_{12} = s_{22} = 1$ are used in (4.29). Two identical lines are drawn with slight offsets for better viewing.

4.3.3 rank(B)=2, rank(A)=3

When the rank of the matrix A is three (thus giving rank$(S) = 2$), we have rather general combination of δ and δ' interactions between each pair of half lines. Let us look at the transmission amplitudes, which are given by

$$\mathcal{T}_{31}(k) = \frac{2t_1^*k^2 + 2\mathrm{i}(s_{22}t_1^* - s_{12}^*t_2^*)k}{k^2E_2 + \mathrm{i}kE_1 + E_0},$$

$$\mathcal{T}_{12}(k) = \frac{-2t_2^*t_1k^2 - 2\mathrm{i}s_{12}k}{k^2E_2 + \mathrm{i}kE_1 + E_0},$$

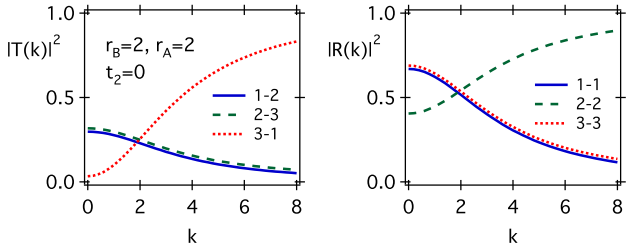

Fig. 5. Transmission and reflection probabilities for Y-junction with δ–δ'–δ' type connection. Parameter values $t_1 = 1/3, t_2 = 0$, $s_{11} = 6, s_{12} = 2, s_{22} = 2/3$ are used in (4.29).

$$\mathcal{T}_{23}(k) = \frac{2t_2k^2 - 2\mathrm{i}(s_{12}^* t_1 - s_{11}t_2)k}{k^2E_2 + \mathrm{i}kE_1 + E_0}, \tag{4.38}$$

where we set

$$\begin{aligned} E_0 &= -\det[S], \\ E_1 &= \mathrm{tr}[S] + s_{22}t_1^*t_1 - s_{12}t_1^*t_2 - s_{12}^*t_2^*t_1 + s_{11}t_2^*t_2 \\ E_2 &= 1 + t_1^*t_1 + t_2^*t_2. \end{aligned} \tag{4.39}$$

The guaranteed presence of δ-like connection between all lines can be seen from the zero energy blockade $\mathcal{T}_{ij}(0) = 0$ for all i and j. The presence or absence of δ'-like component is controlled by t_i since we have $\mathcal{T}_{31}(\infty) \propto t_1^*$, $\mathcal{T}_{12}(\infty) \propto t_2^*t_1$ and $\mathcal{T}_{23}(\infty) \propto t_2$. A numerical example of this case is shown in Fig. 6.

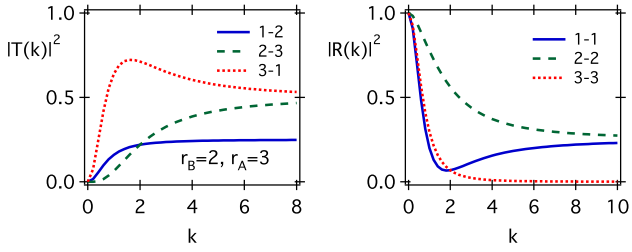

Fig. 6. Transmission and reflection probabilities for Y-junction with $\mathrm{rank}(B) = 2$, $\mathrm{rank}(A) = 3$. Parameter values $t_1 = t_2 = 1/\sqrt{2}$, $s_{11} = s_{12} = 1$, $s_{22} = -2$ are used in (4.29).

4.4 rank(B)=3

We have the ST form

$$\begin{pmatrix} \varphi_1' \\ \varphi_2' \\ \varphi_3' \end{pmatrix} = \begin{pmatrix} s_{11} & s_{12} & s_{13} \\ s_{12}^* & s_{22} & s_{23} \\ s_{13}^* & s_{23}^* & s_{33} \end{pmatrix} \begin{pmatrix} \varphi_1 \\ \varphi_2 \\ \varphi_3 \end{pmatrix}. \tag{4.40}$$

From (2.3), we have $A = S$, and thus $\mathrm{rank}(A) = \mathrm{rank}(S)$. We have four possibilities:

4.4.1 **rank(B)=3, rank(A)=0**

This corresponds to rank(S) = 0, and the boundary condition becomes

$$\Psi' = 0 \tag{4.41}$$

which is the disjoint Neumann condition $\varphi_1' = \varphi_2' = \varphi_3' = 0$.

4.4.2 **rank(B)=3, rank(A)=1**

When the rank of the matrix A is one, namely three rows of the RHS are linearly dependent on each other, we have

$$\begin{pmatrix} \varphi_1' \\ \varphi_2' \\ \varphi_3' \end{pmatrix} = \begin{pmatrix} s & cs & ds \\ c^*s & c^*cs & c^*ds \\ d^*s & d^*cs & d^*ds \end{pmatrix} \begin{pmatrix} \varphi_1 \\ \varphi_2 \\ \varphi_3 \end{pmatrix}. \tag{4.42}$$

Multiplying the both sides by

$$\begin{pmatrix} 1/s & 0 & 0 \\ -c^* & 1 & 0 \\ -d^* & 0 & 1 \end{pmatrix}, \tag{4.43}$$

we arrive at a reverse ST form as

$$\begin{pmatrix} \bar{s} & 0 & 0 \\ -c^* & 1 & 0 \\ -d^* & 0 & 1 \end{pmatrix} \begin{pmatrix} \varphi_1' \\ \varphi_2' \\ \varphi_3' \end{pmatrix} = \begin{pmatrix} 1 & c & d \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \varphi_1 \\ \varphi_2 \\ \varphi_3 \end{pmatrix}, \tag{4.44}$$

with $\bar{s} = 1/s$. We have $c^*d^*\varphi_1' = d^*\varphi_2' = c^*\varphi_3'$, and $\varphi_1 + c\varphi_2 + d\varphi_3 = \bar{s}\varphi_1'$, signifying the *generalized pure δ' interaction*[8] ammended by the Fülöp-Tsutsui scaling. This is also evident from the transmission amplitudes, which are given by

$$\begin{aligned} \mathcal{T}_{31}(k) &= \frac{-2d^*s}{-\mathrm{i}k + s(1 + c^*c + d^*d)}, \\ \mathcal{T}_{12}(k) &= \frac{-2cs}{-\mathrm{i}k + s(1 + c^*c + d^*d)}, \\ \mathcal{T}_{23}(k) &= \frac{-2c^*ds}{-\mathrm{i}k + s(1 + c^*c + d^*d)}. \end{aligned} \tag{4.45}$$

The formulae imply $\mathcal{T}_{ij}(\infty) = 0$ and $\mathcal{T}_{ij}(k) = Const.$ as $k \to 0$ (See Figs. 7 and 8).

4.4.3 **rank(B)=3, rank(A)=2**

When the rank of the matrix A is two, and thus that of S is two, the last row of RHS of (4.40) is equal to some combination of the first two. We then have

$$\begin{pmatrix} \varphi_1' \\ \varphi_2' \\ \varphi_3' \end{pmatrix} = \begin{pmatrix} s & q & cs + dq \\ q^* & r & cq^* + dr \\ c^*s + d^*q^* & c^*q + d^*r & f \end{pmatrix} \begin{pmatrix} \varphi_1 \\ \varphi_2 \\ \varphi_3 \end{pmatrix} \tag{4.46}$$

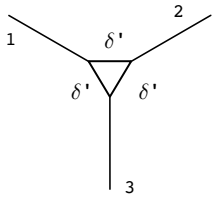

Fig. 7. Pure δ' type connection between all lines, obtained from ST form with $\mathrm{rank}(B) = 3$ and $\mathrm{rank}(A) = 1$.

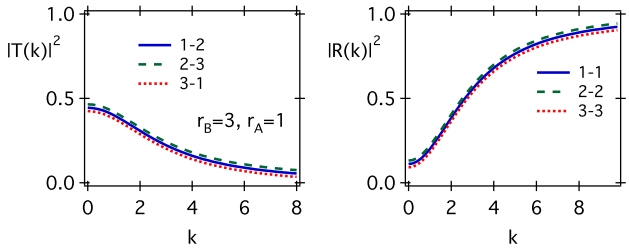

Fig. 8. Transmission and reflection probabilities for Y-junction with pure δ' type connection between all lines. Parameter values $s_{11} = s_{12} = s_{13} = s_{22} = s_{23} = s_{33} = 1$ are used in (4.40).

with $f = c^*cs + c^*dq + d^*cq^* + d^*dr$. Multiplying both sides by

$$\begin{pmatrix} r/(sr-q^*q) & -q/(sr-q^*q) & 0 \\ -q^*/(sr-q^*q) & s/(sr-q^*q) & 0 \\ -c^* & -d^* & 1 \end{pmatrix}, \tag{4.47}$$

we obtain a reverse ST form

$$\begin{pmatrix} \bar{s} & \bar{q} & 0 \\ \bar{q}^* & \bar{r} & 0 \\ -\bar{t}_1^* & -\bar{t}_2^* & 1 \end{pmatrix} \begin{pmatrix} \varphi_1' \\ \varphi_2' \\ \varphi_3' \end{pmatrix} = \begin{pmatrix} 1 & 0 & \bar{t}_1 \\ 0 & 1 & \bar{t}_2 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \varphi_1 \\ \varphi_2 \\ \varphi_3 \end{pmatrix}, \tag{4.48}$$

with identification $\bar{s} = r/(sr - q^*q)$, $\bar{q} = -q/(sr - q^*q)$, $\bar{r} = s/(sr - q^*q)$, $\bar{t}_1 = c$, and $\bar{t}_2 = d$.

This is obviously dual to the case of $\mathrm{rank}(B) = 2$, $\mathrm{rank}(A) = 3$, given by (4.29). Now the presence of δ'-like connection between all lines are guaranteed, and the presence or absence of δ-like component is controlled by c and d. The transmission amplitudes, given by

$$\begin{aligned} \mathcal{T}_{31}(k) &= \frac{2\mathrm{i}k(c^*s + d^*q^*) - 2c^*(sr - q^*q)}{k^2 + \mathrm{i}kF_1 + F_0}, \\ \mathcal{T}_{12}(k) &= \frac{2\mathrm{i}kq + 2cd^*(sr - q^*q)}{k^2 + \mathrm{i}kF_1 + F_0}, \\ \mathcal{T}_{23}(k) &= \frac{2\mathrm{i}k(cq^* + dr) - 2d(sr - q^*q)}{k^2 + \mathrm{i}kF_1 + F_0}, \end{aligned} \tag{4.49}$$

where we set

$$F_0 = -(sr - q^*q)(1 + c^*c + d^*d),$$
$$F_1 = s + r + c^*cs + c^*dq + d^*cq^* + d^*dr, \tag{4.50}$$

corroborate this assertion with high energy blockade $\mathcal{T}_{ij}(\infty) = 0$ for all i and j, and also with the zero energy expressions $\mathcal{T}_{31}(0) \propto c^*$, $\mathcal{T}_{12}(0) \propto d^*c$ and $\mathcal{T}_{23}(0) \propto d$. A numerical example of this case is shown in Fig. 9.

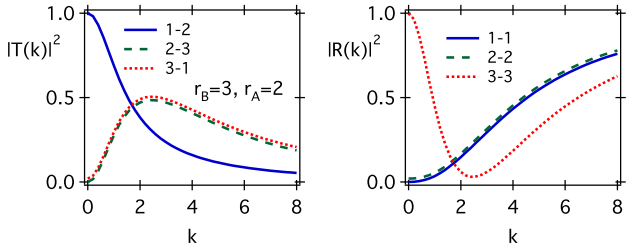

Fig. 9. Transmission and reflection probabilities for Y-junction with rank$(B) = 3$, rank$(A) = 2$. Parameter values $s_{11} = s_{12} = s_{22} = s_{33} = 1$, $s_{13} = s_{23} = 2$ are used in (4.40).

4.4.4 rank(B)=3, rank(A)=3

When the ranks of the matrices A and B are both equal to $n = 3$, we have the generic connection condition for a quantum particle residing on a joint three lines, namely the combinations of δ and δ' interactions. Let us look at the transmission amplitudes, which are given

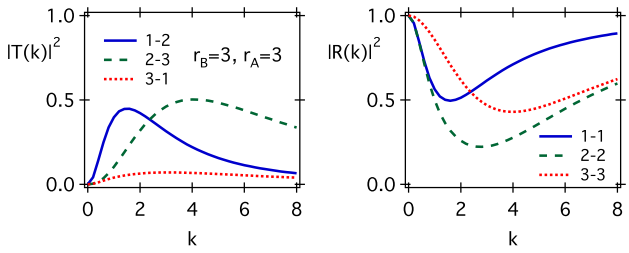

Fig. 10. Transmission and reflection probabilities for Y-junction with rank$(B) = 3$, rank$(A) = 3$, the generic condition. In the left side, solid line represents $|\mathcal{T}_{12}(k)|^2$, dashed line $|\mathcal{T}_{23}(k)|^2$, and dotted line $|\mathcal{T}_{31}(k)|^2$. In the right, solid line represents $|\mathcal{R}_1(k)|^2$, dashed line $|\mathcal{R}_2(k)|^2$, and dotted lin $|\mathcal{R}_3(k)|^2$. Parameter values $s_{11} = -1/3$, $s_{12} = -1$, $s_{13} = 1$, $s_{22} = 1$, $s_{23} = -3$, $s_{33} = -4$ are used in (4.40).

by

$$\mathcal{T}_{ij}(k) = \frac{-2\mathrm{i}k^2 s_{ij} + 2k\det[\mathcal{S}_{ji}]}{k^3 + \mathrm{i}k^2\mathrm{tr}[S] - k\sum_i \det[\mathcal{S}_{ii}] - \mathrm{i}\det[S]}. \tag{4.51}$$

We have $\mathcal{T}_{ij}(0) = \mathcal{T}_{ij}(\infty) = 0$ for all $i \neq j$ signifying the guaranteed presence of both δ-like and δ'-like components in the connections between all lines.

This expression, along with the analogous expression for $n = r_A = r_B = 2$ case, invites an easy straightforward extension to general n. A numerical example of this case is shown in Fig. 10.

5. Conclusion

Our main finding in this article on quantum Y-junction is the fact that the couplings between each pair of outgoing lines are individually tunable. The ST form of vertex boundary condition, which gives the prescription for minimal construction of singular vertex as a limit of finite potentials, is also found to be instrumental in identifying the type of coupling between all pairs of outgoing lines. Crucial quantity to identify the physics of singular vertex is to be found in the rank of matrices A and B appearing in the ST form.

Specifically, the pure δ-type coupling is constructed from $\mathrm{rank}(B) = 1$ boundary condition, while the pure δ'-type coupling is constructed from $\mathrm{rank}(A) = 1$.

Boundary condition corresponding to ST form for $n = 3$ with $\mathrm{rank}(A) = \mathrm{rank}(B) = 2$ is identified as containing Y-junction with both δ–δ–δ' type and δ'–δ'–δ type singular verteces as limiting cases of parameter values $\bar{t}_i = 0$ and $t_i = 0$, respectively. Spectral filtering of quantum waves is achieved by these types of singular vertices.

The extension of our treatment to quantum singular vertex of degree $n = 4$, or "X-junction", and then to that with higher n appears tedious, but is within reach once the need of detail analysis is required as a model of quantum single electron devices. We hope that this work becomes a stepping stone for such extensions. Obviously, the experimental realization and demonstration with quantum wires and quantum dots are highly desired. Designing real-world approximation for singular vertex of quantum graph then becomes crucial.[7,9–11)]

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Appendix D

On the spectrum of a bent chain graph

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On the spectrum of a bent chain graph

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Abstract
We study Schrödinger operators on an infinite quantum graph of a chain form which consists of identical rings connected at the touching points by δ-couplings with a parameter $\alpha \in \mathbb{R}$. If the graph is 'straight', i.e. periodic with respect to ring shifts, its Hamiltonian has a band spectrum with all the gaps open whenever $\alpha \neq 0$. We consider a 'bending' deformation of the chain consisting of changing one position at a single ring and show that it gives rise to eigenvalues in the open spectral gaps. We analyze dependence of these eigenvalues on the coupling α and the 'bending angle' as well as resonances of the system coming from the bending. We also discuss the behaviour of the eigenvalues and resonances at the edges of the spectral bands.

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1. Introduction

Quantum graphs, i.e. Schrödinger operators with graph configuration spaces, were introduced in the middle of the last century [RuS53] and rediscovered three decades later [GP88, EŠ89]. Since then they have attracted a lot of attention; they became both a useful tool in numerous applications and a means of making it easy to study fundamental properties such as quantum chaos. We refrain from giving an extensive bibliography and refer to the recent proceedings volume [AGA] which the reader can use to check the state of art in this area.

One of the frequent questions concerns relations between the geometry of a graph Γ and spectral properties of a Schrödinger operator supported by Γ. Put like that, the question is a bit vague and allows different interpretation. On the one hand, we can have in mind the intrinsic

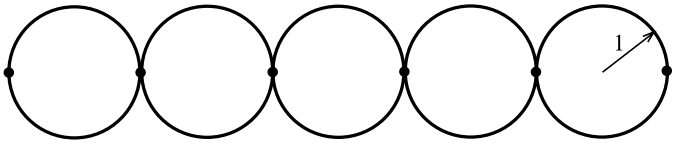

Figure 1. The unperturbed chain graph.

geometry of Γ which enters the problem through the adjacency matrix of the graph and the lengths of its edges. On the other hand, quite often one thinks of Γ as a subset of $\mathbb{R}^n$ with the geometry inherited from the ambient space. In that case geometric perturbations can acquire a rather illustrative meaning and one can ask in which way they influence spectral properties of a quantum particle 'living' on Γ; in such a context one can think of graphs with various local deformations as 'bent', locally 'protruded' or 'squeezed', etc.

This is particularly interesting if the 'unperturbed' system is explicitly solvable being, for instance, an infinite periodic graph. An influence of local spectral perturbations mentioned above is in this setting a rich subject which deserves to be investigated. So far it has been considered only episodically but even such a brief look shows that it may have properties uncommon in the usual theory of Schrödinger operators [KV06]. With this motivation we find it useful to start such a programme by discussing the influence of a 'bending' deformation on a graph which exhibits a one-dimensional periodicity.

To make things as simple as possible at the beginning we will not strive in this paper for generality and we will discuss in detail a simple nontrivial example, allowing for a fully explicit solution, in which the unperturbed system is a 'chain graph' consisting of an array of rings of unit radius, cf figure 1, connected through their touching points. We suppose that there are no external fields. Since values of physical constants are not important in our considerations we put $\hbar = 2m = 1$ and identify the particle Hamiltonian with the (negative) Laplacian acting as $\psi_j \mapsto -\psi_j''$ on each edge of the graph. It is well known that in order to get a self-adjoint operator one has to impose appropriate boundary conditions on the graph vertices. In our model we employ the so-called *δ-coupling* characterized by the conditions

$$\psi_j(0) = \psi_k(0) =: \psi(0), \qquad j,k \in \hat{n}, \qquad \sum_{j=1}^{n} \psi_j'(0) = \alpha\psi(0), \tag{1.1}$$

where $\hat{n} = \{1, 2, \ldots, n\}$ is the index set numbering the edges emanating from the vertex—in our case $n = 4$—and $\alpha \in \mathbb{R} \cup \{+\infty\}$ is the coupling constant supposed to be the same at every vertex of the chain. It is important that the 'straight' graph has spectral gaps[5], thus we *exclude the free boundary conditions* (sometimes called, not quite appropriately, Kirchhoff), i.e. we assume $\alpha \neq 0$.

The geometric perturbation to consider is the simplest possible bending of such a chain obtained by a shift of one of the contact points, as sketched in figure 2, which is parametrized by the bending angle ϑ characterizing the ratio of the two edges constituting the perturbed ring. Our aim is to show that the bending gives rise to eigenvalues in the gaps of the unperturbed spectrum and to analyze how they depend on ϑ. At the same time the bent chain will exhibit resonances and we will discuss behaviour of the corresponding poles.

The contents of the paper are as follows. In the following section we analyze the straight chain. Using the Bloch–Floquet decomposition we will show that the spectrum consists of an

[5] A nontrivial vertex coupling is also related to the problem of approximation of quantum graphs by 'fat graphs' of which the reader can learn more, e.g., in [CE07] or [EP08], references therein, and a paper in preparation by the authors of [EP08].

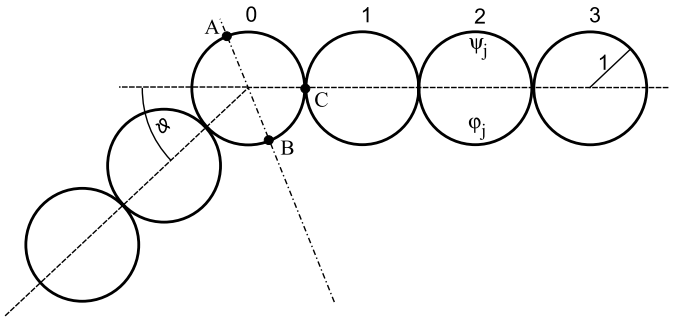

Figure 2. A bent graph.

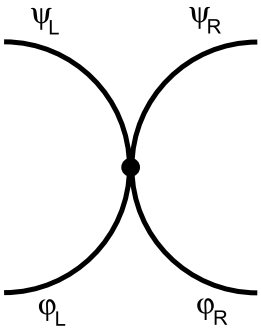

Figure 3. Elementary cell of the periodic system.

infinite number of absolutely continuous spectral bands separated by open gaps, plus a family of infinitely degenerate eigenvalues at band edges. In section 3 we will analyze the discrete spectrum due to the bending showing that in each gap it gives rise to at most two eigenvalues. Section 4 describes their dependence on the bending angle as well as complex solutions to the spectral condition corresponding to resonances in the bent chain. In section 5 we discuss further the angular dependence with attention to singular points where the solutions coincide with the band edges. Finally, in the concluding remarks we draw a parallel of our results with properties of quantum waveguides.

2. An infinite periodic chain

First we consider a 'straight' chain Γ_0 as sketched in figure 1; without loss of generality we may suppose that the circumference of each ring is 2π. The state Hilbert space of a nonrelativistic and spinless particle living on Γ_0 is $L^2(\Gamma_0)$. We suppose that the particle is free, not interacting with an external potentials on the edges, and denote by H_0 its Hamiltonian, i.e. it acts as the negative Laplacian on each graph link and its domain consists of all functions from $W^{2,2}_{\mathrm{loc}}(\Gamma_0)$ which satisfy the δ boundary conditions (1.1) at the vertices of Γ_0; we suppose that the coupling constant α is the same at each vertex[6].

In view of the periodicity of Γ_0, the spectrum of H_0 can be computed using the Bloch–Floquet decomposition. Let us consider an elementary cell with the wavefunction components being denoted according to figure 3 and ask about the spectrum of the Floquet components

[6] The coupling constant α is kept fixed and for the sake of simplicity we will not use it to label the Hamiltonian neither in the straight nor in the bent case.

of H_0. Since the operator acts as a negative second derivative, each component of the eigenfunction with energy $E = k^2 \neq 0$ is a linear combination of the functions $\mathrm{e}^{\pm \mathrm{i}kx}$. The momentum k is conventionally chosen positive for $E > 0$, while for E negative we put $k = \mathrm{i}\kappa$ with $\kappa > 0$ (the case $E = 0$ will be mentioned separately). For a given $E \neq 0$, the wavefunction components on the elementary cell are therefore given by

$$\begin{aligned} \psi_L(x) &= C_L^+ \mathrm{e}^{\mathrm{i}kx} + C_L^- \mathrm{e}^{-\mathrm{i}kx}, & x &\in [-\pi/2, 0] \\ \psi_R(x) &= C_R^+ \mathrm{e}^{\mathrm{i}kx} + C_R^- \mathrm{e}^{-\mathrm{i}kx}, & x &\in [0, \pi/2] \\ \varphi_L(x) &= D_L^+ \mathrm{e}^{\mathrm{i}kx} + D_L^- \mathrm{e}^{-\mathrm{i}kx}, & x &\in [-\pi/2, 0] \\ \varphi_R(x) &= D_R^+ \mathrm{e}^{\mathrm{i}kx} + D_R^- \mathrm{e}^{-\mathrm{i}kx}, & x &\in [0, \pi/2]. \end{aligned} \tag{2.1}$$

As we have said, at the contact point the δ-coupling (1.1) is assumed, i.e.

$$\psi_L(0) = \psi_R(0) = \varphi_L(0) = \varphi_R(0) \qquad -\psi_L'(0) + \psi_R'(0) - \varphi_L'(0) + \varphi_R'(0) = \alpha \cdot \psi_L(0).$$

On the other hand, at the 'free' ends of the cell the Floquet conditions are imposed,

$$\begin{aligned} \psi_R(\pi/2) &= \mathrm{e}^{\mathrm{i}\theta} \psi_L(-\pi/2) & \psi_R'(\pi/2) &= \mathrm{e}^{\mathrm{i}\theta} \psi_L'(-\pi/2) \\ \varphi_R(\pi/2) &= \mathrm{e}^{\mathrm{i}\theta} \varphi_L(-\pi/2) & \varphi_R'(\pi/2) &= \mathrm{e}^{\mathrm{i}\theta} \varphi_L'(-\pi/2) \end{aligned} \tag{2.3}$$

with θ running through $[-\pi, \pi)$; alternatively we may say that the quasimomentum $\frac{1}{2\pi}\theta$ runs through $[-1/2, 1/2)$, the Brillouin zone of the problem.

Substituting (2.1) into (2.2) and (2.3), one obtains after simple manipulations

$$C_X^+ \cdot \sin k\pi = D_X^+ \cdot \sin k\pi, \qquad C_X^- \cdot \sin k\pi = D_X^- \cdot \sin k\pi, \tag{2.4}$$

where X stands for L or R, hence $C_X^+ = C_X^-$ and $D_X^+ = D_X^-$ provided $k \notin \mathbb{N}_0 := \{0, 1, 2, \ldots\}$. We will treat the special case $k \in \mathbb{N}$ later, now we will suppose k does not belong to $\mathbb{N}$, the set of natural numbers. Furthermore, from (2.2) and (2.3) we obtain an equation for the phase factor $\mathrm{e}^{\mathrm{i}\theta}$,

$$\mathrm{e}^{2\mathrm{i}\theta} - \mathrm{e}^{\mathrm{i}\theta}\left(2\cos k\pi + \frac{\alpha}{2k}\sin k\pi\right) + 1 = 0, \tag{2.5}$$

which has real coefficients for any $k \in \mathbb{R} \cup \mathrm{i}\mathbb{R}\backslash\{0\}$ and the discriminant equal to

$$D = \left(2\cos k\pi + \frac{\alpha}{2k}\sin k\pi\right)^2 - 4.$$

We have to determine values of k^2 for which there is a $\theta \in [-\pi, \pi)$ such that (2.5) is satisfied, in other words, for which k^2 it has, as an equation in the unknown $\mathrm{e}^{\mathrm{i}\theta}$, at least one root of modulus 1. Note that a pair of solutions of (2.5) always gives 1 when multiplied, regardless of the value of k; hence either both roots are complex conjugates of modulus 1, or one is of modulus greater than 1 and the other has modulus smaller than 1. Obviously, the latter situation corresponds to a positive discriminant, and the former one to the discriminant less or equal to zero. We summarize this discussion as follows:

Proposition 2.1. *If $k^2 \in \mathbb{R}\backslash\{0\}$ and $k \notin \mathbb{N}$, then $k^2 \in \sigma(H_0)$ if and only if the condition*

$$\left|\cos k\pi + \frac{\alpha}{4} \cdot \frac{\sin k\pi}{k}\right| \leqslant 1 \tag{2.6}$$

is satisfied.

In particular, the negative spectrum is obtained by putting $k = \mathrm{i}\kappa$ for $\kappa > 0$ and rewriting the inequality (2.6) in terms of this variable. Note that since $\sinh x \neq 0$ for all $x > 0$, it never

occurs that $\sin k\pi = 0$ for $k \in \mathrm{i}\mathbb{R}^+$, the positive imaginary axis, thus there is no need to treat this case separately like for $k \in \mathbb{R}^+$, cf (2.4) above.

Corollary 2.2. *If $\kappa > 0$, then $-\kappa^2 \in \sigma(H_0)$ if and only if*

$$\left|\cosh \kappa\pi + \frac{\alpha}{4} \cdot \frac{\sinh \kappa\pi}{\kappa}\right| \leqslant 1. \tag{2.7}$$

Let us finally mention the case $k \in \mathbb{N}$ left out above. It is straightforward to check that k^2 is then an eigenvalue, and moreover, that it has an infinite multiplicity. One can construct an eigenfunction which is supported by a single circle, which is given by $\psi(x) = \sin kx$ with $x \in [0, \pi]$ on the upper semicircle and $\varphi(x) = -\sin kx$ with $x \in [0, \pi]$ on the lower one.

Remark 2.3. The condition (2.6) reminds us of the corresponding condition in the Kronig–Penney model with the distance between the interaction sites equal to π, cf [AGHH], the only difference being that the coupling constant is halved, $\frac{1}{2}\alpha$ instead of α. In contrast to that, the point spectrum of the KP model is empty. These facts are easy to understand if we realize that our model has the up-down mirror symmetry, and thus H_0 decomposes into a symmetric and antisymmetric part. The former is unitarily equivalent to the KP model with modified coupling, the latter corresponds to functions vanishing at the vertices, having thus a pure point spectrum. Looking ahead, we remark that the bending perturbation breaks this mirror symmetry.

Finally, in the case $E = 0$ we get in the similar way the equation

$$\mathrm{e}^{2\mathrm{i}\theta} - \mathrm{e}^{\mathrm{i}\theta}\left(2 + \frac{\alpha\pi}{2}\right) + 1 = 0, \tag{2.8}$$

replacing (2.5), whence we infer that $0 \in \sigma(H_0)$ if and only if

$$\left|1 + \frac{\alpha\pi}{4}\right| \leqslant 1, \tag{2.9}$$

hence zero can belong to the continuous part of the spectrum only and it happens *iff* $\alpha \in [-8/\pi, 0]$. In conclusion, we can make the following claim about $\sigma(H_0)$.

Theorem 2.4. *The spectrum of H_0 consists of infinitely degenerate eigenvalues equal to n^2 with $n \in \mathbb{N}$, and absolutely continuous spectral bands with the following properties:*

If $\alpha > 0$, then every spectral band is contained in an interval $(n^2, (n+1)^2]$ with $n \in \mathbb{N}_0 := \mathbb{N} \cup \{0\}$, and its upper edge coincides with the value $(n+1)^2$.

If $\alpha < 0$, then in each interval $[n^2, (n+1)^2)$ with $n \in \mathbb{N}$ there is exactly one spectral band the lower edge of which coincides with n^2. In addition, there is a spectral band with the lower edge (being the overall spectral threshold) equal to $-\kappa^2$, where κ is the largest solution of

$$\left|\cosh \kappa\pi + \frac{\alpha}{4} \cdot \frac{\sinh \kappa\pi}{\kappa}\right| = 1. \tag{2.10}$$

The position of the upper edge of this band depends on α. If $-8/\pi < \alpha < 0$, then it is equal to k^2 where k is the solution of

$$\cos k\pi + \frac{\alpha}{4} \cdot \frac{\sin k\pi}{k} = -1$$

contained in $(0, 1)$. On the other hand, for $\alpha < -8/\pi$ the upper edge is negative, $-\kappa^2$ with κ being the smallest solution of (2.10), and for $\alpha = -8/\pi$ it equals zero.

Finally, $\sigma(H_0) = [0, +\infty)$ holds if $\alpha = 0$.

Proof. The degenerate bands, in other words, the eigenvalues of infinite multiplicity, were found already and it is straightforward to check that no other eigenvalues exist. The continuous spectrum can be in view of remark 2.3 treated as in [AGHH], nevertheless, we sketch the argument not only to make the paper self-contained, but also in view of following sections where some ideas and formula of the present proof will be used again.

Consider first the positive part of the continuous spectrum. The condition (2.6) clearly determines bands with one endpoint at n^2, $n \in \mathbb{N}$, where the sign of α decides whether it is the upper or lower one. If $\alpha < 0$, the presence of a band in (0,1) depends on $|\alpha|$. Denoting $g(x) := \cos x\pi + \frac{\alpha}{4} \cdot \frac{\sin x\pi}{x}$ we want to show that $B := \{x \in (0, 1) : |g(x)| \leqslant 1\}$ is either empty or an interval with zero as its edge. It is obvious that g maps $(0, 1)$ continuously into $(-\infty, 1)$; we will check that $g(x_0) = -1$ implies $g'(x_0) < 0$. We first note that the premise implies $\cos x_0\pi = -1 - \frac{\alpha}{4} \cdot \frac{\sin x_0\pi}{x_0}$; taking the square of this relation we find after simple manipulations that $\sin x_0\pi = -2\big(\frac{\alpha}{4x_0} + \frac{4x_0}{\alpha}\big)^{-1}$ and $\cos x_0\pi = \big(\frac{\alpha}{4x_0} - \frac{4x_0}{\alpha}\big)\big(\frac{\alpha}{4x_0} + \frac{4x_0}{\alpha}\big)^{-1}$. Evaluating $g'(x_0)$ and substituting these expressions we get

$$g'(x_0) = \frac{\alpha\pi}{4x_0}\left(1 - \frac{\sin \pi x_0}{\pi x_0}\right) < 0.$$

These properties together with the continuity of g imply that if B is not empty, then it is an interval with the left endpoint zero. It is also clear that B is nonempty *iff* $g(0+) > -1$ which gives the condition $\alpha > -8/\pi$. In contrast, B is empty if $\alpha < -8/\pi$ and the borderline case $\alpha = -8/\pi$ was mentioned above.

Let us next focus on the negative part using $\tilde{g}(x) := \cosh x\pi + \frac{\alpha}{4} \cdot \frac{\sinh x\pi}{x}$ and ask about $\tilde{B} := \{x \in (0, \infty) : |\tilde{g}(x)| \leqslant 1\}$. It is easy to check that $\tilde{g}(x) = -1$ iff $\tanh \frac{x\pi}{2} = \frac{4x}{|\alpha|}$ and $\tilde{g}(x) = 1$ iff $\coth \frac{x\pi}{2} = \frac{4x}{|\alpha|}$. It implies that there is exactly one x_1 such that $\tilde{g}(x_1) = 1$, and that the equation $\tilde{g}(x) = -1$ has one solution x_{-1} in the case $\alpha < -8/\pi$ and no solution in the case $\alpha \in [-8/\pi, 0)$. Since obviously $0 < x_{-1} < x_1$ and $\tilde{g}(0+) := \lim_{x\to 0_+} \tilde{g}(x) = 1 + \alpha\pi/4$, we infer that $\tilde{B}$ is a bounded interval. Its closure contains zero *iff* $\alpha \in [-8/\pi, 0)$ because then $\tilde{g}(0+) \in [-1, 1)$. In such a case the lowest spectral band is the closure of $B \cup \tilde{B}$, otherwise it is the closure of $\tilde{B}$ only. □

3. The perturbed system

3.1. General considerations

Let us suppose now that the straight chain of the previous section suffers a bending perturbation as shown in figure 2. We call the perturbed graph Γ_ϑ; it differs from Γ_0 by replacing the arc lengths π of a fixed ring, conventionally numbered as zero, by $\pi \pm \vartheta$. The bending angle ϑ is supposed to take values from $(0, \pi)$, regardless of the fact that for $\vartheta \geqslant 2\pi/3$ it is not possible to consider Γ_ϑ embedded in the plane as sketched—one can certainly realize such a 'bending' in an alternative way, for instance, by deforming the selected ring.

The state Hilbert space of the perturbed system is $L^2(\Gamma_\vartheta)$ and the Hamiltonian is H_ϑ obtained by a natural modification of H_0; our aim is to determine its spectrum. Since Γ_ϑ has the mirror symmetry w.r.t. the axis of the zeroth ring passing through the points $x = \frac{1}{2}(\pi \pm \vartheta)$, the operator H_ϑ can be reduced by parity subspaces into a direct sum of an even part, H^+, and odd one, H^-; for the sake of simplicity we drop mostly the subscript ϑ in the following.

All the components of the wavefunction at energy k^2 are linear combinations of $\mathrm{e}^{\pm \mathrm{i}kx}$. As we have said we use the ring labelling with zero corresponding to the perturbed one; the mirror symmetry allows us to study a half of the system only, say, with non-negative indices.

The wavefunction on each ring will be a pair of functions ψ_j and φ_j, where j is the circle index, ψ_j corresponds to the upper semicircle and φ_j to the lower one,

$$\begin{aligned} \psi_j(x) &= C_j^+ \,\mathrm{e}^{\mathrm{i}kx} + C_j^- \,\mathrm{e}^{-\mathrm{i}kx}, \qquad x \in [0,\pi] \\ \varphi_j(x) &= D_j^+ \,\mathrm{e}^{\mathrm{i}kx} + D_j^- \,\mathrm{e}^{-\mathrm{i}kx}, \qquad x \in [0,\pi], \end{aligned} \tag{3.1}$$

for $j \in \mathbb{N}$. The situation is different in the case $j = 0$, where the variables run over modified intervals,

$$\begin{aligned} \psi_0(x) &= C_0^+ \,\mathrm{e}^{\mathrm{i}kx} + C_0^- \,\mathrm{e}^{-\mathrm{i}kx}, \qquad x \in \left[\frac{\pi-\vartheta}{2}, \pi\right] \\ \varphi_0(x) &= D_0^+ \,\mathrm{e}^{\mathrm{i}kx} + D_0^- \,\mathrm{e}^{-\mathrm{i}kx}, \qquad x \in \left[\frac{\pi+\vartheta}{2}, \pi\right]. \end{aligned} \tag{3.2}$$

There are δ-couplings with the parameter α in the points of contact, i.e.

$$\psi_j(0) = \varphi_j(0) \qquad \psi_j(\pi) = \varphi_j(\pi) \tag{3.3}$$

and

$$\psi_j(0) = \psi_{j-1}(\pi) \tag{3.4}$$

$$\psi_j'(0) + \varphi_j'(0) - \psi_{j-1}'(\pi) - \varphi_{j-1}'(\pi) = \alpha \cdot \psi_j(0). \tag{3.5}$$

Substituting (3.1) into (3.3) we obtain

$$C_j^+ \cdot \sin k\pi = D_j^+ \cdot \sin k\pi \qquad \text{and} \qquad C_j^- \cdot \sin k\pi = D_j^- \cdot \sin k\pi,$$

thus for $k \notin \mathbb{N}_0$ we have $C_j^+ = D_j^+$ and $C_j^- = D_j^-$. The case $k \in \mathbb{N}_0$ can be treated analogously with the 'straight' case: it is easy to see that squares of integers are infinitely degenerate eigenvalues and the eigenfunctions can be supported by any ring, now with the exception of the zeroth one. From now on, we suppose $k \notin \mathbb{N}_0$.

Using the coupling conditions (3.4) and (3.5), we arrive at a 'transfer matrix' relation between coefficients of the neighbouring rings,

$$\begin{pmatrix} C_j^+ \\ C_j^- \end{pmatrix} = \underbrace{\begin{pmatrix} \left(1+\frac{\alpha}{4\mathrm{i}k}\right)\mathrm{e}^{\mathrm{i}k\pi} & \frac{\alpha}{4\mathrm{i}k}\,\mathrm{e}^{-\mathrm{i}k\pi} \\ -\frac{\alpha}{4\mathrm{i}k}\,\mathrm{e}^{\mathrm{i}k\pi} & \left(1-\frac{\alpha}{4\mathrm{i}k}\right)\mathrm{e}^{-\mathrm{i}k\pi} \end{pmatrix}}_{M} \cdot \begin{pmatrix} C_{j-1}^+ \\ C_{j-1}^- \end{pmatrix}, \tag{3.6}$$

valid for all $j \geqslant 2$, which yields

$$\begin{pmatrix} C_j^+ \\ C_j^- \end{pmatrix} = M^{j-1} \cdot \begin{pmatrix} C_1^+ \\ C_1^- \end{pmatrix}. \tag{3.7}$$

It is clear that the asymptotical behaviour of the norms of $\left(C_j^+, C_j^-\right)^T$ is determined by spectral properties of the matrix M. Specifically, let $\left(C_1^+, C_1^-\right)^T$ be an eigenvector of M corresponding to an eigenvalue μ, then $|\mu| < 1$ ($|\mu| > 1$, $|\mu| = 1$) means that $\left\|\left(C_j^+, C_j^-\right)^T\right\|$ decays exponentially with respect to j (respectively, it is exponentially growing, or independent of j).

The wavefunction components on the jth ring for both $H^{\pm}$ (as well as on the $(-j)$th by the mirror symmetry) are determined by C_j^+ and C_j^-, and thus by $\left(C_1^+, C_1^-\right)^T$ by virtue of (3.7). If $\left(C_1^+, C_1^-\right)^T$ has a non-vanishing component related to an eigenvalue of M of modulus larger than 1, it determines neither an eigenfunction nor a generalized eigenfunction of $H^{\pm}$. On the other hand, if $\left(C_1^+, C_1^-\right)^T$ is an eigenvector, or a linear combination of eigenvectors,

of the matrix M with modulus less than 1 (respectively, equal to 1), then the coefficients $C_j^{\pm}$ determine an eigenfunction (respectively, a generalized eigenfunction) and the corresponding energy E belongs to the point (respectively, continuous) spectrum of the operator $H^{\pm}$. To perform the spectral analysis of M, we employ its characteristic polynomial at energy k^2,

$$\lambda^2 - 2\lambda\left(\cos k\pi + \frac{\alpha}{4k}\sin k\pi\right) + 1, \tag{3.8}$$

which we have encountered already in the relation (2.5); it shows that M has an eigenvalue of modulus less than 1 *iff* the discriminant of (3.8) is positive, i.e.

$$\left|\cos k\pi + \frac{\alpha}{4k}\sin k\pi\right| > 1,$$

and a pair of complex conjugated eigenvalues of modulus 1 *iff* the above quantity is $\leqslant 1$. In the former case the eigenvalues of M are given by

$$\lambda_{\frac{1}{2}} = \cos k\pi + \frac{\alpha}{4k}\sin k\pi \pm \sqrt{\left(\cos k\pi + \frac{\alpha}{4k}\sin k\pi\right)^2 - 1},$$

satisfying $\lambda_2 = \lambda_1^{-1}$, hence $\lambda_2 < 1$ holds if $\cos k\pi + \frac{\alpha}{4k}\sin k\pi > 1$ and $\lambda_1 < 1$ if this quantity is < -1. Moreover, the corresponding eigenvectors of M are

$$v_{1,2} = \begin{pmatrix} \frac{\alpha}{4ik}\,\mathrm{e}^{-ik\pi} \\ \lambda_{1,2} - \left(1 + \frac{\alpha}{4ik}\right)\mathrm{e}^{ik\pi} \end{pmatrix}.$$

Remark 3.1. Comparing to (2.6) we see that the perturbation does not affect the spectral bands, and also, that new eigenvalues coming from the perturbation can appear only in the gaps. These facts are obvious, of course, from general principles. Using the natural identification of $L^2(\Gamma_0)$ and $L^2(\Gamma_\vartheta)$ we see that H_0 and H_ϑ differ by a shift of the point where a boundary condition is applied, hence their resolvent difference has a finite rank (in fact, rank two). Consequently, their essential spectra coincide and each spectral gap of H_0 contains at most two eigenvalues of H_ϑ, see [We, sec. 8.3, cor. 1].

3.2. Spectrum of H^+

The operator H^+ corresponds to the wavefunctions *even* w.r.t. the symmetry axis, hence we may consider a half of the graph with the Neumann conditions at the boundary (i.e., the points A, B in figure 2),

$$\psi_0'\left(\frac{\pi - \vartheta}{2}\right) = 0, \qquad \varphi_0'\left(\frac{\pi + \vartheta}{2}\right) = 0.$$

At the contact point of the zeroth and the first ring (denoted by C) there is a δ-coupling with the parameter α,

$$\psi_0(\pi) = \varphi_0(\pi) = \psi_1(0) \tag{3.9}$$

$$\psi_1'(0) + \varphi_1'(0) - \psi_0'(\pi) - \varphi_0'(\pi) = \alpha \cdot \psi_0(\pi). \tag{3.10}$$

Substituting to these conditions from (3.1) and (3.2) and using the equality $\varphi_1'(0) = \psi_1'(0)$, we obtain $\left(C_1^+, C_1^-\right)^T$ up to a multiplicative constant,

$$\begin{pmatrix} C_1^+ \\ C_1^- \end{pmatrix} = \begin{pmatrix} \frac{\cos k\pi + \cos k\vartheta}{\sin k\pi} + \mathrm{i}\left(1 - \frac{\alpha(\cos k\pi + \cos k\vartheta)}{2k\sin k\pi}\right) \\ \frac{\cos k\pi + \cos k\vartheta}{\sin k\pi} - \mathrm{i}\left(1 - \frac{\alpha(\cos k\pi + \cos k\vartheta)}{2k\sin k\pi}\right) \end{pmatrix}.$$

The right-hand side is well defined except for $\sin k\pi = 0$, but this case has already been excluded from our considerations; we know that for $k \in \mathbb{N}$ the number k^2 is an eigenvalue of infinite multiplicity.

Following the above discussion $k^2 \in \sigma_p(H^+)$ requires that the vector $\big(C_1^+, C_1^-\big)^T$ is an eigenvector of M corresponding to the eigenvalue λ of the modulus less than 1. Using the above explicit form of the eigenvectors and solving the equation

$$\begin{vmatrix} \frac{\cos k\pi+\cos k\vartheta}{\sin k\pi} + \mathrm{i}\big(1 - \frac{\alpha(\cos k\pi+\cos k\vartheta)}{2k\sin k\pi}\big) & \frac{\alpha}{4\mathrm{i}k}\,\mathrm{e}^{-\mathrm{i}k\pi} \\ \frac{\cos k\pi+\cos k\vartheta}{\sin k\pi} - \mathrm{i}\big(1 - \frac{\alpha(\cos k\pi+\cos k\vartheta)}{2k\sin k\pi}\big) & \lambda - \big(1 + \frac{\alpha}{4\mathrm{i}k}\big)\mathrm{e}^{\mathrm{i}k\pi} \end{vmatrix} = 0$$

we arrive at the condition

$$(\cos k\vartheta + \cos k\pi)\cdot\left(\frac{\alpha}{4k}\sin k\pi \pm \sqrt{\Big(\cos k\pi + \frac{\alpha}{4k}\sin k\pi\Big)^2 - 1}\right) = \sin^2 k\pi,$$

with the sign given by the sign of $\cos k\pi + \frac{\alpha}{4k}\sin k\pi$. Since $\sin k\pi \neq 0$, the second factor at the *lhs* is also nonzero and the last equation is equivalent to

$$\cos k\vartheta = -\cos k\pi + \frac{\sin^2 k\pi}{\frac{\alpha}{4k}\sin k\pi \pm \sqrt{\big(\cos k\pi + \frac{\alpha}{4k}\sin k\pi\big)^2 - 1}}; \tag{3.11}$$

for the sake of brevity we denote the expression at the *rhs* by $f(k)$.

The relation (3.11) is our main tool to analyze the discrete spectrum and we are going to discuss now its solutions. We start with an auxiliary result noting that, as a consequence of theorem 2.4, the set of positive k for which the inequality $|\cos k\pi + \frac{\alpha}{4k}\sin k\pi| \geqslant 1$ is satisfied is an infinite disjoint union of closed intervals. We denote them I_n with $n \in \mathbb{N}$ and recall that $n \in I_n$. If $\alpha > 0$ we denote by I_0 the interval with the edge at zero corresponding to the non-negative part of the lowest spectral gap of H_0.

Proposition 3.2. *The function f introduced above maps each $I_n\backslash\{n\}$ into the interval $(-1, 1)\cup\{(-1)^n\}$. Moreover, $f(x) = (-1)^n$ holds for $x \in I_n\backslash\{n\}$ iff $|\cos x\pi + \frac{\alpha}{4x}\sin x\pi| = 1$, and $\lim_{x\in I_n, x\to n} f(x) = (-1)^{n+1}$.*

Proof. According to (3.11), the function f is continuous in each interval $I_n\backslash\{n\}$, thus it maps the interval $I_n\backslash\{n\}$ again to an interval. The claim then follows from the following easy observations. First, $f(x) = (-1)^n$ *iff* x is the non-integer boundary point of I_n (if $\alpha < 0$ and $|\alpha|$ is sufficiently large, the left edge of I_1 is moved to zero and one checks that $\lim_{x\to 0} f(x) = -1$). Furthermore, for all $x \in I_n\backslash\{n\}$ we have $f(x) \neq (-1)^{n-1}$, and finally, $\lim_{x\to n, x\in I_n} f(x) = (-1)^{n-1}$. □

Proposition 3.2 guarantees the existence of at least one solution of (3.11) in each interval $I_n\backslash\{n\}$, except for the case when ϑ satisfies $\cos n\vartheta = (-1)^{n-1}$, or equivalently, except for the angles $\vartheta = \frac{n+1-2\ell}{n}\pi$, $\ell = 1, \ldots, \big[\frac{n+1}{2}\big]$. Later we will show that for these angles there is indeed no solution of the equation (3.11) in $I_n\backslash\{n\}$, while for the other angles in $(0, \pi)$ there is exactly one.

In a similar way one can proceed with the negative part of the spectrum. If $k = \mathrm{i}\kappa$ where $\kappa > 0$, the condition (3.11) acquires the form

$$\cosh\kappa\vartheta = -\cosh\kappa\pi - \frac{\sinh^2\kappa\pi}{\frac{\alpha}{4\kappa}\sinh\kappa\pi \pm \sqrt{\big(\cosh\kappa\pi + \frac{\alpha}{4\kappa}\sinh\kappa\pi\big)^2 - 1}}, \tag{3.12}$$

where the upper sign in the denominator refers to $\cosh\kappa\pi + \frac{\alpha}{4\kappa}\sinh\kappa\pi > 1$, and the lower one to $\cosh\kappa\pi + \frac{\alpha}{4\kappa}\sinh\kappa\pi < -1$. Let us denote the *rhs* of (3.12) by $\tilde{f}(\kappa)$, then we have the following counterpart to proposition 3.2.

Proposition 3.3. *If* $\alpha \geqslant 0$, *then* $\tilde{f}(\kappa) < -\cosh \kappa\vartheta$ *holds for all* $\kappa > 0$ *and* $\vartheta \in (0, \pi)$. *On the other hand, for* $\alpha < 0$ *we have*

If $\lim_{\kappa\to 0} \left(\cosh \kappa\pi + \frac{\alpha}{4\kappa} \sinh \kappa\pi\right) < -1$, *then there is a right neighbourhood of zero where* $\tilde{f}(x) = -1 - C(\alpha)x^2 + o(x^2)$ *with the constant explicitly given by* $C(\alpha) := \left(\frac{1}{2} + \left(\frac{\alpha\pi}{4} + \sqrt{\left(\frac{\alpha\pi}{4}\right)^2 + \frac{\alpha\pi}{2}}\right)^{-1}\right)\pi^2$. *Moreover,* $\tilde{f}(\kappa) = -1$ *holds for* $\kappa > 0$ *iff* $\cosh \kappa\pi + \frac{\alpha}{4\kappa} \sinh \kappa\pi = -1$.

The interval $\left\{\kappa : \cosh \kappa\pi + \frac{\alpha}{4\kappa} \sinh \kappa\pi \geqslant 1 \wedge \kappa \cdot \tanh \kappa\pi < -\alpha/2\right\}$ *is mapped by the function* $\tilde{f}$ *onto* $[1, +\infty)$.

If $\kappa \tanh \kappa\pi > -\alpha/2$, *then* $\tilde{f}(\kappa) < -\cosh \kappa\vartheta$ *holds for all* $\kappa > 0$ *and* $\vartheta \in (0, \pi)$.

Proof. The statement for $\alpha \geqslant 0$ is obvious, assume further that $\alpha < 0$. The first claim follows from the Taylor expansions of the functions involved in $\tilde{f}$, the last uses the equality $\cosh^2 \kappa - \sinh^2 \kappa = 1$. The set determined by the conditions $\cosh \kappa\pi + \frac{\alpha}{4\kappa} \sinh \kappa\pi \geqslant 1$ and $\kappa \cdot \tanh \kappa\pi < -\alpha/2$ is obviously an interval and $\tilde{f}$ is continuous on it. Since $\cosh \kappa\pi + \frac{\alpha}{4\kappa} \sinh \kappa\pi = 1$ implies $\tilde{f}(\kappa) = 1$ and for $\kappa_0 \cdot \tanh \kappa_0\pi = -\alpha/2$ it holds $\lim_{x\to\kappa_0^-} \tilde{f} = +\infty$, the second claim follows immediately. Finally, if $\kappa \cdot \tanh \kappa\pi > -\alpha/2$, then $\cosh \kappa\pi + \frac{\alpha}{4\kappa} \sinh \kappa\pi > 1$ and $\frac{\alpha}{4\kappa} \sinh \kappa\pi \pm \sqrt{\left(\cosh \kappa\pi + \frac{\alpha}{4\kappa} \sinh \kappa\pi\right)^2 - 1} > 0$, thus $\tilde{f}(\kappa) < -\cosh \kappa\pi < -\cosh \kappa\vartheta$ holds for all $\kappa > 0$ and $\vartheta \in (0, \pi)$. □

In particular, the first claim concerning $\alpha < 0$ together with the continuity of $\tilde{f}$ implies that if the set $\left\{\kappa : \cosh \kappa\pi + \frac{\alpha}{4\kappa} \sinh \kappa\pi \geqslant 1\right\}$ is nonempty (and thus an interval), the graph of $\tilde{f}$ on this set lies below the value -1 touching it exactly at the endpoints of this interval.

Corollary 3.4. *If* $\alpha \geqslant 0$, *then* H^+ *has no negative eigenvalues. On the other hand, for* $\alpha < 0$ *the operator* H^+ *has at least one negative eigenvalue which lies under the lowest spectral band and above the number* $-\kappa_0^2$, *where* κ_0 *is the (unique) solution of* $\kappa \cdot \tanh \kappa\pi = -\alpha/2$.

Proof. The eigenvalues are squares of solutions to the equation $\cosh \kappa\vartheta = \tilde{f}(\kappa)$. The absence of negative eigenvalues for $\alpha \geqslant 0$ follows directly from the first claim in proposition 3.3. The same proposition implies that there is exactly one interval mapped by $\tilde{f}$ onto $[1, +\infty)$, hence there is at least one solution of $\cosh \kappa\vartheta = \tilde{f}(\kappa)$ in this interval. □

3.3. Spectrum of H^- *and a summary*

The operator H^- which corresponds to the odd part of the wavefunction can be treated in an analogous way. The boundary conditions on the zero circle are now Dirichlet ones,

$$\psi_0\left(\frac{\pi - \vartheta}{2}\right) = 0, \qquad \varphi_0\left(\frac{\pi + \vartheta}{2}\right) = 0.$$

One can easily find the spectral condition,

$$-\cos k\vartheta = -\cos k\pi + \frac{\sin^2 k\pi}{\frac{\alpha}{4k} \sin k\pi \pm \sqrt{\left(\cos k\pi + \frac{\alpha}{4k} \sin k\pi\right)^2 - 1}}; \tag{3.13}$$

in comparison with (3.11) corresponding to H^+ there is a difference in the sign of the cosine on the left-hand side. Since we already know the behaviour of the right-hand side, cf proposition 3.2, we can infer, similarly as for H^+, that there is at least one solution of (3.13) in each interval I_n except for the case when $-\cos n\vartheta = (-1)^{n-1}$, i.e. when $\vartheta = \frac{n-2\ell}{n}\pi$, $\ell = 1, \ldots, \left[\frac{n}{2}\right]$.

Following the analogy with the symmetric case further we can employ proposition 3.2 to conclude that in each interval I_n there is at least one solution of $-\cos k\vartheta = f(\kappa)$. The only exception is the interval I_1 for $\alpha < 0$: for $|\alpha|$ sufficiently small it holds $-\cos k\vartheta < f(k)$ in the whole I_1; we will comment on this situation in more detail in the following section devoted to resonances. The negative part of the point spectrum of H^- is determined by the condition

$$-\cosh\kappa\vartheta = -\cosh\kappa\pi - \frac{\sinh^2\kappa\pi}{\frac{\alpha}{4\kappa}\sinh\kappa\pi \pm \sqrt{\left(\cosh\kappa\pi + \frac{\alpha}{4\kappa}\sinh\kappa\pi\right)^2 - 1}}, \tag{3.14}$$

where we set $k = \mathrm{i}\kappa$ for $\kappa \in \mathbb{R}^+$. It follows from proposition 3.3 that (3.14) has a solution for negative α only, and it happens if (i) the positive spectral gap touching zero extends to negative values, and (ii) the bending angle ϑ is small enough. In other words, if there is a number κ_0 solving $\cosh\kappa\pi + \frac{\alpha}{4\kappa}\sinh\kappa\pi = -1$, the energy plot w.r.t. ϑ obtained as the implicit solutions of (3.14) is a curve departing from $(\vartheta, E) = \left(0, -\kappa_0^2\right)$; in the following section we will show that it is analytic and following it one arrives at the point $(\vartheta, E) = (\pi, 1)$.

Let us summarize the discussion of the discrete spectrum. We have demonstrated that for each of the operators $H^\pm$ there generally arises at least one eigenvalue in every spectral gap closure. We have also explained that such an eigenvalue can lapse into a band edge equal to n^2, $n \in \mathbb{N}$, and thus be in fact absent. The eigenvalues of H^+ and H^- may also coincide, in this case they become a single eigenvalue of multiplicity two. One can check directly that it happens only if

$$k \cdot \tan k\pi = \frac{\alpha}{2}.$$

The study of the resonances, performed in the following section, will help us to find more precise results concerning the number of eigenvalues. We will show that there are at *most* two of them in each spectral gap. However, to make the explanation clearer, we refer already at this moment to figures 4–6 illustrating the numerical solution of the spectral condition for different signs of the coupling constant, as well as the resonances of the system.

4. Resonances and analyticity

Proceeding further with the discussion we want to learn more about the angle dependence of the perturbation effects. First we note, however, that the added eigenvalues are not the only consequence of the chain bending. One has to investigate all solutions of (4.1), not only the real ones which correspond to $\sigma_p(H^+)$, but also complex solutions describing *resonances*[7] of $H^\pm$.

Proposition 4.1. *Given a non-integer $k > 0$, the conditions (3.11) and (3.12) for $H^\pm$, respectively, are equivalent to*

$$\frac{\alpha}{2k}(1 \pm \cos k\vartheta\cos k\pi)(\pm\cos k\vartheta + \cos k\pi) = \sin k\pi \cdot (1 \pm 2\cos k\vartheta\cos k\pi + \cos^2 k\vartheta). \tag{4.1}$$

Proof. First we note that changing the square root sign in denominator of (3.11) does not give rise to a real solution. Indeed, if the sign of the right-hand side of (3.11) is changed, the obtained expression is of modulus greater than 1, hence it cannot be equal to $\cos k\vartheta$. This

[7] The notion of resonance in the chain–graph system can be introduced in different, mutually equivalent, ways similarly as in [EL07].

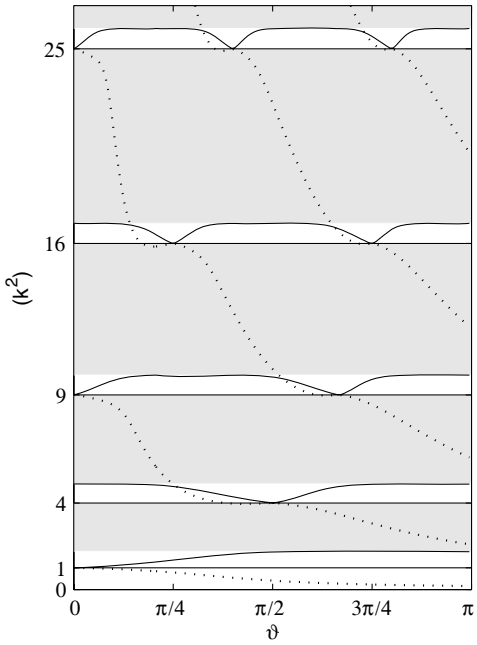

Figure 4. The spectrum of H^+ as a function of ϑ for repulsive coupling, $\alpha = 3$. The shaded regions are spectral bands, the dashed lines show real parts of the resonance pole positions discussed in section 4.

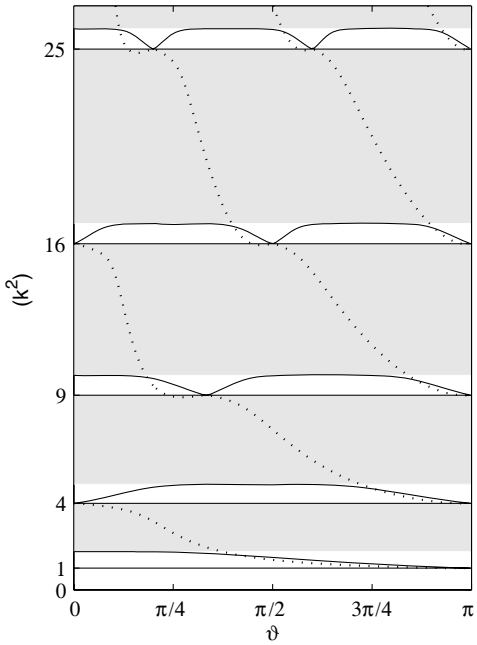

Figure 5. The spectrum of H^- in the same setting as in figure 4.

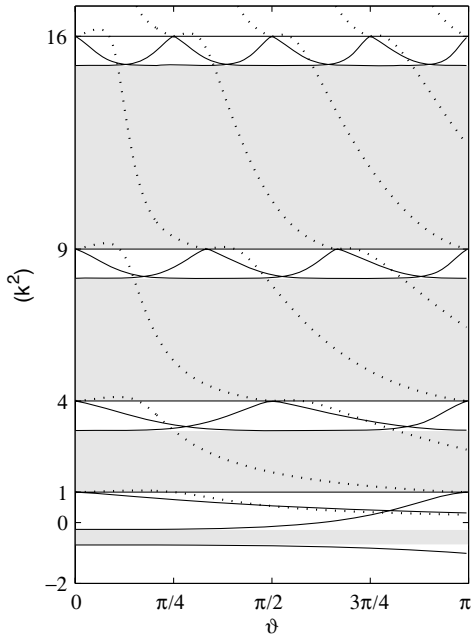

Figure 6. The spectrum of H as a function of ϑ for attractive coupling, $\alpha = -3$.

further implies that one need not specify the sign in the denominator of (3.11) by the sign of $\cos k\pi + \frac{\alpha}{4k}\sin k\pi$, and therefore we can express the square root and subsequently square both sides of the obtained relation. After simple manipulations, we arrive at (4.1); note that for all $k \in \mathbb{R}^+\backslash\mathbb{N}$, the denominator of (3.11) is nonzero. The equivalence of (3.11) and (4.1) for $k \in \mathbb{C}\backslash\mathbb{N}$ is obvious for (4.1) considered with the complex square root, i.e. without restrictions on the sign in the denominator. The argument for H^- is analogous. □

Now we are ready to state and prove the analyticity properties. Since the cases of different symmetries are almost the same, apart from the position of the points where the analyticity fails, we will mention the operator H^+ only.

Proposition 4.2. *Curves given by the implicit equation (4.1) for H^+ are analytic everywhere except at $(\vartheta, k) = \left(\frac{n+1-2\ell}{n}\pi, n\right)$, where $n \in \mathbb{N}$, $\ell \in \mathbb{N}_0$, $\ell \leqslant \left[\frac{n+1}{2}\right]$. Moreover, the real solution in the nth spectral gap is given by a function $\vartheta \mapsto k$ which is analytic, except at the points $\frac{n+1-2\ell}{n}\pi$.*

Proof. First we will demonstrate the analyticity of the curves $\vartheta \mapsto k \in \mathbb{C}$. This is easily done using equation (3.11); we have to prove that at each point (ϑ, k) solving the equation $G(\vartheta, k) = 0$ with

$$G(\vartheta, k) = -\cos k\vartheta - \cos k\pi + \frac{\sin^2 k\pi}{\frac{\alpha}{4k}\sin k\pi \pm \sqrt{\left(\cos k\pi + \frac{\alpha}{4k}\sin k\pi\right)^2 - 1}}$$

the derivative $\frac{\partial G}{\partial \vartheta}$ is nonzero. We have $\frac{\partial G}{\partial \vartheta} = k \cdot \sin(k\vartheta) = 0$ *iff* $\sin k\vartheta = 0$, i.e. $k\vartheta = m\pi, m \in \mathbb{Z}$. This implies $G(\vartheta, k) = (-1)^{m+1} - \cos k\pi$, and since $G(\vartheta, k) = 0$

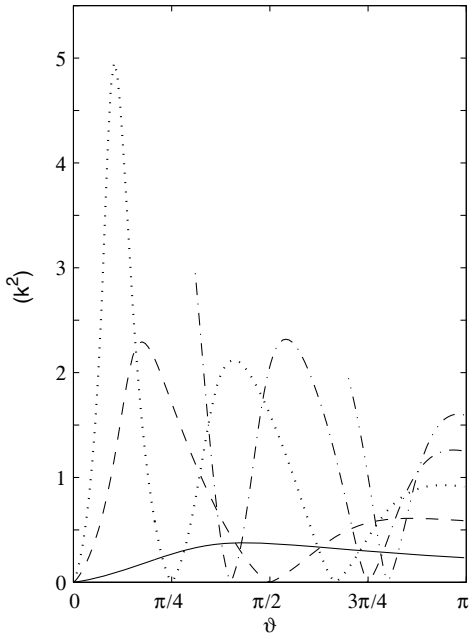

Figure 7. The imaginary parts of resonance pole positions in the same setting as in the previous picture; for the sake of lucidity only the curves corresponding to H^+ are plotted.

should be satisfied, k is an integer of the same parity as $m+1$. For $k \in \mathbb{N}$, G is not defined and we use (4.1); it is easy to check that any solution (ϑ, k) of (4.1) with $k \in \mathbb{N}$ corresponds to

$$\vartheta = \frac{k+1-2\ell}{k}\pi, \qquad \ell \in \mathbb{N}, \quad \ell \leqslant \left[\frac{k+1}{2}\right].$$

To prove that real solutions are analytic functions, it suffices to check that, except at the points $(\varphi, k) = \left(\frac{n+1-2\ell}{n}\pi, n\right)$, for each (ϑ, k) solving $F(\vartheta, k) = 0$ with

$$\begin{aligned} F(\vartheta, k) := {} & \alpha(1+\cos k\vartheta \cos k\pi)(\cos k\vartheta + \cos k\pi) \\ & - 2k \sin k\pi \cdot (1 + 2\cos k\vartheta \cos k\pi + \cos^2 k\vartheta) \end{aligned}$$

it holds $\frac{\partial F}{\partial k} \neq 0$. Computing the derivative one obtains an expression which can be cast in the form

$$\begin{aligned} & 2\sin^2 k\pi \cdot (1 + 2\cos k\vartheta \cos k\pi + \cos^2 k\vartheta)^2 + \alpha \cdot [\pi(\cos k\vartheta + \cos k\pi)^4 \\ & \quad + \sin^2 k\pi \cdot (\cos k\vartheta + \cos k\pi)^2 + \vartheta \sin^2 k\pi \sin^2 k\vartheta (1 + \cos k(\pi - \vartheta)) \\ & \quad + (\pi - \vartheta) \sin^2 k\pi \sin^2 k\vartheta (1 + \cos k\vartheta \cos k\pi)]. \end{aligned}$$

This is always non-negative, and vanishes *iff*

$$(\cos k\pi = 1 \wedge \cos k\vartheta = -1) \vee (\cos k\pi = -1 \wedge \cos k\vartheta = 1),$$

i.e. *iff* $k \in \mathbb{Z}$ and $k\pi = k\vartheta + (2\ell - 1)\pi$, $\ell \in \mathbb{Z}$, proving this the sought claim. □

The resonance dependence on the bending angle ϑ is again visualized in figures 4–6 where the real parts are shown; the imaginary parts corresponding to the situation of figure 4 are plotted on figure 7.

5. More on the angle dependence

The above results raise naturally the question about the behaviour of the curves at the singular points $[\vartheta, k] = \left[\frac{n+1-2\ell}{n}\pi, n\right]$ with $n \in \mathbb{N}$, $\ell \in \mathbb{N}$, $\ell \leqslant \left[\frac{n+1}{2}\right]$, where they touch the band edges and where the eigenvalues and resonances may cross. Now we are going to examine the asymptotic expansion at these points and to look how many curves 'stem' from them.

Consider again first the part H^+. Let $k_0 \in \mathbb{N}$ and $\vartheta_0 := \frac{n+1-2\ell}{n}\pi$ for some $\ell \in \mathbb{N}$, and put

$$k := k_0 + \varepsilon, \qquad \vartheta := \vartheta_0 + \delta.$$

After substituting into (4.1) with the plus signs and employing Taylor expansions of the cos and sin functions we arrive at the relation

$$\frac{\alpha}{4}\left(k_0^4\delta^4 + 4k_0^3\vartheta_0\delta^3\varepsilon + 6k_0^2\vartheta_0^2\delta^2\varepsilon^2\right) - k_0\pi^3\varepsilon^3 = \mathcal{O}(\delta\varepsilon^3) + \mathcal{O}(\varepsilon^4) + \mathcal{O}(\delta^3\varepsilon).$$

Using the theory of algebroidal functions and Newton polygon, we find that in the neighbourhood of (ϑ_0, k_0), the asymptotical behaviour of solutions is given by the terms of the order δ^4 and ε^3. In other words, up to a higher-order term we have $\frac{\alpha}{4}k_0^4\delta^4 = k_0\pi^3\varepsilon^3$, and therefore

$$\left(\frac{\varepsilon\pi}{k_0}\right)^3 = \frac{\alpha}{4}\delta^4.$$

Note that $\alpha \in \mathbb{R}$, $k_0 > 0$, $\delta \in \mathbb{R}$, i.e. only ε may be complex here, hence the last equation admits exactly three types of solutions:

- $\varepsilon = \sqrt[3]{\frac{\alpha}{4}\frac{k_0}{\pi}}\delta^{4/3}$ (a real solution corresponding to the spectrum)
- $\varepsilon = \mathrm{e}^{\pm\mathrm{i}\frac{2}{3}\pi}\sqrt[3]{\frac{\alpha}{4}\frac{k_0}{\pi}}\delta^{4/3}$ (imaginary solutions corresponding to resonances).

Let us remark that since (4.1) has a symmetry with respect to the complex conjugation of k, the imaginary solution comes in pairs. This is why we find pairs of curves outside the real plane, conventionally just one of them is associated with a resonance.

Returning to properties of eigenvalues in a fixed spectral gap, we have so far demonstrated that each real curve describing a solution of (4.1) is a graph of a function analytic except at the singular points, cf proposition 4.2. Furthermore, at each singular point only one pair of branches meets (with respect to the variable ϑ); it follows that there is exactly one solution in each spectral gap *closure*. Assuming for definiteness $\alpha > 0$ we can say that the complete graph of solutions of (4.1) has the following structure:

- It consists of curves that are analytic and not intersecting, except at the points $(\vartheta, k) = \left(\frac{n+1-2\ell}{n}\pi, n\right)$, where $n \in \mathbb{N}$, $\ell \in \mathbb{N}$, $\ell \leqslant \left[\frac{n+1}{2}\right]$; these are the only ramification points.
- The real curves branches join the points $\left(\frac{n+1-2\ell}{n}\pi, n\right)$ and $\left(\frac{n+1-2\ell-2}{n}\pi, n\right)$, i.e. the consecutive points on the lines $k = n \in \mathbb{N}$.
- The curves branches outside the plane $\Im(k) = 0$ join the points $\left(\frac{\ell}{n-\ell}\pi, n-\ell\right)$ and $\left(\frac{\ell+1}{n-\ell-1}\pi, n-\ell-1\right)$, i.e. the consecutive points laying on the hyperbolas $(\vartheta+\pi)\cdot k = n\cdot\pi$, $k \in \mathbb{R}$, $n \in \mathbb{N}$, n odd, cf figure 7.

Furthermore, we have seen that the behaviour of eigenvalues in the vicinity of the singular points is as follows,

$$k \approx k_0 + \sqrt[3]{\frac{\alpha}{4}\frac{k_0}{\pi}}|\vartheta - \vartheta_0|^{4/3},$$

and this is valid for in the particular case $\vartheta_0 = 0$, $k_0 \in \mathbb{N}$, as well provided the band edge k_0 is odd.

However, H^+ has an eigenvalue near $\vartheta_0 = 0$ also in the gaps adjacent to even numbers. In these cases the curve starts at the point $(0, k_0)$ for k_0 being the solution of $\left|\cos k\pi + \frac{\alpha}{4k}\sin k\pi\right| = 1$ in $(n, n+1)$, n even. The asymptotic behaviour of k for ϑ close to zero is then different, namely:

Theorem 5.1. *Suppose that $n \in \mathbb{N}$ is even and k_0 is as described above, i.e. k_0^2 is the right endpoint of the spectral gap adjacent to n^2. Then the behaviour of the solution of (4.1) in the neighbourhood of $(0, k_0)$ is given by*

$$k = k_0 - C_{k_0,\alpha}\cdot\vartheta^4 + \mathcal{O}(\vartheta^5),$$

where $C_{k_0,\alpha} := \frac{k_0^2}{8\pi}\cdot\left(\frac{\alpha}{4}\right)^3 (k_0\pi + \sin k_0\pi)^{-1}$.

Proof. The argument is straightforward, it suffices to use Taylor expansions in (4.1). □

The analogous asymptotic behaviour applies to k^2, the energy distance of the eigenvalue from the band edge is again proportional to ϑ^4 in the leading order. Note that this is true in any spectral gap, but of course, the error term depends in general on the gap index.

We refrain from discussing in detail the odd part H^- of the Hamiltonian. The corresponding results are practically the same, the only difference is that the roles of the even and odd gaps are interchanged.

Most of what we have discussed above modifies easily to the case of attractive coupling with the obvious changes: for $\alpha < 0$ the spectral gaps lay now *below* the numbers n^2, $n \in \mathbb{N}$. Of particular interest is the spectral gap adjacent to the value one, because with the increase of $|\alpha|$ its lower edge moves towards zero and may become negative for $|\alpha|$ large enough. The even part H^+ has similar properties as before: the eigenvalue curve goes from $(0, 1)$ to (π, k_0), where $k_0 \in (0, 1)$, and there two complex conjugated branches with $\Re(k) > 0$ one of which describes a resonance.

However, the odd part H^- requires a more detailed examination. We know that there is an eigenvalue curve going to the point $[\pi, 1]$. If the entire spectral gap is above zero, this curve joins it with $\left[0, k_0^2\right]$, where k_0^2 is the lower edge of the gap. On the other hand, if $|\alpha|$ is large enough the eigenvalue curve starts from $[0, -\kappa_0]$, where $-\kappa_0^2$ is again the lower gap edge; to show that even in this case the curve joins the points $[0, -\kappa_0]$ and $[\pi, 1]$ analytically, it suffices to prove that the solutions of (4.1) with the negative sign preserves analyticity when it crosses the line $k^2 = 0$.

The spectral condition (3.13) for H^- is valid for $k \neq 0$. If we put all terms to the left-hand side denoting it as $\mathcal{G}^-(\vartheta, k)$, i.e.

$$\mathcal{G}^-(\vartheta, k) = -\cos k\vartheta + \cos k\pi - \frac{\sin^2 k\pi}{\frac{\alpha}{4k}\sin k\pi \pm \sqrt{\left(\cos k\pi + \frac{\alpha}{4k}\sin k\pi\right)^2 - 1}}$$

with the sign in the denominator properly chosen, we have $\lim_{k\to 0}\mathcal{G}^-(\vartheta, k)k^{-l} = 0$ for $l = 0, 1$ while for $l = 2$ the limit is real-valued and non-vanishing. It follows that to find the behaviour at the crossing point one has to examine the function given implicitly by $\tilde{G}(\vartheta, k) = 0$, where

$$\tilde{G}(\vartheta, k) = \begin{cases} \dfrac{\mathcal{G}^-(\vartheta, k)}{k^2} & \text{for} \quad k \neq 0 \\ \lim\limits_{k\to 0}\dfrac{\mathcal{G}^-(\vartheta, k)}{k^2} & \text{for} \quad k = 0. \end{cases}$$

This is continuous and it can be easily checked that it has continuous partial derivatives with respect to ϑ and k in the neighbourhood of any solution of $\tilde{G}(\vartheta, k) = 0$ with $k = 0$. In

particular, the derivative w.r.t. ϑ equals $k^{-1}\sin k\vartheta$ for all $k \neq 0$, thus at a point $[\vartheta_0, 0]$ solving $\tilde{G}(\vartheta, k) = 0$ we have

$$\frac{\partial \tilde{G}(\vartheta_0, 0)}{\partial \vartheta} = \lim_{k\to 0} \frac{\sin k\vartheta_0}{k} = \vartheta_0 \neq 0,$$

in other words, the solution of $\tilde{G}(\vartheta, k) = 0$ is analytic also at the point $[\vartheta_0, 0]$. Needless to say, this claim which we have checked directly here can also be obtained by means of the analytic perturbation theory [Ka66].

Finally, note that by proposition 4.2 the solutions of (4.1) with both the positive and negative signs are analytic in the whole open half-plane $\Re(k) < 0$, and consequently, no resonance curves can be found there.

6. Concluding remarks

We have reasons to believe that the spectral and resonance properties due to geometric perturbations of the considered type hold much more generally. In this paper we have decided, however, to treat the present simple example because it allowed us to find a rather explicit solution to the problem.

The problem can be viewed from different perspectives. As an alternative one may interpret the chain graph as a *decoration* of a simple array-type graph, or if you wish, the Kronig–Penney model, in the sense of [AI00, Ku05]. The results of the paper then say that *a local modification* of the decoration can produce a discrete spectrum in the gaps and the other effects discussed here.

It is also interesting to draw a parallel between the quantum graphs discussed here and *quantum waveguides*, i.e. Laplacians in tubular domains. Although the nature of the two systems is very different, they nevertheless share some properties, in particular, the existence of bound states below the essential spectrum threshold due to a local bend. This effect is well studied for Dirichlet quantum waveguides where it is known for a gentle bend the binding energy is proportional to the fourth power of the bending angle [DE95], i.e. it has exactly the same behaviour as described by theorem 5.1.

Bent quantum waveguides with mixed (or Robin) boundary conditions were also studied [Ji06] and it was shown that the effect of *binding through bending* is present for any repulsive boundary. In our case an eigenvalue below the lowest band exists whenever $\alpha \neq 0$ which inspires another look at the waveguide case. It appears that the argument of [Ji06] works again and proves the existence of curvature-induced bound states in all cases except the Neumann boundary which is an analogue of the case $\alpha = 0$ here.

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