Spectral and Scattering Problems for Differential Operators on Quantum Star Graphs

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MUHAMMAD DANISH ZIA
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Department of Mathematics
Syed Babar Ali School of Science and Engineering
Lahore University of Management Sciences
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DEDICATED

TO

MY FAMILY

Abstract

Spectral theory is a generalization of ideas of eigenvalues and eigenvectors of square matrices to broader classes of linear operators defined in a variety of infinite dimensional vector spaces. Spectrum of non-compact quantum star graphs, star shaped metric graph equipped with differential operators and set of vertex conditions, is studied. The selection of vertex or boundary conditions play a vital role in making the operators self-adjoint as well as ensuring that edges are connected or coupled with each other. Generally, a closed and densely defined self-adjoint linear differential operator defined on a separable Hilbert space has real spectrum which consists of a set of negative eigenvalues with finite multiplicity and a continuous part covering the positive semi-axis. The number of negative eigenvalues are finite if the potential function(s) are rapidly decaying at the boundary or a countable infinite set if the potential decays slowly with zero as the only accumulation point. In case of complex-valued potential the corresponding non-selfadjoint graph has complex eigenvalues.

For Schrödinger operators we develop trace formulas for resolvent difference of perturbed and unperturbed operators. Which lead to explicit expressions for perturbation determinant, Levinson's formula and spectral shift function for star shaped quantum graphs. These mathematical objects are of central importance in the study of scattering problems. Moreover, among many spectral problems associated with differential operators, one is, to find the bounds on the series of moments of negative eigenvalues in terms of potentials and boundary parameters of the operator. We derive sharp upper bounds for a fourth order differential operator with two real-valued potentials on semi-axis with the "Generic" three parameters self-adjoint boundary conditions at zero. Such bounds are commonly known as Lieb-Thirring inequalities. We also obtain bounds for eigenvalues of star graphs with complex valued potentials having n edges with δ and δ' vertex conditions. For two edge graphs sharp and explicit bounds on the complex eigenvalues are obtained in terms of potential and boundary parameters.

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List of Papers

The following papers are included in this thesis.

PAPER I: **Sharp spectral inequalities for fourth order differential operators on semi-axis.** MD Zia and M Usman, *Mathematical Physics, Analysis and Geometry* 22(4) pp.1-13 (2019).

PAPER II: **A trace formula, perturbation determinant and Levinson's theorem for a class of star graphs.** MD Zia and M Usman, submitted (2021).

PAPER III: **Perturbation determinant and Levinson's formula for Schrödinger operators with generalized point interaction.** MD Zia and M Usman, submitted (2021).

PAPER IV: **Eigenvalue bounds for quantum star graphs with complex potentials.** MD Zia and M Usman, (manuscript under preparation).

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Chapter 1

Introduction

This thesis is devoted to the study of some aspects of spectral and scattering theory of quantum star graphs. A quantum star graph Γ is a metric graph with finitely many edges of infinite length connected at a single vertex. Generally, a quantum graph is a triplet (Γ, H, S) with H a differential operator and S a set of vertex conditions. We are interested in the mathematical objects associated with the discrete spectrum of second and fourth order differential operators defined on quantum star graph. Our objective in this chapter is to fix the notation, introduce the reader to the main ideas, and review some of the known results.

The chapter is organized as follows. In Section 1, we introduce the quantum graphs. Sections 2-6 introduce and discuss the main objects of our study including perturbation determinant, spectral shift function, Levinson's formula, Lieb-Thirring inequalities and eigenvalue bounds.

1.1 Quantum graphs

A quantum graph is a triplet consisting of

- a metric graph (defined below)
- a differential operator acting on the edges and
- some boundary or matching conditions at the vertices.

Metric graphs

In discrete mathematics, a graph G consists of two sets, the set of vertices $V = \{v_i\}$ and the set of edges $E = \{e_i\}$. Each edge e_i is identified with a pair of vertices it is connecting.

The length of edges do not play any role. One can generalize discrete graphs by assigning a length to each edge or identifying each edge with an interval of the real line. In this way, a distance function or a metric can be defined on such graphs. The metric can be the length of smallest path connecting two points on the graph. The two points are not necessarily vertices of the graph. This new continuous version, instead of discrete, of the graph is called a metric graph. Edges of infinite length are usually identified with the interval $[0, \infty)$ and are called open edges. Such edges are attached to only one vertex at $x_e = 0$. A metric graph with one or more open edges is called a non-compact metric graph. A star graph is a metric graph of finitely many open edges connected at a single vertex zero.

Definition 1.1.1. *A graph Γ is called a metric graph, if each edge e connecting vertices v_i and v_j of Γ is considered as an interval $[0, l_e]$. The coordinate on edge e is denoted as x_e. The vertex v_i is at $x_e = 0$ and v_j at $x_e = l_e$.*

The above definition makes it possible to consider the functions on metric graphs and define spaces of functions. The coordinate x_e along the edge e enables us to define some Lebesgue measure dx_e on Γ. With this measure we can define the space of square integrable functions on metric graphs.

Definition 1.1.2. *The Hilbert space of all square integrable functions on Γ is denoted by $L^2(\Gamma)$ and consists of functions ψ defined on Γ and satisfying*

$$||\psi||^2_{L_2(\Gamma)} := \sum_{e \in E} ||\psi||^2_{L_2(e)} < \infty.$$

This means that $L^2(\Gamma)$ is orthogonal direct sum of $L_2(e)$. In a similar fashion one can define any other space of functions on Γ.

The operators

In this thesis we consider second and fourth order differential operators defined on a domain of functions from the Hilbert space $L_2(\Gamma)$, where Γ is a star graph. Specifically we are interested in the Schrödinger operators $-\Delta + V$ and the fourth order operators $(-\Delta)^2 + \partial(U\partial) + V$.

The dynamics of particles or waves traveling along any axis are usually described by a particular type of a differential operator. The most commonly studied operators on graphs are given by the following differential expressions:

- The Laplace operator

$$H_0 := -\frac{d^2}{dx^2}.$$

- The Schrödinger operator
$$H_V := -\frac{d^2}{dx^2} + V(x).$$
- The perturbed bi-Laplacian
$$\mathbb{H}_V := \frac{d^4}{dx^4} + V(x)$$
or more generally
$$\mathbb{H}_{U,V} := \frac{d^4}{dx^4} + \frac{d}{dx}\left(U(x)\frac{d}{dx}\right) + V(x).$$

Vertex conditions

The above operators and the Hilbert space $L^2(\Gamma)$ do not give any information about the connectivity of different edges with each other. The connectivity of a graph is therefore established by prescribing vertex or matching conditions. Moreover, the vertex conditions are also necessary to ensure that an operator is self-adjoint. Specifically, the role of vertex conditions is:

- to connect the functions on different edges of the graph and
- to make the differential operator acting on Γ self-adjoint.

Let Γ be a star graph with finitely many edges e_j joined at a single vertex $\{v\}$ and consider the Schrödinger operator H_V on Γ with a real-valued potential function V. For $\psi \in L^2(\Gamma)$ we denote the restriction of ψ on edge e_j by ψ_j. At a vertex v, $\psi(v)$ is denoted as a column vector

$$\psi(v) := (\psi_1(v), \ldots, \psi_n(v))^T.$$

If ψ is continuous on Γ then all components have the same value. Similarly we can define

$$\psi'(v) := (\psi_1'(v), \ldots, \psi_n'(v))^T,$$

as a column vector of derivatives in the outward direction on the edges attached to v.

The operator H_V can be made self-adjoint by considering functions from the space $W^{2,2}(\Gamma\backslash\{v\})$ satisfying certain vertex conditions involving $\psi(v)$ and $\psi'(v)$. The most general form of such conditions can be expressed in terms of two $n \times n$ matrices A_v and B_v as

$$A_v\psi(v) + B_v\psi'(v) = 0. \tag{1.1.1}$$

To ensure that the number of independent vertex conditions are equal to the degree n of vertex, the matrices must satisfy maximal rank condition, which is

$$\text{Rank}(A_v, B_v) = n. \tag{1.1.2}$$

The Schrödinger operator acting on Γ is self-adjoint if and only if, the matrix product $A_v B_v^*$ is self-adjoint along with the conditions (1.1.1) and (1.1.2). There are several other equivalent formulations for the most general self-adjoint vertex conditions, see for example [3, 5, 4, 41, 42].

In case of a vertex of degree two the most general form of properly connecting self-adjoint vertex conditions are given by

$$\begin{bmatrix} \psi_1(0) \\ \psi_1'(0) \end{bmatrix} = \mathcal{A} \begin{bmatrix} \psi_2(0) \\ \psi_2'(0) \end{bmatrix} \tag{1.1.3}$$

where $\mathcal{A} = e^{i\phi} \begin{bmatrix} a & b \\ c & d \end{bmatrix}$ and $\psi = (\psi_1, \psi_2)^T \in L^2([0,\infty)) \oplus L^2([0,\infty))$ and the real parameters $\phi \in [-\pi/2, \pi/2]$, $a, b, c, d \in \mathbb{R}$ satisfying $ad - bc = -1$. The above conditions are commonly known as the generalized point interaction, first introduced by Šeba [89]. There are several other equivalent formulations for the generalized point interaction, see for example [25] and references therein.

Examples of self-adjoint vertex conditions

Here, we enlist the most commonly used self-adjoint vertex conditions. Starting with the following δ-conditions with strength a at a vertex $v = 0$

$$\begin{aligned} \psi(0) := \psi_1(0) = \cdots = \psi_n(0), \\ \sum_{j=1}^{n} \psi_j'(0) = a\psi(0). \end{aligned} \tag{1.1.4}$$

This condition can be considered analogous to the conditions for the Schrödinger operator considered on a real line with δ-type potential [6]. When $a = 0$, this condition becomes the well known Kirchhoff condition. The condition (5.2.3) makes the operator H_V self-adjoint if and only if $a \in \mathbb{R}$.

Another most frequently used vertex conditions are the Dirichlet vertex conditions. These conditions require that the value of the function must vanish at the vertex when

approaching towards it from any edge. This condition can be described as

$$\begin{aligned} \psi(0) := \psi_1(0) = \cdots = \psi_n(0), \\ \psi(0) = 0. \end{aligned} \tag{1.1.5}$$

The Dirichlet vertex conditions (1.1.5), may seem different then the δ-conditions (5.2.3), but in fact they are the limiting case of (5.2.3) and can be obtained by dividing second sub-condition of (5.2.3) by a and letting $a \to \infty$. The Dirichlet vertex conditions are also the example of decoupling vertex conditions because they separate the edges joined at vertex. If the Dirichlet vertex conditions are applied to a vertex then the Schrödinger operator on the whole graph Γ becomes the direct sum of Schrödinger operators acting on separated edges with the Dirichlet vertex condition at end. Hence, the shape of graph becomes insignificant. The spectrum of the graph becomes the union of the spectrum of the separated edges.

If we interchange the role of function values and its derivative values in conditions (5.2.3), we get new conditions known in literature as δ'-conditions, defined as:

$$\begin{aligned} \psi'(0) := \psi_1'(0) = \cdots = \psi_n'(0), \\ \sum_{j=1}^{n} \psi_j(0) = b\psi'(0). \end{aligned} \tag{1.1.6}$$

The conditions (1.1.6) are self-adjoint if and only if, $b \in \mathbb{R}$.

The following two conditions were proposed as an alternative to δ and δ' conditions by Exner in [23], see also [83]

$$\begin{aligned} \psi_j(0) - \psi_k(0) = d(\psi_j'(0) - \psi_k'(0)), \quad j,k = 1,\ldots,n, \\ \sum_{j=1}^{n} \psi_j'(0) = 0. \end{aligned} \tag{1.1.7}$$

We call these conditions as $\hat{\delta}$-conditions. If we interchange the role of function values and its derivative values in conditions (1.1.7), we get the following conditions

$$\begin{aligned} \psi_j'(0) - \psi_k'(0) = c(\psi_j(0) - \psi_k(0)), \quad j,k = 1,\ldots,n, \\ \sum_{j=1}^{n} \psi_j(0) = 0. \end{aligned} \tag{1.1.8}$$

These conditions become analog to δ'-conditions when we set strength to zero. Therefore, we denote these conditions as $\hat{\delta}'$-conditions.

In Chapter 4, we consider fourth order differential operator $\mathbb{H}_{U,V}$ on the half line with the following "Generic" three parameter family of self-adjoint boundary conditions (see [96])

$$\varphi''(0) = \sigma_0\varphi(0) + \sigma_1\varphi'(0),$$
$$\varphi'''(0) = -\sigma_2\varphi(0) - \sigma_0\varphi'(0),$$

σ_0, σ_1 and σ_2 are all real parameters.

Spectrum

For a linear operator H defined on a Hilbert space $\mathcal{H}$ the resolvent set $\rho(H)$ of the operator H is defined to be the set of all $\lambda \in \mathbb{C}$ such that $H - \lambda\mathbb{I}$ has a bounded inverse in $\mathcal{H}$. The complement of $\rho(H)$ in $\mathbb{C}$ is called the spectrum of H. Spectrum is real if the operator is self-adjoint.

Typically, for a self-adjoint Schrödinger operator $H = -\Delta + V$ on a star graph Γ the spectrum has two parts, i.e., continuous part which covers the whole positive semi axis and the discrete part having negative eigenvalues. The total number of negative eigenvalues is finite if the potential V decays fast i.e. either V is compactly supported or $\int_\Gamma (1+|x|)V(x)dx < \infty$. It is countably infinite with zero as the only accumulation point, if it decays slowly.

1.2 Scattering on star graph

We start by considering a simplest star graph with single edge and a single vertex, i.e. real half-line $\mathbb{R}^+ = [0, \infty)$ and discuss some known results. Consider the Hamiltonian

$$H := -\frac{d^2}{dx^2} + V(x),$$

with boundary condition $u(0) = 0$, where $V(x)$ is real-valued and represents a compactly supported potential function. The potential free operator with same boundary condition is denoted and defined as

$$H_0 := -\frac{d^2}{dx^2}.$$

First we consider the corresponding eigenvalue problem in the form of following ordinary differential equation with the Dirichlet condition

$$\begin{aligned} u''(x) - V(x)u(x) &= -\kappa^2 u(x), \qquad \kappa \in \mathbb{C}, x > 0, \\ u(0) &= 0, \end{aligned} \tag{1.2.1}$$

where derivatives in x are denoted by $'$(prime). We consider two types of solutions of this differential equation, one denoted by $\phi(x,\kappa)$, which satisfies the following conditions

$$\phi(0,\kappa) = 0, \quad \phi'(0,\kappa) = 1,$$

is called the regular solution and the other one denoted by $f(x,\kappa)$ satisfying the asymptotic

$$f(x,\kappa) \sim e^{ix\kappa}, \quad x \to \infty,$$

is called the Jost solution. Their Wronskian is defined as

$$w(\kappa) := w(\phi(\cdot,\kappa), f(\cdot,\kappa)) = \phi'(x,\kappa)f(x,\kappa) - \phi(x,\kappa)f'(x,\kappa).$$

It is independent of x and is known as the Jost function. Further, we denote the resolvent of the operator H by $R(z)$ and the resolvent of $H_0(z)$ by $R_0(z)$. The following theorem represents the formula for trace of difference of resolvents on half line, for the Dirichlet boundary conditions in terms of Jost function.

Theorem 1.2.1 ([97], Proposition 5.3)**.** *If the potential function $V(x)$ satisfies the condition*

$$\int_0^\infty |V(x)|dx < \infty.$$

Then,

$$\operatorname{Tr}(R(z) - R_0(z)) = -\frac{\dot{w}(\kappa)}{2\kappa w(\kappa)}, \qquad \operatorname{Im}\kappa > 0,$$

where derivatives in κ are denoted by $\cdot$ (dot).

S. Demirel and M. Usman in [19], studied the same problem with the Robin boundary condition $u'(0) = \gamma u(0)$, where $\gamma \in \mathbb{R}$. The parameter γ describes the strength of the interaction of the particle with the boundary. Negative γ correspond to an attractive interaction and positive γ to a repulsive one. An analog of the above theorem for the case of Robin boundary conditions is stated below.

Theorem 1.2.2 ([19], Theorem 1.1). *Let* $\int_0^\infty |V(x)|dx < \infty$ *then*

$$\mathrm{Tr}(R(z) - R_0(z)) = \frac{1}{2\kappa}\left(\frac{\dot{w}(\kappa)}{w(\kappa)} + \frac{i}{\gamma - i\kappa}\right), \quad \kappa = z^{1/2}, \quad \mathrm{Im}\,\kappa > 0.$$

We now consider the scattering problem on a star shaped graph with finitely many edges e_j of infinite length and denote it by Γ. We follow the results obtained in [33]. Further literature on scattering problem for quantum graphs can be found in [27, 33, 34, 40]. Consider

$$-U''(x) + V(x)U(x) = ZU(x), \qquad Z = \kappa^2 \in \mathbb{C}, \quad x \in \Gamma. \tag{1.2.2}$$

Let $\psi_i(x) = \{\psi_{i,1}(x_1, \kappa), \ldots, \psi_{i,n}(x_n, \kappa)\}, i = 1, \ldots, n$ be the solution of (1.2.2). These solutions is called a scattering solution if it solves (1.2.2) with some vertex condition and has following asymptotes at infinity

$$\begin{aligned}
\psi_{i,j}(x_j, \kappa) &= A_{i,j}(\kappa)e^{ix_j\kappa} + o(1), x_j \to \infty, i \neq j,\\
\psi_{i,i}(x_i, \kappa) &= B_{i,i}(\kappa)e^{ix_i\kappa} + e^{-ix_i\kappa} + o(1), x_i \to \infty, i = 1, \ldots, n,
\end{aligned}$$

where $A_{i,j}(\kappa)$ are called the transmission coefficients and $B_{i,i}(\kappa)$ are called the reflection coefficients. A matrix with its diagonal entries as reflection coefficients and off-diagonal entries as transmission coefficients is called the scattering matrix and is denoted by $S(\kappa)$. The study of a scattering problem is incomplete without considering the irregular solutions of (1.2.2) also known as Jost solutions, which satisfy the following integral equations

$$\begin{aligned}
f_{1,i}(x_i, \kappa) &= e^{ix_i\kappa} - \int_{x_i}^{\infty} \kappa^{-1}\sin((x_i - y_i)\kappa) f_{1,i}(y_i, \kappa)V_i(y_i)dy_i,\\
f_{2,i}(x_i, \kappa) &= e^{-ix_i\kappa} - \int_{0}^{x_i} \kappa^{-1}\sin((x_i - y_i)\kappa) f_{2,i}(y_i, \kappa)V_i(y_i)dy_i,
\end{aligned}$$

with asymptotic behavior, when $x_i \to \infty$ as

$$f_{1,i}(x_i, \kappa) \sim e^{ix_i\kappa} + o(1), \qquad f_{2,i}(x_i, \kappa) \sim a_i(\kappa)e^{-ix_i\kappa} + b_i(\kappa)e^{ix_i\kappa} + o(1),$$

where

$$\begin{aligned}
a_i(\kappa) &= 1 - \frac{1}{2i\kappa}\int_0^\infty e^{iy_i\kappa} f_{2,i}(y_i, \kappa)V_i(y_i)dy_i,\\
b_i(\kappa) &= \frac{1}{2i\kappa}\int_0^\infty e^{-iy_i\kappa} f_{2,i}(y_i, \kappa)V_i(y_i)dy_i.
\end{aligned}$$

The solutions $f_{1,i}(x_i, \kappa), f_{2,i}(x_i, \kappa)$ are same as the Jost solutions of the Schrödinger operator for the whole line with zero potential on the negative axis and $V_i(x_i)$ for $x \geq 0$.

For a star shaped graph with 3 edges, the solution $\psi_1(x,\kappa)$ is defined as follows:

$$\begin{aligned}
\psi_{1,1}(x_1,\kappa) &= \overline{f_{1,1}(x_1,\kappa)} + B_{1,1}(\kappa) f_{1,1}(x_1,\kappa),\\
\psi_{1,2}(x_2,\kappa) &= A_{1,2}(\kappa) f_{1,2}(x_2,\kappa),\\
\psi_{1,3}(x_3,\kappa) &= A_{1,3}(\kappa) f_{1,3}(x_3,\kappa).
\end{aligned}$$

$\psi_1(x,\kappa)$ is analytic in upper-half plane, where $\mathrm{Im}\kappa > 0$. Jost solution can be used to construct the scattering solutions for $i = 2,\ldots,n$. The resulting transmission and reflection coefficients are given as

$$\begin{aligned}
A_{i,j}(\kappa) &= \frac{2i\kappa}{f_{1,i}(0,\kappa) f_{1,j}(0,\kappa) K(\kappa)}, \quad i \neq j,\\
B_{i,i}(\kappa) &= \frac{2i\kappa}{f_{1,i}^2(0,\kappa) K(\kappa)} - \frac{1}{f_{1,i}(0,\kappa) a_i(\kappa)} + \frac{b_i(\kappa)}{a_i(\kappa)}, \quad i,j = 1,\ldots,n,
\end{aligned}$$

where $K(\kappa) = \sum_{i=1}^{n} \dfrac{f'_{1,i}(0,\kappa)}{f_{1,i}(0,\kappa)}$.

An extensive study for the Schrödinger operator on the whole line with generalization to multi-dimensional operators can be found in [12, 14, 35, 53]. Here, we present some explicit results for trace formulas of resolvent difference found in literature.

Let $H := -\Delta + V$ and $H_0 := -\Delta$, then the resolvents for perturbed and free operator are denoted and defined by $R(z) := (H - z)^{-1}$ and $R_0(z) := (H_0 - z)^{-1}$ respectively. While studying continuous spectrum, an explicit expression for $\mathrm{Tr}(R(z) - R_0(z))$ is of central importance because it provides base for the development of perturbation determinant which eventually lead to explicit expressions for spectral shift function and Levinson's formula.

For a star shaped quantum graphs with n edges joined at a single vertex S. Demirel in [18] considered second order Schrödinger operator with continuity and Kirchhoff type boundary conditions at vertex

$$\psi_1(0) = \ldots = \psi_n(0) := \psi(0), \qquad \sum_{j=1}^{n} \psi'_j(0) = 0.$$

They obtained the following expression

Theorem 1.2.3 ([18], Theorem 1.1)**.** *Let Γ be a star graph equipped with continuity and Kirchhoff conditions at zero and assume that $\int_{e_j} |V(x_j)| dx_j < \infty$, $e_j = [0,\infty)$ is satisfied for $1 \leq j \leq n$. Then, for the Schrödinger operator on $L_2(\Gamma)$ the following trace formula holds,*

$$\mathrm{Tr}(R_\Gamma(z) - R_{0\Gamma}(z)) = \frac{1}{2\kappa}\frac{d}{d\kappa} \ln\left(\frac{K(\kappa)}{\kappa} \prod_{j=1}^{n} w_j(\kappa)\right), \quad \mathrm{Im}\,\kappa > 0,$$

where $K(\kappa) = \sum_{j=1}^{n} \frac{f_j'(0,\kappa)}{f_j(0,\kappa)}$ *and* $w_j(\kappa) = f_j(0,\kappa)$.

Perturbation determinant

Krein (see e.g. [58, 59, 60, 61, 62]) introduced the concept of perturbation determinant for operators in infinite dimensional Hilbert spaces. Kuroda in [64] also independently developed the perturbation determinant, which on one side plays an important role in the study of spectral shift functions [10, 11] and on the other side is used to investigate certain other characteristics of non self-adjoint operators like completeness of root vectors etc [58, 59].

Perturbation determinant (modified) for a pair of self-adjoint Schrödinger operator $H = -\Delta + V$ and $H_0 = -\Delta$ is defined as

$$D(z) := \det(I + \sqrt{V} R_0(z) \sqrt{|V|}), \qquad z \in \rho(H_0),$$

where $\sqrt{V} = \mathrm{sgn} V \sqrt{|V|}$. If $V \in L^1([0,\infty))$ then $D(z)$ is well-defined because $\sqrt{|V|R_0(z)}$ is a Hilbert-Schmidt operator and thus $\sqrt{V}R_0(z)\sqrt{|V|}$ belongs to trace class. Some useful facts about the perturbation determinant that can be found e.g. in [58], are as follows.

- $D(z)$ is holomorphic in $\mathrm{Im}(z) > 0$
- $D(z)$ has a zero in z of order r if and only if, z^2 is an eigenvalue of multiplicity r of H.
- $\mathrm{Tr}(R(z) - R_0(z)) = \frac{\frac{d}{dz} D(z)}{D(z)}$.

In literature presented in [49, 37, 80, 90], it is shown that a perturbation determinant which is also a Fredholm determinant in an infinite dimensional space becomes a Wronski determinant, which is a simple determinant in a finite dimensional space. From theorem 1.2.1, it was found that Jost function $w(\kappa)$ plays the role of perturbation determinant in Dirichlet case, and from theorem 1.2.2, it was found that under Robin conditions the perturbation determinant not only depends on Jost function but also depends on the parameter of the conditions. In that case the perturbation determinant is given by

$$D(z) = \frac{w(\sqrt{z})}{\gamma - i\sqrt{z}}.$$

For a star shaped graph equipped with Kirchhoff vertex conditions, the perturbation determinant is given as under

$$D(z) = \frac{K(\sqrt{z})}{in\sqrt{z}} \prod_{j=1}^{n} w_j(\sqrt{z}).$$

Spectral shift function

The notion of the spectral shift function was introduced by physicist I.M. Lifshits in [76]. He considered the finite rank perturbations V of the Laplace operator H_0 and developed the formulas and quantities for the magnitude of eigenvalues shift due to the perturbation. Later, M.G. Krein elaborated the notion of spectral shift function in [58] for more general situation; he showed that for self-adjoint operators H and H_0 with trace class difference, there exists a unique real function $\xi(\lambda; H, H_0)$ (it is called the spectral shift function for the pair $\{H, H_0\}$) such that the following trace formula holds

$$\mathrm{Tr}(f(H) - f(H_0)) = \int_{\mathbb{R}} \xi(\lambda; H, H_0) f'(\lambda) d\lambda, \tag{1.2.3}$$

for all functions $f \in C_0^\infty(\mathbb{R})$. To prove the existence of the spectral shift function, he introduced the concept of perturbation determinant $D(z)$ and proved the inversion formula

$$\xi(\lambda; H, H_0) = \pi^{-1} \lim_{\epsilon \to 0^+} \mathrm{Im}(\ln(D(\lambda + i\epsilon))).$$

Some worthy points to note about that spectral shift function are

- $\xi(\lambda; H, H_0) \in L_1(\mathbb{R})$, which means that it is an equivalence class of Lebeque measurable functions.
- $\xi(\lambda; H, H_0)$ is unique up to a constant for a perturbation V of trace class.
- $\xi(\lambda; H, H_0)$ can be extended in different ways. One way is to develop the function f so that (1.2.3) hold. Another way is to extend the class of perturbations V.

Here we enlist some most simple properties of the spectral shift function. Let H_a, H_b and H_c such that $V_1 := H_b - H_a$ and $V_2 := H_c - H_b$ are bounded linear operators on a Hilbert space. Then for $\lambda \in \mathbb{R}$

$$\xi(\lambda; H_c, H_a) = \xi(\lambda; H_c, H_b) + \xi(\lambda; H_b, H_a).$$

Particularly,

$$\xi(\lambda; H_c, H_a) = -\xi(\lambda; H_a, H_c).$$

Additionally, if $H_b \leq H_c$ then,

$$\xi(\lambda; H_b, H_a) \leq \xi(\lambda; H_c, H_a).$$

Following inequality also holds

$$||\xi(\cdot; H_c, H_a) - \xi(\cdot; H_b, H_a)||_1 \leq ||H_c - H_b||_1.$$

A number of additional properties of the spectral shift function and its applications can be found in [32, 48, 50, 56, 82, 91].

Levinson's formula

Levinson's theorem is a relation between the number of bound states of a quantum mechanical system and an expression related to the scattering part of that system. Its original formulation was established by N. Levinson in [70] in the context of a Schrödinger operator with a spherically symmetric potential $V(r)$, but subsequently numerous authors extended the validity of such a relation in various contexts or for various models.

For a wavefunction to behave nicely at the origin and at the infinity, it is required that the spherically symmetric potential $V(r)$ must satisfy the following asymptotic condition

$$\int_0^\infty r|V(r)|dr < \infty, \tag{1.2.4}$$

and for the Jost function to be analytic in the complex momentum plane of momentum k it is further required that $V(r)$ satisfy

$$\int_0^\infty r^2|V(r)|dr < \infty. \tag{1.2.5}$$

If the condition (1.2.4) is not satisfied, then the Levinson's theorem does not hold. However, the conditon (1.2.5) is additionally required for Jost function's analytic continuity and its a very strong condition for Levinson's theorem. If the conditions (1.2.4) and (1.2.5) are satisfied, then the phase shift $\eta(k)$ at $k = 0$ is related with the number of bound states N as:

$$\eta(\infty) - \eta(0) = (N + 1/2)\pi, \quad \text{if a half bound state occurs}$$

and

$$\eta(\infty) - \eta(0) = N\pi, \quad \text{for all other cases.}$$

This is called the Levinson's theorem for a Schrödinger equation. A half bound state is a zero momentum state in which a wave function is finite but not square integrable.

Different proofs of the Levinson's theorem and its generalization can be found in literature, see for example [7, 79, 81, 93]. Generally, different approaches are adopted in order to prove the Levinson's theorem, some of which are using Jost function, using Green function and by Sturm–Liouville theorem. We will briefly review these techniques.

In [47], Jauch applied the operator formulism method of the Scattering Theory to prove the Levinson's theorem. He claimed that as the potential changes, the total number of eigenstates remains unchanged. In other words, as the potential changes, the scattering state is transformed from the bound state and vice versa. Guang in [39], generalized the Levinson's theorem for Klein-Gordan equation and Dirac equation using the retarded

Green function. Unfortunately, his proof for the relativistic cases had some mistakes. Zhong [101] gave the first correct proof of the Levinson's theorem for the Dirac equation. Yang in [98], considered first order coupled partial differential equations and developed a new version of Sturm-Liouville theorem, this new form made the proof of the Levinson's theorem for Schrödinger equation [100] very simple. Due to this technique, the Levinson's theorem was free from the term $\eta(\infty)$ and $V(r)$ was released to fulfill the condition (1.2.5).

In the remaining part of this section, we present explicit versions of the Levinson's theorem which provide motivation for the development of the Levinson's theorem for the star graphs with different vertex conditions.

Yafaev in [97], considered the scattering problem for the half line and developed the Levinson's theorem for Dirichlet condition which is given as follows:

Theorem 1.2.4 ([97], Theorem 6.1)**.** *Let $\mathcal{N}$ denotes the number of negative eigenvalues of H and $\int_0^\infty (1+|x|)V(x)dx < \infty$ is satisfied. Then*

$$\eta(\infty) - \eta(0) = \begin{cases} \pi\mathcal{N} & if \quad w(0) \neq 0, \\ \pi(\mathcal{N} + 1/2) & if \quad w(0) = 0. \end{cases}$$

The Levinson's theorem for the Robin type boundary condition was developed by Demirel [19] in which it was observed that phase shift depend on the parameter of the boundary condition γ and was given as follows:

Theorem 1.2.5 ([19], Theorem 5.5)**.** *Let $\mathcal{N}$ denotes the number of negative eigenvalues of H and $\int_0^\infty (1+|x|)V(x)dx < \infty$ is satisfied. Then for $w(0) \neq 0$*

$$\eta(\infty) - \eta(0) = \begin{cases} \pi\mathcal{N} & if\gamma > 0, \\ \pi(\mathcal{N} - 1/2) & if\gamma = 0, \\ \pi(\mathcal{N} - 1) & if\gamma < 0 \end{cases}$$

and for $w(0) = 0$

$$\eta(\infty) - \eta(0) = \begin{cases} \pi(\mathcal{N} + 1/2) & if\gamma > 0, \\ \pi\mathcal{N} & if\gamma = 0, \\ \pi(\mathcal{N} - 1/2) & if\gamma < 0. \end{cases}$$

Demirel in [18], considered the star graph with the Kirchhoff vertex conditions and presented the Levinson's theorem as:

Theorem 1.2.6 ([18], Theorem 1.3)**.** *Suppose $\int_{e_j}(1+|x_j|)|V(x_j)|dx_j < \infty$ and let N be the number of negative eigenvalues of H and m be the multiplicity of the resonance at $\kappa = 0$. If $m = 1$, also suppose that $\int_{e_j}(1+x_j^2)|V(x_j)|dx_j < \infty, 1 \leq j \leq n$. Then*

$$\eta(\infty) - \eta(0) = \pi\left(N + \frac{m-1}{2}\right).$$

1.3 Lieb-Thirring inequalities

The upper bounds on the moments of negative eigenvalues are commonly known as Lieb-Thirring inequalities. These inequalities were first developed by E. H. Lieb and W. E. Thirring [75], which bound absolute power sum of negative eigenvalues of the Schrödinger operator in the form of constant multiple of integrals of the potential function. These inequalities generally state that, for a Schrödinger operator in $L^2(\mathbb{R}^d), d \geq 1$, the values $\lambda_0 \leq \lambda_1 \leq \ldots \leq 0$ (not necessarily finite) denote the sequence of negative eigenvalues. For m and d satisfying one of the conditions, $\{m \geq \frac{1}{2}, d = 1\}, \{m > 0, d = 2\}, \{m \geq 0, d \geq 3\}$ there exists a constant $L_{m,d}$, known as Lieb-Thirring constant, which depends only on m and d, such that

$$\sum_{j \geq 0} |\lambda_j|^m \leq L_{m,d} \int_{\mathbb{R}^d} V(x)_-^{m+\frac{d}{2}} dx, \tag{1.3.1}$$

where $V(x)_- := \max\{-V(x), 0\}$. When $m = 0$, (1.3.1) provides bound on total number of negative eigenvalues of the Schrödinger operator.

When proving stability of matter, E.H. Lieb and W.E. Thirring [75] developed (1.3.1) for $m > \frac{1}{2}$ and $d = 1, m > 0, d \geq 2$. T. Weidl proved it for the case $m = 1/2, d = 1$. M. Cwikel [16], Lieb [73] and G.V. Rosenbljum [84] proved the same inequality independently for the case $m = 0, d \geq 3$ by adopting different techniques, which in literature is known as CLR bound. The smallest known value for $L_{0,d}$ is in [73, 72].

If $V(x) \in L^{m+\frac{d}{2}}(\mathbb{R}^d)$, then (1.3.1) can be represented by the Weyl type asymptotic formula

$$\begin{aligned} \lim_{\alpha \to +\infty} \frac{1}{\alpha^{m+\frac{d}{2}}} \mathrm{Tr}\,(-\Delta + \alpha V)_-^m &= \lim_{\alpha \to +\infty} \frac{1}{\alpha^{m+\frac{d}{2}}} \iint_{\mathbb{R}^d \times \mathbb{R}^d} \left(|\kappa|^2 + \alpha V\right)_-^m \frac{dx d\kappa}{(2\pi)^d} \\ &= L_{m,d}^{cl} \int_{\mathbb{R}^d} V_-^{m+\frac{d}{2}} dx. \end{aligned}$$

The constant $L_{m,d}^{cl}$ is also known as classical constant and is defined as

$$L_{m,d}^{cl} = \frac{\Gamma(m+1)}{2^d \pi^{d/2} \Gamma(\frac{d}{2} + m + 1)}, \quad m \geq 0.$$

The constant $L_{m,d}^{cl}$ is finite for all $m \geq 0$, while (1.3.1) is valid only for the particular cases mentioned above. Both the constants are related as follows:

$$L_{m,d} = R_{m,d} L_{m,d}^{cl},$$

where $R_{m,d}$ is a non-increasing, monotone function of m [2]. So, if $R_{\gamma,d} = 1$ for some γ then $L_{m,d} = L_{m,d}^{cl}$ for all $m \geq \gamma$.

An intriguing and generally open problem is to find the sharp constant $L_{m,d}$, particularly to discover those cases wherein $L_{m,d} = L^{cl}_{m,d}$. With the help of Buslaev-Faddeev-Zakharov (BFZ) trace formulae [15, 99], it is found in [75] that $R_{m,d} = 1$ for $m \geq \frac{3}{2}, d = 1$ and $R_{m,d} > 1$ for $d = 1, \frac{1}{2} \leq m < \frac{3}{2}$ [75] or $d \in \mathbb{N}, m < 1$ [43]. From the Berezin-Lieb inequality [9, 71, 67], it is proved that on any arbitrary $I_d \subset \mathbb{R}^d$, $R_{m,d} = 1$, if $m \geq 1$. This technique is adopted in [69] for the matrices of pseudo-differential operators with constant coefficients in $\mathbb{R}^d$ having the Dirichlet boundary conditions. For the subclass of the Schrödinger operators with characteristic functions of finite measure sets taken as potentials, the Lieb constant [73] in the CLR inequality is improved using the BL inequality [66].

In [65], $R_{m,d} = 1$ for $m \geq 1$ and $d \in \mathbb{N}$ is proved for a class of the quadratic potentials. The sharp value for the Lieb-Thirring constant $L_{m,d}$ except for the case $\{d = 1, m \geq \frac{3}{2}\}$ can be found in [45], in which it is shown that $L_{\frac{1}{2},1} = L^{cl}_{\frac{1}{2},1} = \frac{1}{2}$. For $d > 1$, the equation $L_{\frac{3}{2},d} = L^{cl}_{\frac{3}{2},d}$ is proved by A. Laptev and T. Weidl in [69] and for $d = 1$ it is proved in [75].

Lieb and Thirring in [74] initially proved $R_{1,d} \leq 4\pi$, after that a lot of contributions were asserted to enhance the upper bound for $R_{1,d}$ [72, 22, 13, 45, 21]. In 1991, Eden-Foias [22] proved $R_{1,d} \leq \sqrt{3}\pi \approx 1.814$ for $d = 1$, Dolbeault, Laptev and Loss in 2007 [21] extended this result for $d \geq 1$. In 2018, Rupert frank [30] significantly improved $R_{1,d}$. For all $d \geq 1$, the best constant for the Lieb–Thirring inequality satisfies $R_{1,d} \leq 1.456$.

Moving towards the fourth order operators, J. Hoppe, A. Laptey and J. Ostensson in [44] considered the linear fourth order self-adjoint operators $L := \partial^4 + \partial u \partial + v$ with two real valued, rapidly decaying functions u and v.

They factorized the operators L in to two linear second order operators A and A^* as $L := A^*A + E_0$, where E_0 denotes the lowest negative eigenvalue of double multiplicity of the operator L. They also calculated a non-linear functional $Q[u, v]$ that governs the loss or gain of (doubly degenerate) eigenvalues of fourth order differential operators L. By Removing the eigenvalues, they obtained a sharp Lieb-Thirring inequality for a class of operators L, whose negative eigenvalues are of multiplicity two.

Theorem 1.3.1 ([44], Theorem 4.1)**.** *Let the operator L has n negative eigenvalues of multiplicity two. Assume that $Q[u_n, v_n] \geq 0$, where u_n and v_n are obtained by using the removal of eigenvalues. Then*

$$\sum_{j=1}^{n} |E_j|^{7/4} \leq 2L^{cl}_{4,7/4,1} Q[u, v].$$

Following the arguments as in [44], if we commute the two operators A and A^*, we get a new operator L_1, i.e., $AA^* = L_1 - E_0$. This new operator L_1, with new potential

functions u_1 and v_1, satisfies the Dirichlet boundary conditions and is isospectral to the original operator L, except the lowest negative eigenvalue E_0 which does not belong to the spectrum of L_1. Further, one can remove all the negative eigenvalues of the operator L. By adapting the commutation method, our findings are as follows:

- The negative eigenvalues of double multiplicity of the operator L coincide with the negative eigenvalues of double multiplicity of the operator L_1, except for the spectral value of the ground state energy, which does not belong to the spectrum of L_1.

- Let $U, V \in C_0^{\infty}(\mathbb{R}_+)$ and $\{E_j\}_{j=1}^{n}$ be n negative eigenvalues of double multiplicity of the operator L. Assume that $Q[U_j, V_j] \geq 0$, where U_j and V_j are the potentials associated with the operator L_j that one obtains after removing first j eigenvalues of the original operator L, then the following inequality holds

$$\frac{16}{3}|E_1|\sigma_2 L^{cl}_{4,7/4,1} + \sum_{j=1}^{n} |E_j|^{7/4} \leq 2L^{cl}_{4,7/4,1}\left(Q[U,V] + \Omega(\sigma_0,\sigma_1,\sigma_2)\right), \tag{1.3.2}$$

  where, $\Omega(\sigma_0, \sigma_1, \sigma_2)$ is a real valued function. The above inequality is known as Lieb Thirring inequality in literature.

1.4 Bounds on complex eigenvalues

In the recent years, there has been an increasing interest in estimating eigenvalue bounds for the Schrödinger operator having complex-value potential. First effort in this regards was made by L. Spurch accredited in [51]. He proved that any negative eigenvalue λ of the one-dimensional Schrödinger operator H with real valued potential function V satisfies the following inequality

$$|\lambda|^{\frac{1}{2}} \leq \frac{1}{2}\int_{-\infty}^{\infty} |V(x)|\, dx. \tag{1.4.1}$$

If $V(x) = b\delta(x-a)$, where $a \in \mathbb{R}$ and $b > 0$, then (1.4.1) becomes equality. It was observed in [1] that inequality (1.4.1) also holds for all complex eigenvalues in $\mathbb{C}\backslash[0,\infty)$, if V is complex valued potential.

The above result can also be developed for semi-axis. By using (1.4.1) and the variational principle for the self-adjoint operators in $L^2[0,\infty)$ with the Dirichlet boundary conditions, the following inequality holds

$$|\lambda|^{\frac{1}{2}} \leq \frac{1}{2}\int_{0}^{\infty} |V(x)|\, dx, \tag{1.4.2}$$

the constant $\frac{1}{2}$ is sharp but not attainable.

Rupert in [31], observed that, for complex valued potentials, inequality (1.4.2) is not true in general, rather he gave the following inequality:

$$|\lambda|^{\frac{1}{2}} \leq f\left(\cot\left(\frac{\theta}{2}\right)\right) \int_0^\infty |V(x)|\, dx,$$

where $f(v) = \sup_{u\geq 0} \left|e^{ivu} - e^{-u}\right|, v \in \mathbb{R}$. The equality is obtained, when $V(x) = d\delta(x-c)$ where, $d \in \mathbb{C}$ and $c > 0$.

For the higher dimensional Schrödinger operator, we refer to references [29, 68, 85, 86]. In Chapter 5, we developed the estimates on bounds of complex eigenvalues of the non self-adjoint Schrödinger operator acting on a star graph with complex valued potential.

Chapter 2

1D Schrödinger operators with GPI

In this chapter we consider the one dimensional Schrödinger operator with properly connecting generalized point interaction (GPI) at the origin. We derive a trace formula for trace of difference of resolvents of perturbed and unperturbed Schrödinger operators in terms of a Wronskian which results into an explicit expression for perturbation determinant. For large enough real argument, we estimate the trace norm of the resolvent difference of the perturbed and unperturbed Schrödinger operator which leads to a representation for spectral shift function in terms of perturbation determinant. Under certain integrability condition on the potential function, we calculate low energy asymptotics for the perturbation determinant and prove the Levinson's theorem.

2.1 Introduction and main results

Let $H_V^{\mathcal{A}}$ be the Schrödinger operator

$$H_V^{\mathcal{A}} = H_0^{\mathcal{A}} + V, \quad H_0^{\mathcal{A}} = -\frac{d^2}{dx^2} \tag{2.1.1}$$

on the real-line which is realized as a union of two positive semi-axis $e_j = [0, \infty)$, $j = 1, 2$ coupled at 0. The potential function V is assumed to be real-valued and satisfies

$$\int_{e_j} |V_j(x)| dx < \infty, \tag{2.1.2}$$

where, V_j is the restriction of V on e_j, $j = 1, 2$. The operator (2.1.1) is self-adjoint for all functions from the space $L^2([0,\infty)) \oplus L^2([0,\infty))$ satisfying the conditions

$$\begin{bmatrix} \psi_1(0) \\ \psi_1'(0) \end{bmatrix} = \mathcal{A} \begin{bmatrix} \psi_2(0) \\ \psi_2'(0) \end{bmatrix} \tag{2.1.3}$$

where $\mathcal{A} = e^{i\varphi} \begin{bmatrix} a & b \\ c & d \end{bmatrix}$ and $\psi = (\psi_1, \psi_2)^T \in L^2([0,\infty)) \oplus L^2([0,\infty))$ and the real parameters $\varphi \in [-\pi/2, \pi/2]$, $a, b, c, d \in \mathbb{R}$ satisfying $ad - bc = -1$.

The above conditions are commonly known as the generalized point interaction, first introduced by Šeba [89]. There are several other equivalent formulations for the generalized point interaction, see for example [25] and references therein. The free Hamiltonian $H_0^{\mathcal{A}}$ with conditions (2.1.3) describes certain second order differential operators with generalized functions in coefficients. The Schrödinger operator with δ potential of strength α, for instance, corresponds to the unperturbed operator $H_0^{\mathcal{A}}$ with $\varphi = 0$, $a = 1$, $b = 0$, $c = \alpha$ and $d = -1$. Similarly, δ' potential of strength β corresponds to $\varphi = 0$, $a = -1$, $b = \beta$, $c = 0$ and $d = 1$. Differential operators of this kind are closely related to exactly solvable models in quantum mechanics, atomic physics, and acoustics [6, 20].

The present chapter is devoted to deriving explicit expression for perturbation determinant for the pair of operators $H_V^{\mathcal{A}}$ and $H_0^{\mathcal{A}}$ and its relationship with spectral shift function and Levinson's theorem. These mathematical objects play an important role in the study of direct and inverse scattering theory [33, 40, 41, 42] as well as in solid state physics in connection with Friedel sum rule and excess charge [54]. Krěin [58] (see also [64]) introduced the concept of perturbation determinant and it is an important tool in studying trace formulas of higher order. For a detailed study on these topics for Schrödinger operator on the half-line as well as on the whole real line we refer to the monograph [97] (see also reference [19]) and for a quantum star graph we refer to [18]. Our aim in this chapter is to generalize these results for Schrödinger operators on the real-line, which can also be seen as a two edge star graph, satisfying the most general properly connecting self-adjoint matching conditions at zero.

Using Krěin's resolvent formula (see [6] and [24]), we first prove a trace formula that expresses the trace of the difference between the perturbed and corresponding unperturbed resolvents in terms of a Wronskian. This trace formula allows us to derive an explicit expression for the perturbation determinant. The perturbation determinant is an interesting object in the spectral theory of Schrödinger operators, as the zeros of perturbation

determinant coincide with the eigenvalues of the Schrödinger operator and the multiplicity of each eigenvalue is equal to the order of the corresponding zero of the perturbation determinant [5]. Estimate on the trace norm of the resolvent difference of the operators $H_V^{\mathcal{A}}$ and $H_0^{\mathcal{A}}$ obtained in [94] allows one to express the spectral shift function in terms of perturbation determinant. For a real argument, perturbation determinant is used to define the phase shift function. The so called Levinson's formula is derived for the Schrödinger operator $H_V^{\mathcal{A}}$ in terms of its phase shift function. This formula, also called a zero order trace formula gives a relationship between the number of negative eigenvalues and the scattering data via phase shift function.

To state our main results we first consider the half-line Schrödinger operators $H_{e_j}^D = -\frac{d^2}{dx^2} + V_j$, $j = 1, 2$, with Dirichlet boundary condition at 0 and let $H_V^D = H_{e_1}^D \oplus H_{e_2}^D$ denotes the decoupled Schrödinger operator on the whole line. The resolvent $(H_V^D - z)^{-1}$ is denoted by $R_V^D(z)$. Under the condition (2.1.2) the differential equation

$$-u_j'' + V_j u = \kappa^2 u, \quad j = 1, 2$$

has two particular solutions, namely, the regular solution and the Jost solution. The regular solution φ_j is characterized by the conditions

$$\varphi_j(0, \kappa) = 0, \quad \varphi_j'(0, \kappa) = 1$$

and the Jost solution f_j by the asymptotics $f_j(x, \kappa) \sim e^{i\kappa x}$, as $x \to \infty$. We denote the resolvent $(H_V^{\mathcal{A}} - z)^{-1}$ of the perturbed operator $H_V^{\mathcal{A}}$ by $R_V^{\mathcal{A}}(z)$ and the resolvent $(H_0^{\mathcal{A}} - z)^{-1}$ of the unperturbed operator $H_0^{\mathcal{A}}$ by $R_0^{\mathcal{A}}(z)$. Moreover, the (modified) perturbation determinant is defined as

$$D(z) := \det(\mathbb{I} + \sqrt{V} R_0^{\mathcal{A}}(z) \sqrt{|V|}), \quad z \in \rho(H_0^{\mathcal{A}}),$$

where, $\sqrt{V} = \mathrm{sgn} V \sqrt{|V|}$.

Our first main result is the following trace formula for the difference of two resolvents in terms of Jost solutions f_j and their derivatives

Theorem 2.1.1. *If the potential V satisfies* (2.1.2) *then the following trace formula holds*

$$Tr(R_V^{\mathcal{A}}(z) - R_0^{\mathcal{A}}(z)) = -\frac{1}{2\kappa} \left(\frac{d}{d\kappa} \ln \left(\frac{w_1(\kappa) w_2(\kappa) L(\kappa)}{(a-d)\kappa + (b\kappa^2 + c)i} \right) \right), \quad \kappa = z^{1/2}, \quad Im\, \kappa > 0 \tag{2.1.4}$$

where

$$L(\kappa) = a\frac{f_1'(0,\kappa)}{f_1(0,\kappa)} - d\frac{f_2'(0,\kappa)}{f_2(0,\kappa)} + b\frac{f_1'(0,\kappa)f_2'(0,\kappa)}{f_1(0,\kappa)f_2(0,\kappa)} - c$$

and $w_j(\kappa) = f_j(0,\kappa)$, $j = 1, 2$. *Moreover, for* $z \in \rho(H_V)$ *and* $Im\, z^{1/2} > 0$, *the perturbation determinant* $D(\kappa)$ *of the operator* $H_V^{\mathcal{A}}$ *with respect to* $H_0^{\mathcal{A}}$ *is given by*

$$D(z) = \frac{L(\sqrt{z})w_1(\sqrt{z})w_2(\sqrt{z})}{(a-d)\sqrt{z}i - (bz+c)}. \tag{2.1.5}$$

In Section 4 we study the behaviour of $D(z)$ as $|z| \to 0$ and prove the zero order trace formula, commonly known as the Levinson's formula, for the operator $H_V^{\mathcal{A}}$. We will need the following constants:

$$\begin{aligned}
\alpha_1 &= \left(b\left(\frac{f_1'(0,0)}{f_2(0,0)} + \frac{f_2'(0,0)}{f_1(0,0)}\right) - a\frac{f_2(0,0)}{f_1(0,0)} + d\frac{f_1(0,0)}{f_2(0,0)}\right)i, \qquad (2.1.6)\\
\alpha_2 &= af_1'(0,0)f_2(0,0) + bf_1'(0,0)f_2'(0,0),\\
\alpha_3 &= (cf_2(0,0) + df_2'(0,0))\dot{f}_1(0,0),\\
\alpha_4 &= af_1'(0,0)\dot{f}_2(0,0) - d\dot{f}_1(0,0)f_2'(0,0),
\end{aligned}$$

where dot denotes the derivative with respect to κ.

Theorem 2.1.2. *Assume that*

$$\int_{e_j} (1+x)|V_j(x)|\, dx < \infty, \quad j = 1, 2 \tag{2.1.7}$$

and let N *be the number of negative eigenvalues of the operator* $H_V^{\mathcal{A}}$. *Then, the following formula holds*

$$\eta(\infty) - \eta(0) = \begin{cases} \pi\left(N - \dfrac{P-Q}{2}\right), & w_j(0) \neq 0,\ j = 1, 2,\\ \pi\left(N - \dfrac{P-R}{2}\right), & w_1(0) = 0, w_2(0) \neq 0,\\ \pi\left(N - \dfrac{P-S}{2}\right), & w_1(0) \neq 0, w_2(0) = 0,\\ \pi\left(N - \dfrac{P-T}{2}\right), & w_j(0) = 0,\ j = 1, 2. \end{cases}$$

Here, η *is the so-called phase shift function,* P, Q, R, S *and* T *are functions which are*

defined as

$$P = \begin{cases} 0 & c \neq 0 \\ 1 & c = 0, a - d \neq 0 \\ 2 & c = 0, a - d = 0, b \neq 0, \end{cases} \qquad Q = \begin{cases} 0 & L(0) \neq 0 \\ 1 & L(0) = 0, \alpha_1 \neq 0 \\ 2 & L(0) = 0, \alpha_1 = 0, b \neq 0, \end{cases}$$

$$R = \begin{cases} 0 & \alpha_2 \neq 0 \\ 1 & \alpha_2 = 0, \end{cases} \qquad S = \begin{cases} 0 & \alpha_3 \neq 0 \\ 1 & \alpha_3 = 0, \end{cases}$$

$$T = \begin{cases} 0 & b \neq 0 \\ 1 & b = 0, \alpha_4 \neq 0 \\ 2 & b = 0, \alpha_4 = 0, c \neq 0. \end{cases}$$

2.2 Perturbation determinant

Our main purpose in this section is to derive the trace formula (2.1.4) and the explicit expression (2.1.5) for the perturbation determinant of operator $H_V^{\mathcal{A}}$ with respect to H_0 in terms of the Jost solutions f_j and their derivatives f_j'. For this purpose we use the Krein's resolvent formula which allows us to describe the kernel of $R_V^{\mathcal{A}}(z)$ in terms of the kernel of $R_V^D(z)$. More precisely, for $\operatorname{Im}\kappa \geq 0$, the Krein's formula states

$$R_{j,l}^{\mathcal{A}}(x,y;z) := R_{j,l}^D(x,y;z) + \lambda_{j,l} f_j(x,\kappa) f_l(y,\kappa), \quad j,l = 1,2, \quad z = \kappa^2 \in \rho(H_V^{\mathcal{A}}) \cap \rho(H_V^D), \tag{2.2.1}$$

where $R_{j,l}^{\mathcal{A}}$ and $R_{j,l}^D$ denote the kernel of 2×2 matrix integral operators $R_V^{\mathcal{A}}$ and R_V^D, respectively. The values of the coefficients $\lambda_{j,l}$ are given by the following lemma

Lemma 2.2.1. *Let $\psi(x) := \int_0^\infty R(x,y;z)u(y)\,dy$ and $u = (u_1(x), u_2(x))^T \in L^2([0,\infty)) \oplus L^2([0,\infty))$. If $\psi(x)$ satisfies $H_V^{\mathcal{A}}\psi = \kappa^2\psi + u$ and conditions (2.1.3) then $\lambda_{j,l}$ in (2.2.1) are given by*

$$\begin{bmatrix} \lambda_{1,1} & \lambda_{1,2} \\ \lambda_{2,1} & \lambda_{2,2} \end{bmatrix} = \begin{bmatrix} a + b\dfrac{f_2'(0,\kappa)}{f_2(0,\kappa)} & \dfrac{(ad-bc)e^{i\varphi}}{L(\kappa)f_1(0,\kappa)f_2(0,\kappa)} \\ -\dfrac{}{L(\kappa)f_1^2(0,\kappa)} & \\ \dfrac{e^{-i\varphi}}{L(\kappa)f_1(0,\kappa)f_2(0,\kappa)} & b\dfrac{f_1'(0,\kappa)}{f_1(0,\kappa)} - d \\ & -\dfrac{}{L(\kappa)f_2^2(0,\kappa)} \end{bmatrix}$$

where $L(\kappa) = a\frac{f_1'(0,\kappa)}{f_1(0,\kappa)} - d\frac{f_2'(0,\kappa)}{f_2(0,\kappa)} + b\frac{f_1'(0,\kappa)f_2'(0,\kappa)}{f_1(0,\kappa)f_2(0,\kappa)} - c$.

Proof. It is a well-known fact (see for example [18]), that the resolvent of the operator $H^D_{e_j}$ is an integral operator with symmetric kernel

$$R^D_{e_j}(x,y;z) = \frac{\varphi_j(x,\kappa)f_j(y,\kappa)}{w_j(\kappa)}, \qquad x \le y, \qquad \kappa = \sqrt{z}. \tag{2.2.2}$$

Therefore the resolvent R^D_V is a matrix integral operator with kernel

$$R^D_{j,l}(x,y;z) = \delta_{j,l}R^D_j(x,y;z) \qquad j,l = 1,2. \tag{2.2.3}$$

For simplicity, we use the following notation

$$R^{\mathcal{A}}_{j,l}(x,y;z) = R^{\mathcal{A}}_{j,l}, \quad \varphi_j(x,\kappa) = \varphi_j(x), \quad f_j(y,\kappa) = f_j(y) \quad \text{and} \quad w_j(\kappa) = w_j.$$

By substituting (2.2.2) and (2.2.3) into (2.2.1) and expressing it in matrix form we get

$$\begin{bmatrix} R^{\mathcal{A}}_{1,1} & R^{\mathcal{A}}_{1,2} \\ R^{\mathcal{A}}_{2,1} & R^{\mathcal{A}}_{2,2} \end{bmatrix} = \begin{bmatrix} \frac{\varphi_1(x)f_1(y)+w_1\lambda_{1,1}f_1(x)f_1(y)}{w_1} & \lambda_{1,2}f_1(x)f_2(y) \\ \lambda_{2,1}f_2(x)f_1(y) & \frac{\varphi_2(x)f_2(y)+w_2\lambda_{2,2}f_2(x)f_2(y)}{w_2} \end{bmatrix}.$$

Multiplying u from right and using the definition of function ψ the above expression becomes

$$\begin{bmatrix} \psi_1(x) \\ \psi_2(x) \end{bmatrix} = \begin{bmatrix} \int_0^\infty \{\frac{\varphi_1(x)f_1(y)}{w_1}u_1(y) + \sum_{i=1}^2 \lambda_{1,i}f_1(x)f_i(y)u_i(y)\}dy \\ \int_0^\infty \{\frac{\varphi_2(x)f_2(y)}{w_2}u_2(y) + \sum_{i=1}^2 \lambda_{2,i}f_2(x)f_i(y)u_i(y)\}dy \end{bmatrix}$$

which is equivalent to the following system of equations

$$\psi_j(x) = \int_0^\infty \left\{ \frac{\varphi_j(x)f_j(y)}{w_j}u_j(y) + \sum_{i=1}^n \lambda_{j,i}f_j(x)f_i(y)u_i(y) \right\} dy, \qquad j = 1,2.$$

In order to determine $\lambda_{j,l}$ uniquely, we first express conditions (2.1.3) as a system of two equations and first apply the sub-condition

$$\psi_1(0) = e^{i\varphi}(a\psi_2(0) + b\psi_2'(0))$$

on ψ and Dirichlet condition on φ. This yields the following expression

$$\int_0^\infty \left\{ \sum_{i=1}^2 \lambda_{1,i}f_1(0)f_i(y)u_i(y) \right\} dy = \tag{2.2.4}$$

$$e^{i\varphi}\left(a\int_0^\infty \left\{ \sum_{i=1}^2 \lambda_{2,i}f_2(0)f_i(y)u_i(y) \right\} dy + b\int_0^\infty \left\{ \frac{f_2(y)u_2(y)}{f_2(0)} + \sum_{i=1}^2 \lambda_{2,i}f_2'(0)f_i(y)u_i(y) \right\} dy \right).$$

Applying the second sub-condition

$$\psi_1'(0) = e^{i\varphi}(c\psi_2(0) + d\psi_2'(0))$$

on ψ and Dirichlet condition on φ, we obtain

$$\int_0^\infty \left\{ \frac{f_1(y)u_1(y)}{f_1(0)} + \sum_{i=1}^{2} \lambda_{1,i} f_1'(0) f_i(y) u_i(y) \right\} dy = \tag{2.2.5}$$

$$e^{i\varphi} \left(c \int_0^\infty \left\{ \sum_{i=1}^{2} \lambda_{2,i} f_2(0) f_i(y) u_i(y) \right\} dy + d \int_0^\infty \left\{ \frac{f_2(y)u_2(y)}{f_2(0)} + \sum_{i=1}^{2} \lambda_{2,i} f_2'(0) f_i(y) u_i(y) \right\} dy \right).$$

Comparing the coefficients of $u_i(y)f_i(y)$ in (2.2.4) and (2.2.5), we get the following set of equations

$$\begin{aligned}
f_1(0)\lambda_{1,2} - e^{i\varphi}\left(a f_2(0)\lambda_{2,2} - b\left(\frac{1}{f_2(0)} + f_2'(0)\lambda_{2.2} \right) \right) &= 0 \\
f_1(0)\lambda_{1,1} - e^{i\varphi}\left(a f_2(0)\lambda_{2,1} + b f_2'(0)\lambda_{2,1} \right) &= 0 \\
f_1'(0)\lambda_{1,2} - e^{i\varphi}\left(c f_2(0)\lambda_{2,2} - d\left(\frac{1}{f_2(0)} + f_2'(0)\lambda_{2.2} \right) \right) &= 0 \\
\frac{1}{f_1(0)} + f_1'(0)\lambda_{1,1} - e^{i\varphi}\left(c f_2(0)\lambda_{2,1} + d f_2'(0)\lambda_{2,1} \right) &= 0
\end{aligned}$$

We obtain the values of $\lambda_{j,l}$ $j,l = 1,2$ by solving the above set of equations. □

Using (2.2.3) and Lemma (2.2.1) we can express the resolvent kernel of $H_V^{\mathcal{A}}$ given by (2.2.1) as

$$\begin{bmatrix} R_{1,1}^{\mathcal{A}} & R_{1,2}^{\mathcal{A}} \\ R_{2,1}^{\mathcal{A}} & R_{2,2}^{\mathcal{A}} \end{bmatrix} = \begin{bmatrix} R_{e_1}^D - \dfrac{a + b\dfrac{f_2'(0)}{f_2(0)}}{L(\kappa) f_1^2(0)} f_1^2(x) & \dfrac{(ad-bc)e^{i\varphi}}{L(\kappa) f_1(0) f_2(0)} f_1(x) f_2(y) \\ \dfrac{e^{-i\varphi}}{L(\kappa) f_1(0) f_2(0)} f_2(x) f_1(y) & R_{e_2}^D - \dfrac{b\dfrac{f_1'(0)}{f_1(0)} - d}{L(\kappa) f_2^2(0)} f_2^2(x) \end{bmatrix}. \tag{2.2.6}$$

Here, for simplicity, we used the notation $R_{i,j}^{\mathcal{A}}(x,y;\kappa) = R_{i,j}^{\mathcal{A}}$, $R_{e_i}^D(x,y;\kappa) = R_{e_i}^D$ and $f_i(x,\kappa) = f_i(x)$.

For unperturbed operator i.e., when $V_j(x) \equiv 0$, we may let

$$f_j(x,\kappa) = e^{ix_j\kappa} \Rightarrow L(\kappa) = (a-d)i\kappa - \left(b\kappa^2 + c \right).$$

Hence

$$\begin{bmatrix} R^{\mathcal{A}}_{0,(1,1)} & R^{\mathcal{A}}_{0,(1,2)} \\ R^{\mathcal{A}}_{0,(2,1)} & R^{\mathcal{A}}_{0,(2,2)} \end{bmatrix} = \begin{bmatrix} R^{D}_{0,e_1} - \frac{a+i\kappa b}{(a-d)i\kappa-(b\kappa^2+c)}e^{2i\kappa x} & \frac{(ad-bc)}{(a-d)i\kappa-(b\kappa^2+c)}e^{i(x+y+\varphi)\kappa} \\ \frac{1}{(a-d)i\kappa-(b\kappa^2+c)}e^{i(x+y-\varphi)\kappa} & R^{D}_{0,e_2} - \frac{i\kappa b-d}{(a-d)i\kappa-(b\kappa^2+c)}e^{2i\kappa x} \end{bmatrix}. \tag{2.2.7}$$

we now prove Theorem (2.1.1).

Proof of Theorem 2.1.1. The operator difference $R^D_V(z) - R^D_0(z)$ is a trace class operator and the second term on the right hand side of (2.2.1) is a finite rank perturbation. Therefore, the difference $R^{\mathcal{A}}_V(z) - R^{\mathcal{A}}_0$ is a trace class operator. The operator $H^{\mathcal{A}}_V$ can be seen as a particular case of a more general matrix valued Schrödinger operator considered in [94] on the half-line when potential is a diagonal matrix. The fact that $R^{\mathcal{A}}_V(z) - R^{\mathcal{A}}_0$ is trace class also follows from Lemma 9.1 of [94]. Representation (2.2.1) with values of $\lambda_{j,l}$ given by lemma (2.2.1) allows us to compute the trace of the resolvent difference of operators $H^{\mathcal{A}}_V$ and $H^{\mathcal{A}}_0$.

Using (2.2.6) and (2.2.7) the trace of the difference of $R^{\mathcal{A}}_V$ and $R^{\mathcal{A}}_0$ can be written as

$$\begin{aligned} \mathrm{Tr}(R^{\mathcal{A}}_V(z) - R^{\mathcal{A}}_0(z)) = &\sum_{j=1}^{2} \int_0^\infty \left(R^D_{e_j}(x,x,z) - R^D_{0,e_j}(x,x,z) \right) dx \\ &- \int_0^\infty \left(\frac{a + b\dfrac{f_2'(0)}{f_2(0)}}{L(\kappa) f_1^2(0)} f_1^2(x) + \frac{b\dfrac{f_1'(0)}{f_1(0)} - d}{L(\kappa) f_2^2(0)} f_2^2(x) \right) dx \\ &+ \int_0^\infty \left(\frac{(a-d+2i\kappa b)}{(a-d)i\kappa - (b\kappa^2 + c)} e^{2ix\kappa} \right) dx. \end{aligned} \tag{2.2.8}$$

The first term on the right hand side of (2.2.8) is given by (c.f. Remark 1.2 of [18])

$$\sum_{j=1}^{2} \int_0^\infty \left(R^D_{e_j}(x,x,z) - R^D_{0,e_j}(x,x,z) \right) dx = -\frac{1}{2\kappa} \sum_{j=1}^{2} \frac{\dot{w}_j(\kappa)}{w_j(\kappa)}. \tag{2.2.9}$$

To compute the first term in the second integral on the right hand side of (2.2.8) we use the following equation which is true for any arbitrary solutions $u_j(x,\kappa)$ and $v_j(x,\kappa)$ of $H^D_{e_j}\psi_j = \kappa^2\psi_j$

$$u_j(x,\kappa)v_j(x,\kappa) = \frac{(u_j'(x,\kappa)\dot{v}_j(x,\kappa) - u_j(x,\kappa)\dot{v}_j'(x,\kappa))'}{2\kappa}. \tag{2.2.10}$$

If we let $u_j = v_j = f_j$ we obtain

$$\int_0^\infty f_j^2(x,\kappa)dx = \frac{[f_j'(x,\kappa)\dot{f}_j(x,\kappa) - f_j(x,\kappa)\dot{f}_j'(x,\kappa)]_0^\infty}{2\kappa}.$$

If V_j is compactly supported potential then the Jost solution $f_j(x,\kappa) = e^{i\kappa x}$ and hence

$$f_j'(x,\kappa)\dot{f}_j(x,\kappa) - f_j(x,\kappa)\dot{f}_j'(x,\kappa) = ie^{2i\kappa x}.$$

For $\mathrm{Im}\kappa > 0$, $ie^{2i\kappa x} \to 0$ as $x \to \infty$. Therefore, we are left with

$$\begin{aligned}\int_0^\infty f_j^2(x,\kappa)dx &= \frac{f_j(0,\kappa)\dot{f}_j'(0,\kappa) - f_j'(0,\kappa)\dot{f}_j(0,\kappa)}{2\kappa} \\ &= \frac{f_j^2(0,\kappa)}{2\kappa}\frac{d}{d\kappa}\frac{f_j'(0,\kappa)}{f_j(0,\kappa)}.\end{aligned}$$

This implies

$$\begin{aligned}&\int_0^\infty \left(\frac{a + b\dfrac{f_2'(0)}{f_2(0)}}{L(\kappa)f_1^2(0)} f_1^2(x) + \frac{b\dfrac{f_1'(0)}{f_1(0)} - d}{L(\kappa)f_2^2(0)} f_2^2(x) \right) dx \\ &= \frac{1}{2\kappa L(\kappa)} \left(\left(a + b\frac{f_2'(0)}{f_2(0)} \right) \frac{d}{d\kappa}\frac{f_1'(0,\kappa)}{f_1(0,\kappa)} + \left(b\frac{f_1'(0)}{f_1(0)} - d \right) \frac{d}{d\kappa}\frac{f_2'(0,\kappa)}{f_2(0,\kappa)} \right) \\ &= \frac{\dot{L}(\kappa)}{2\kappa L(\kappa)}. \end{aligned} \tag{2.2.11}$$

By a density argument the above result can be extended to all potentials satisfying the condition $\int_0^\infty |V_j(x)|dx < \infty$.

Now it only remains to compute the last integral on the right hand side of (2.2.8), which is

$$\int_0^\infty \left(\frac{(a - d + 2i\kappa b)}{(a-d)i\kappa - b\kappa^2 + c} e^{2ix\kappa} \right) dx = \frac{(a - d + 2i\kappa b)}{2\kappa((a-d)\kappa + (b\kappa^2 + c)i)}. \tag{2.2.12}$$

Substituting values from (2.2.9), (2.2.11) and (2.2.12) in (2.2.8), we get

$$\begin{aligned}\mathrm{Tr}(R_V^{\mathcal{A}}(z)-R_0^{\mathcal{A}}(z)) &= -\frac{1}{2\kappa}\left(\sum_{j=1}^{2}\frac{\dot{w}_j(\kappa)}{w_j(\kappa)}+\frac{\dot{L}(\kappa)}{L(\kappa)}-\frac{(a-d+2i\kappa b)}{(a-d)\kappa+(b\kappa^2+c)i}\right)\\ &= -\frac{1}{2\kappa}\left(\sum_{j=1}^{2}\frac{d}{d\kappa}\ln(w_j(\kappa))+\frac{d}{d\kappa}\ln(L(\kappa))-\frac{d}{d\kappa}\ln((a-d)\kappa+(b\kappa^2+c)i)\right)\\ &= -\frac{1}{2\kappa}\left(\frac{d}{d\kappa}\ln\left(\frac{L(\kappa)}{(a-d)\kappa+(b\kappa^2+c)i}\prod_{j=1}^{2}w_j(\kappa)\right)\right).\end{aligned}$$

The second term on the right hand side of (2.2.1) with values of $\lambda_{j,l}$ given by lemma (2.2.1) is a finite rank operator and if the potential function V satisfy condition (2.1.2) then the operator $\sqrt{|V|}(H_0^{\mathcal{A}})^{-1/2}$ is Hilbert-Schmidt and therefore, $\sqrt{V}R_0^{\mathcal{A}}\sqrt{|V|}$ is trace class. This implies that the perturbation determinant $D(z)$ is well defined. The perturbation determinant and trace of the resolvent difference $R_V^{\mathcal{A}}(z)-R_0^{\mathcal{A}}(z)$ are related by the following expression

$$\mathrm{Tr}(R_V^{\mathcal{A}}(z)-R_0^{\mathcal{A}}(z))=\frac{\frac{d}{dz}D(z)}{D(z)},\quad z\in\rho(H_V^{\mathcal{A}})\cap\rho(H_0^{\mathcal{A}}).$$

In order to find an explicit expression for the perturbation determinant we choose $\kappa=\sqrt{z}$ such that Im $(z)>0$. It follows from Theorem (2.1.1) that

$$\frac{\frac{d}{dz}(D(z))}{D(z)}=\frac{\frac{d}{dz}\left(\frac{L(\sqrt{z})}{(a-d)\sqrt{z}+(bz+c)i}\prod_{j=1}^{2}w_j(\sqrt{z})\right)}{\frac{L(\sqrt{z})}{(a-d)\sqrt{z}+(bz+c)i}\prod_{j=1}^{2}w_j(\sqrt{z})}.$$

From here we deduce that

$$D(z)=A\frac{L(\sqrt{z})}{(a-d)\sqrt{z}+(bz+c)i}\prod_{j=1}^{2}w_j(\sqrt{z}),\qquad A\in\mathbb{C}.$$

To find the value of the complex coefficient A, we use the following asymptotic of perturbation determinant

$$\lim_{|\mathrm{Im}(z)|\to\infty}D(z)=1.$$

This asymptotic holds if $\sqrt{|V|R_0^{\mathcal{A}}(z)}$ is Hilbert-Schmidt operator (see [97]). For the asymptotic behaviour of $w_j(\sqrt{z})$ as $|\sqrt{z}|\to\infty$, we refer to [19], which provides

$$w_j(\sqrt{z})=f_j(0,\sqrt{z})=1+O(|\sqrt{z}|^{-1}).$$

Further, it is easy to find that

$$L(\sqrt{z}) = (a-d)\sqrt{z}i - (bz+c) + O(1), \quad |\sqrt{z}| \to \infty. \tag{2.2.13}$$

This implies, $A = \dfrac{1}{i}$. □

2.2.1 spectral shift function

In this section we briefly discuss the relationship between perturbation determinant $D(z)$ and the spectral shift function $\xi(\lambda; H_V^{\mathcal{A}}, H_0^{\mathcal{A}})$. The spectral shift function for the pair of operators $H_V^{\mathcal{A}}$ and $H_0^{\mathcal{A}}$ can be defined by the trace formula

$$\mathrm{Tr}(f(H_V^{\mathcal{A}} - H_0^{\mathcal{A}})) := \int_{-\infty}^{\infty} \xi(\lambda; H_V^{\mathcal{A}}, H_0^{\mathcal{A}}) f'(\lambda)\, d\lambda \tag{2.2.14}$$

for all $f \in C_0^{\infty}(\mathbb{R})$.

Theorem 9.2 of [94] explicitly characterize the spectral shift function in the more general case of matrix valued Schrödinger operators with general self-adjoint conditions at the origin. It was proved that the trace formula (2.2.14) holds for a bigger class of functions satisfying $f'(\lambda) = O(\lambda^{-1/2-\epsilon})$, $f''(\lambda) = O(\lambda^{-1-\epsilon})$, $\epsilon > 0$, $\lambda \to \infty$ and

$$\int_{-\infty}^{\infty} |\xi(\lambda; H_V^{\mathcal{A}}, H_0^{\mathcal{A}})|(1+|\lambda|)^{-1/2-\epsilon}\, d\lambda < \infty, \quad \epsilon > 0.$$

One of the main ingredient in the proof of Theorem 9.2 of [94] is the following estimate[1] (cf. inequality (9.2) of [94], see also (5.11) of [97])

$$||R_V^{\mathcal{A}}(-t) - R_0^{\mathcal{A}}(-t)||_1 \le C_\epsilon t^{-\frac{3}{2}+\epsilon}, \quad \epsilon > 0, \quad t \to \infty. \tag{2.2.15}$$

The above estimate implies

$$\int_1^{\infty} t^{-m} ||R_V^{\mathcal{A}}(-t) - R_0^{\mathcal{A}}(-t)||_1 < \infty$$

which holds for all $m > -1/2$. Proposition (3.3) of [18] then implies

$$\xi(\lambda;\, H_V^{\mathcal{A}}, H_0^{\mathcal{A}}) = \pi^{-1} \lim_{\epsilon \to 0} \arg D(\lambda + i\epsilon),$$

where $\arg D(z) = \mathrm{Im} \ln D(z)$ is defined by the condition $\ln D(z) \to 0$ as $\mathrm{dist}\{z, \sigma(H_0)\} \to \infty$. Moreover,

$$\ln D(z) = \int_{-\infty}^{\infty} \xi(\lambda;\, H_V^{\mathcal{A}}, H_0^{\mathcal{A}})(\lambda - z)^{-1}\, d\lambda, \quad z \in \rho(H_0^{\mathcal{A}}) \cap \rho(H_V^{\mathcal{A}}).$$

[1] The interested reader can consult Appendix (A) where explicit derivation of this estimate is provided.

2.3 Levinson's formula

In this section we derive a zero order trace formula, commonly known as Levinson's formula, which describes the number of negative eigenvalues of an operator in terms of phase shift function which is denoted by η and it is defined, for real k, as $\eta(k) := \arg D(k)$. The Levinson's formula derived in this section is closely related to the Levinson's formulas obtained in Theorem 9.3 of [5] and Theorem 9.3 of [94]. Levinson's formula obtained in [5] relates the number of negative eigenvalues with the determinant of the scattering matrix and certain parameters that depend on the boundary conditions. Formula obtained in [94] relates the number of negative eigenvalues with the spectral shift function. The vertex conditions of this chapter can be expressed as a particular case of more general conditions considered in references [5] and [94] and therefore the Levinson's formulas obtained there also holds for the operator $H_V^{\mathcal{A}}$. For higher order trace formulas of integer and half-integer order we refer to [97, 95, 92].

We will need the following low-energy asymptotics of the perturbation determinant

Lemma 2.3.1 (Low energy asymptotics)**.** *Let the potential V satisfies the condition*

$$\int_{e_j} (1+x)|V_j(x)|dx < \infty, \quad 1 \le j \le n. \tag{2.3.1}$$

Then as $\kappa \to 0$ the perturbation determinant satisfies

$$D(\kappa) = \begin{cases} \kappa^{(Q-P)}(1+o(1)) & w_j(0) \neq 0,\ j=1,2, \\ \kappa^{(R-P)}(1+o(1)) & w_1(0)=0, w_2(0)\neq 0, \\ \kappa^{(S-P)}(1+o(1)) & w_1(0)\neq 0, w_2(0)=0, \\ \kappa^{(T-P)}(1+o(1)) & w_j(0)=0,\ j=1,2. \end{cases}$$

Where the functions P, Q, R, S and T constants and functions are defined in Theorem (2.1.2).

Proof. Expression for perturbation determinant is

$$D(\kappa) = \frac{L(\kappa)\prod_{j=1}^{2} w_j(\kappa)}{(a-d)i\kappa - (b\kappa^2 + c)}.$$

We consider the following five different cases

1. $w_j(0) \neq 0$, $j = 1, 2$ and $L(0) \neq 0$.

2. $w_j(0) \neq 0$, $j = 1, 2$ and $L(0) = 0$.

3. $w_1(0) = 0$ and $w_2(0) \neq 0$.

4. $w_1(0) \neq 0$ and $w_2(0) = 0$.

5. $w_j(0) = 0$, $j = 1, 2$.

In the first case $D(\kappa)$ has no zeros and we can let

$$\begin{aligned}
&L(0)\prod_{j=1}^{2} w_j(0) = \tilde{c} \neq 0 \\
&\Rightarrow \lim_{\kappa\to 0} D(\kappa) = \lim_{\kappa\to 0} \frac{\tilde{c}}{(a-d)i\kappa - (b\kappa^2 + c)} \\
&\Rightarrow \lim_{\kappa\to 0} D(\kappa)((a-d)i\kappa - (b\kappa^2 + c)) = \tilde{c} \\
&\Rightarrow \lim_{\kappa\to 0} \frac{D(\kappa)((a-d)i\kappa - (b\kappa^2 + c)) - \tilde{c}}{\tilde{c}} = 0 \\
&\Rightarrow D(\kappa)((a-d)i\kappa - (b\kappa^2 + c)) - \tilde{c} = o(\tilde{c}) \\
&\Rightarrow D(\kappa) = \tilde{c}((a-d)i\kappa - (b\kappa^2 + c))^{-1}(1 + o(1)).
\end{aligned}$$

In the second case, we make use of the following small energy asymptotics (c.f. Theorem 2.3 (iii)of [3])

$$\frac{f_j'(0,\kappa)}{f_j(0,\kappa)} = \frac{f_j'(0,0)}{f_j(0,0)} - \frac{i\kappa}{f_j^2(0,0)} + o(\kappa)$$

which implies

$$\begin{aligned}
L(\kappa) =& a\left(\frac{f_1'(0,0)}{f_1(0,0)} - \frac{i\kappa}{f_1^2(0,0)} + o(\kappa)\right) - d\left(\frac{f_2'(0,0)}{f_2(0,0)} - \frac{i\kappa}{f_2^2(0,0)} + o(\kappa)\right) \\
&+ b\left(\frac{f_1'(0,0)}{f_1(0,0)} - \frac{i\kappa}{f_1^2(0,0)} + o(\kappa)\right)\left(\frac{f_2'(0,0)}{f_2(0,0)} - \frac{i\kappa}{f_2^2(0,0)} + o(\kappa)\right) + c \\
=& a\frac{f_1'(0,0)}{f_1(0,0)} - d\frac{f_2'(0,0)}{f_2(0,0)} + b\frac{f_1'(0,0)}{f_1(0,0)}\frac{f_2'(0,0)}{f_2(0,0)} - c + a\left(\frac{-i\kappa}{f_1^2(0,0)} + o(\kappa)\right) \\
&- d\left(\frac{-i\kappa}{f_2^2(0,0)} + o(\kappa)\right) + b\left[\left(\frac{f_1'(0,0)}{f_1(0,0)f_2^2(0,0)} + \frac{f_2'(0,0)}{f_1^2(0,0)f_2(0,0)}\right)i\kappa\right] \\
&+ b\left(o(\kappa) + o(\kappa^2) - \frac{\kappa^2}{f_1(0,0)f_2(0,0)}\right)
\end{aligned}$$

This yields

$$\begin{aligned}
L(\kappa) =& L(0) + a\left(\frac{-i\kappa}{f_1^2(0,0)} + o(\kappa)\right) - d\left(\frac{-i\kappa}{f_2^2(0,0)} + o(\kappa)\right) \\
&+ b\left[\left(\frac{f_1'(0,0)}{f_1(0,0)f_2^2(0,0)} + \frac{f_2'(0,0)}{f_1^2(0,0)f_2(0,0)}\right)i\kappa + o(\kappa) + o(\kappa^2) - \frac{\kappa^2}{f_1(0,0)f_2(0,0)}\right].
\end{aligned}$$

Therefore,

$$D(\kappa) = \frac{b\kappa^2 + \alpha_1\kappa + o(\kappa) + b(o(\kappa^2))}{(a-d)i\kappa - (b\kappa^2 + c)},$$

where, $\alpha_1 = \left(b\left(\frac{f_1'(0,0)}{f_2(0,0)} + \frac{f_2'(0,0)}{f_1(0,0)} \right) - a\frac{f_2(0,0)}{f_1(0,0)} + d\frac{f_1(0,0)}{f_2(0,0)} \right) i.$

The study of first two cases can be summarized as follows

- If $w_j(0) \neq 0$, $j = 1, 2$ and $L(0) \neq 0$ then the numerator of $D(\kappa)$ is a non zero constant and it will have no zeros.
- If $w_j(0) \neq 0$, $j = 1, 2$ and $L(0) = 0$ then the numerator of $D(\kappa)$ for small κ will have one zero in case $\alpha_1 \neq 0$ and it will have two zeros in case $\alpha_1 = 0$, $b \neq 0$.

This gives us the following low energy asymptotics in the first two cases

$$D(\kappa) = \kappa^{(Q-P)}(1 + o(1)),$$

where

$$Q = Q(b, \alpha_1, L(0)) = \begin{cases} 0 & L(0) \neq 0, \\ 1 & L(0) = 0, \alpha_1 \neq 0 \\ 2 & L(0) = 0, \alpha_1 = 0, b \neq 0 \end{cases}$$

and

$$P = P(a, b, c, d) = \begin{cases} 0 & c \neq 0, \\ 1 & c = 0, a - d \neq 0 \\ 2 & c = 0, a - d = 0, b \neq 0. \end{cases}$$

The function P gives the number of poles of $D(\kappa)$ in the given cases.

Let us now consider the third case, i.e., when $w_1(0) = 0$ and $w_2(0) \neq 0$. We rewrite $D(\kappa)$ as

$$\begin{aligned} D(\kappa) &= \frac{\left(a\frac{f_1'(0,\kappa)}{f_1(0,\kappa)} - d\frac{f_2'(0,\kappa)}{f_2(0,\kappa)} + b\prod_{k=1}^{2}\frac{f_k'(0,\kappa)}{f_k(0,\kappa)} - c \right)\prod_{j=1}^{2} f_j(0,\kappa)}{(a-d)i\kappa - (b\kappa^2 + c)} \\ &= \frac{\left(af_1'(0,\kappa)f_2(0,\kappa) + bf_1'(0,\kappa)f_2'(0,\kappa) - df_1(0,\kappa)f_2'(0,\kappa) - c\prod_{j=1}^{2} f_j(0,\kappa) \right)}{(a-d)i\kappa - (b\kappa^2 + c)} \end{aligned} \quad (2.3.2)$$

and use the following asymptotic for $f_1(x,\kappa)$ (c.f. [17])

$$f_1(0,\kappa) = \kappa \dot{f}_1(0,0) + o(\kappa).$$

This implies

$$D(\kappa) = \frac{(\alpha_2 - c_3\kappa + o(\kappa))}{(a-d)i\kappa - (b\kappa^2 + c)}$$

Where $\alpha_2 = af_1'(0,0)f_2(0,0) + bf_1'(0,0)f_2'(0,0)$ and $c_3 = (cf_2(0,0) + df_2'(0,0))\dot{f}_1(0,0)$. The numerator of $D(\kappa)$ is equal to $\alpha_2 - c_3\kappa + o(\kappa)$ as $\kappa \to 0$. If $\alpha_2 \neq 0$ then the numerator od $D(\kappa)$ has no zeros for small κ and if $\alpha_2 = 0$, then the numerator od $D(\kappa)$ has one zero for small κ. Hence,

$$D(\kappa) = \kappa^{(R-P)}(1 + o(1)), \quad \kappa \to 0,$$

where,

$$R = R(\alpha_2) = \begin{cases} 0 & \alpha_2 \neq 0, \\ 1 & \alpha_2 = 0. \end{cases}$$

For the fourth case we substitute

$$f_2(0,\kappa) = \kappa \dot{f}_2(0,0) + o(\kappa), \kappa \to 0$$

into (2.3.2) and obtain

$$D(\kappa) = \frac{(\alpha_3 + c_5\kappa + o(\kappa))}{(a-d)i\kappa - (b\kappa^2 + c)}.$$

Here, $\alpha_3 = bf_1'(0,0)f_2'(0,0) - df_1(0,0)f_2'(0,0)$ and $c_5 = (af_1'(0,0) - cf_1(0,0))\dot{f}_2(0,0)$. The numerator of $D(\kappa)$ for small κ has no zeros if $\alpha_3 \neq 0$ and it has one zero if $\alpha_3 = 0$. Therefore,

$$D(\kappa) = \kappa^{(S-P)}(1 + o(1)), \quad \kappa \to 0,$$

where,

$$S = S(\alpha_3) = \begin{cases} 0 & \alpha_3 \neq 0, \\ 1 & \alpha_3 = 0. \end{cases}$$

Finally, for the fifth case we substitute the asymptotics

$$f_1(0,\kappa) = \kappa \dot{f}_1(0,0) + o(\kappa) \text{ and } f_2(0,\kappa) = \kappa \dot{f}_2(0,0) + o(\kappa), \quad \kappa \to 0$$

into (2.3.2) and obtain

$$D(\kappa) = \frac{c\left(c_6\kappa^2 + o(\kappa^2)\right) + \alpha_4\kappa + bc_8 + o(\kappa)}{(a-d)i\kappa - (b\kappa^2 + c)}, \quad \kappa \to 0.$$

Here, $c_6 = \dot{f}_1(0,0)\dot{f}_2(0,0) \neq 0$, $c_8 = f_1'(0,0)f_2'(0,0) \neq 0$ (because $f(0,0) = 0 \Rightarrow \dot{f}(0,0)f'(0,0) = -i$ hence $\dot{f}(0,0) \neq 0$ and $f'(0,0) \neq 0$) $\alpha_4 = af_1'(0,0)\dot{f}_2(0,0) - d\dot{f}_1(0,0)f_2'(0,0)$. This implies the numerator of $D(\kappa)$ for small κ has no zeros if $b \neq 0$, it has one zero if $b = 0, \alpha_4 \neq 0$ and it has two zeros if $b = 0$, $\alpha_4 = 0$, $c \neq 0$. This yields

$$D(\kappa) = \kappa^{(T-P)}(1 + o(1)), \quad \kappa \to 0,$$

where

$$T = T(b, c, \alpha_4) = \begin{cases} 0 & b \neq 0, \\ 1 & b = 0, \alpha_4 \neq 0 \\ 2 & b = 0, \alpha_4 = 0, c \neq 0. \end{cases}$$

□

Using the low energy asymptotics of $D(\kappa)$ we now prove the analogue of Levinson's formula for the negative eigenvalues of $H_V^{\mathcal{A}}$, stated in Theorem (2.1.2).

Proof of Theorem 2.1.2. The function $D(\kappa)$ has a zero in κ of order r if and only if κ^2 is an eigenvalue of multiplicity r of the operator $H_V^{\mathcal{A}}$ [5]. As $H_V^{\mathcal{A}}$ is a self-adjoint operator, so the zeros of $D(\kappa)$ lie on the positive imaginary axis and it may have only real eigenvalues.

Let $\Gamma_{R,\epsilon}$ denotes the contour (counterclockwise) consisting of semicircles $C_R^+ = \{|\kappa| = R, \quad \text{Im } \kappa \geq 0\}$ and $C_\epsilon^+ = \{|\kappa| = \epsilon, \quad \text{Im } \kappa \geq 0\}$ and the intervals (ϵ, R) and $(-R, -\epsilon)$. R and ϵ are chosen such that all N negative eigenvalues lie inside the contour $\Gamma_{R,\epsilon}$.

The function $w_j(\kappa)$ is analytic in the upper halfp-plane, therefore, $D(\kappa)$ is analytic inside and on the contour $\Gamma_{R,\epsilon}$. Hence,

$$\int_{\Gamma_{R,\epsilon}} \frac{\frac{d}{d\kappa}D(\kappa)}{D(\kappa)} d\kappa = 2\pi i N. \tag{2.3.3}$$

Note that,

$$\lim_{\substack{\kappa\to\infty \\ \text{Im}}} D(\kappa) = \lim_{\substack{\kappa\to\infty \\ \text{Im}}} \frac{L(\kappa)\prod_{j=1}^{2} w_j(\kappa)}{(a-d)i\kappa - (b\kappa^2+c)} = 1 + O(|\kappa|^{-1}). \tag{2.3.4}$$

The branch of the function $\ln D(\kappa)$ can be fixed by the condition $\ln D(\kappa) \to 0$ as $|\kappa| \to \infty$. For $k \in \mathbb{R}$, we set $D(k) = a(k)e^{i\eta(k)}$, where $a(k) = |D(k)|$ and $\eta(k) = \arg D(k)$. Now

$$\text{var}_{\Gamma_{R,\epsilon}} \arg D(\kappa) = \eta(R) - \eta(\epsilon) + \text{var}_{C_R^+} \arg D(\kappa) + \{\eta(-\epsilon) - \eta(-R)\} + \text{var}_{C_\epsilon^+} \arg D(\kappa).$$

It follows from the representation of $D(k)$ that $\eta(-k) = -\eta(k)$. Hence,

$$\text{var}_{\Gamma_{R,\epsilon}} \arg D(\kappa) = 2(\eta(R) - \eta(\epsilon)) + \text{var}_{C_R^+} \arg D(\kappa) + \text{var}_{C_\epsilon^+} \arg D(\kappa)$$

Equation (2.3.3) implies that

$$\text{var}_{\Gamma_{R,\epsilon}} \arg D(\kappa) = 2\pi N.$$

This implies

$$2\pi N = 2(\eta(R) - \eta(\epsilon)) + \text{var}_{C_R^+} \arg D(\kappa) + \text{var}_{C_\epsilon^+} \arg D(\kappa).$$

Using (2.3.4), one can see that $\lim_{R\to\infty} \text{var}_{C_R^+} \arg D(\kappa) = 0$. We are left with

$$\eta(\infty) - \eta(\epsilon) = \pi N - \frac{1}{2}\text{var}_{C_\epsilon^+} \arg D(\kappa).$$

Now letting $\epsilon \to 0$ and using Lemma (2.3.1), we arrive at

$$\lim_{\epsilon\to 0} \text{var}_{C_\epsilon^+} \arg D(\kappa) = \begin{cases} -(Q-P)\pi & w_j(0) \neq 0,\ j = 1,2, \\ -(R-P)\pi & w_1(0) = 0, w_2(0) \neq 0, \\ -(S-P)\pi & w_1(0) \neq 0, w_2(0) = 0, \\ -(T-P)\pi & w_j(0) = 0,\ j = 1,2. \end{cases}$$

Therefore,

$$\eta(\infty) - \eta(0) = \begin{cases} \pi(N + \dfrac{Q-P}{2}) & w_j(0) \neq 0,\ j = 1,2, \\ \pi(N + \dfrac{R-P}{2}) & w_1(0) = 0, w_2(0) \neq 0, \\ \pi(N + \dfrac{S-P}{2}) & w_1(0) \neq 0, w_2(0) = 0, \\ \pi(N + \dfrac{T-P}{2}) & w_j(0) = 0,\ j = 1,2. \end{cases}$$

□

2.4 examples

In this section we illustrate the trace formula and perturbation determinant obtained in theorem (2.1.1) with some examples.

Example 2.4.1. *For the δ interaction of strength $\alpha \in \mathbb{R}$, we can choose $\varphi = 0$, $a = 1$, $b = 0$, $c = \alpha$ and $d = -1$. Then according to theorem* (2.1.1) *the trace of the resolvent difference is given by*

$$Tr(R_V^{\mathcal{A}}(\kappa) - R_0^{\mathcal{A}}(\kappa)) = -\frac{1}{2\kappa} \ln \left(\frac{f_1'(0,\kappa) f_2(0,\kappa) + f_1(0,\kappa) f_2'(0,\kappa) - \alpha f_1(0,\kappa) f_2(0,\kappa)}{2\kappa + i\alpha} \right)$$

and the expression for perturbation determinant is

$$D(\kappa) = \frac{1}{2i\kappa - \alpha} \left(f_1'(0,\kappa) f_2(0,\kappa) + f_1(0,\kappa) f_2'(0,\kappa) - \alpha f_1(0,\kappa) f_2(0,\kappa) \right).$$

For $\alpha = 0$ the δ conditions are commonly known as Kirchhoff conditions and in this case the above expressions coincide with the results obtained in Theorem (1.1) and Corollary (3.1) of [18] with $n = 2$.

Example 2.4.2. *The δ' conditions are obtained by choosing $\varphi = 0$, $a = -1$, $b = \beta$, $c = 0$ and $d = 1$ in* (2.1.3)*. In this case theorem* (2.1.1) *implies*

$$Tr(R_V^{\mathcal{A}}(\kappa) - R_0^{\mathcal{A}}(\kappa)) = -\frac{1}{2\kappa} \ln \left(\frac{f_1'(0,\kappa) f_2(0,\kappa) + f_1(0,\kappa) f_2'(0,\kappa) - \beta f_1'(0,\kappa) f_2'(0,\kappa)}{2\kappa - i\beta\kappa^2} \right)$$

and perturbation determinant is given by

$$D(\kappa) = \frac{1}{2i\kappa + \beta\kappa^2} \left(f_1'(0,\kappa) f_2(0,\kappa) + f_1(0,\kappa) f_2'(0,\kappa) - \beta f_1'(0,\kappa) f_2'(0,\kappa) \right).$$

In the next two examples we use the notation $D_x\varphi = \varphi^{(1)}$ for the generalized derivative in the sense of [63].

Example 2.4.3. *The Schrödinger operator with the singular density $-D_x\left(1 + \sigma\delta\right) D_x$ is equivalent to the operator $H_V^{\mathcal{A}}$ with $\varphi = 0$, $a = 1$, $b = -\sigma \in \mathbb{R}$, $c = 0$ and $d = -1$ and the perturbation determinant is given by*

$$D(\kappa) = \frac{1}{2i\kappa + \sigma\kappa^2} \left(f_1'(0,\kappa) f_2(0,\kappa) + f_1(0,\kappa) f_2'(0,\kappa) - \sigma f_1'(0,\kappa) f_2'(0,\kappa) \right).$$

Example 2.4.4. *For real σ_1 and σ_2 the two parameters family of Schrödinger operators with singular potential $-D_x^2 + \sigma_1\delta + \sigma_2\delta^{(1)} + V$ is equivalent to the operator $H_V^{\mathcal{A}}$ with $\varphi = 0$, $a = \frac{2+\sigma_2}{2-\sigma_2}$, $b = 0$, $c = \frac{4\sigma_1}{4-\sigma_2^2}$, $d = -\left(\frac{2-\sigma_2}{2+\sigma_2}\right)$ (c.f. Section 3.2.4 of [63]). Theorem* (2.1.1) *implies the following expression for the perturbation determinant*

$$D(\kappa) = \frac{\left(\left(\frac{2+\sigma_2}{2-\sigma_2}\right) f_1'(0,\kappa) f_2(0,\kappa) + \left(\frac{2-\sigma_2}{2+\sigma_2}\right) f_1(0,\kappa) f_2'(0,\kappa) - \left(\frac{4\sigma_1}{4-\sigma_2^2}\right) f_1(0,\kappa) f_2(0,\kappa)\right)}{\left(\frac{8+2\sigma_2^2}{4-\sigma_2^2}\right) i\kappa - \left(\frac{4\sigma_1}{4-\sigma_2^2}\right)}.$$

Chapter 3

Quantum star graphs with PI vertex conditions

We consider Schrödinger operators on quantum star graphs with properly connecting permutation invariant conditions at the central vertex, which amongst others, include δ and δ' conditions. We derive trace formulas for the difference of resolvents of perturbed and unperturbed Schrödinger operators. These formulas lead to explicit expressions for the perturbation determinants and the spectral shift function. Under certain integrability conditions on the potential function, the perturbation determinant along with its low energy asymptotics lead to an analog of Levinson's formula.

3.1 Introduction

In this study, we consider the Schrödinger operator on star shaped graph Γ

$$-\frac{d^2}{dx^2} + V, \quad x \in \Gamma. \tag{3.1.1}$$

Star graph Γ can be imagined as a metric graph with a finite number of n edges of infinite length connected at a single vertex. We identify each edge e_j by the interval $[0, \infty)$ and the common vertex of the star graph by the set $\{0\}$. The restriction of V on an edge e_j is denoted by V_j. We assume that it is a real-valued function on Γ and satisfies

$$\int_{e_j} |V_j(x_j)| dx_j < \infty, \quad j = 1, \cdots, n. \tag{3.1.2}$$

The operator (3.1.1) can be made self-adjoint by specifying certain vertex or matching conditions at the vertex. The most general form of such conditions can be expressed in terms of two $n \times n$ matrices A and B as $A\psi(0) + B\psi'(0) = 0$ where A and B satisfy $AB^\dagger = BA^\dagger$ and $\text{rank}[A \quad B] = n$. Here, $\dagger$ denotes complex conjugate transpose and $\psi(0)$ and $\psi'(0)$ are column vectors of function and its derivative values at zero along each edge, respectively. There are several other equivalent formulations for the most general self-adjoint vertex conditions, see for example [3, 5, 4, 41, 40, 42]. In this chapter, however, we consider a class of properly connecting vertex conditions which are permutation invariant i.e. they do not distinguish between the edges incident to the vertex and do not degenerate to decoupled Dirichlet, Neumann or Robin conditions. Vertex conditions (3.1.3)–(3.1.6), below, describe all properly connecting permutation invariant vertex conditions.

1. The δ conditions:

$$\begin{aligned} &\psi(0) := \psi_1(0) = \cdots = \psi_n(0), \\ &\sum_{j=1}^{n} \psi_j'(0) = a\psi(0), \quad a \in \mathbb{R}. \end{aligned} \tag{3.1.3}$$

2. The δ' conditions:
   If we interchange the role of function values and derivative values at zero in conditions (3.1.3), we get the following self-adjoint permutation invariant conditions which are commonly known as δ'-conditions

$$\begin{aligned} &\psi'(0) := \psi_1'(0) = \cdots = \psi_n'(0), \\ &\sum_{j=1}^{n} \psi_j(0) = b\psi'(0), \quad b \in \mathbb{R}. \end{aligned} \tag{3.1.4}$$

3. The $\hat{\delta}$ conditions:

$$\begin{aligned} &\psi_j(0) - \psi_k(0) = d(\psi_j'(0) - \psi_k'(0)) \quad j,k = 1,\ldots,n, \quad 0 \neq d \in \mathbb{R}, \\ &\sum_{j=1}^{n} \psi_j'(0) = 0. \end{aligned} \tag{3.1.5}$$

   The above permutation invariant conditions with strength $d = 0$ become δ-conditions with zero strength. Therefore $\hat{\delta}$ notation is used to denote these conditions.

4. The $\hat{\delta}'$ conditions:
   Interchanging the role of function values and derivative values at the vertex zero in conditions (3.1.5), we obtain the following self-adjoint conditions

$$\psi_j'(0) - \psi_k'(0) = c(\psi_j(0) - \psi_k(0)) \quad j,k = 1,\dots,n, \quad 0 \neq c \in \mathbb{R},$$
$$\sum_{j=1}^{n} \psi_j(0) = 0. \tag{3.1.6}$$

   as these conditions become analog to δ'-conditions when we set strength c to zero, we therefore, denote these conditions as $\hat{\delta}'$-conditions. Conditions (3.1.5) were proposed in [23] as an alternative to the (3.1.4) in the description of quantum particles on graphs, see also [83].

We denote the Schrödinger operators given by the differential expression (3.1.1) subject to the vertex conditions (3.1.3), (3.1.4), (3.1.5) and (3.1.6) by $H_{V,\Gamma}^{\delta_a}, H_{V,\Gamma}^{\delta_b'}, H_{V,\Gamma}^{\hat{\delta}_d}$ and $H_{V,\Gamma}^{\hat{\delta}_c'}$, respectively. The associated unperturbed operators, that is when $V = 0$, are denoted by $H_{0,\Gamma}^{\delta_a}, H_{0,\Gamma}^{\delta_b'}, H_{0,\Gamma}^{\hat{\delta}_d}$ and $H_{0,\Gamma}^{\hat{\delta}_c'}$.

The present chapter is devoted to derive explicit expressions for perturbation determinant and Levinson's formula for the above operators defined on star graphs. We first prove a trace formula that expresses the trace of the difference between the perturbed and corresponding unperturbed resolvents in terms of a Wronskian. This trace formula allows us to derive an explicit expression for the (modified) perturbation determinant, which is an important mathematical object in the study of spectral as well as scattering theory. The zeros of perturbation determinant coincide with the eigenvalues of the Schrödinger operator and the multiplicity of each eigenvalue is equal to the order of the corresponding zero of the perturbation determinant [5]. For a real argument, perturbation determinant is used to define the phase shift function. The so called Levinson's formula is derived for the above defined Schrödinger operators in terms of phase shift function. This formula, also called a zero order trace formula gives a relationship between the number of negative eigenvalues and the scattering data via phase shift function. The obtained Levinson's formula is closely related to the Levinson's formulas obtained in theorem 9.3 of [5] and theorem 9.3 of [94].

Schrödinger operator on star graph is equivalent to the matrix Schrödinger operator on the half-line. Recently, there has been a great deal of interest in the spectral and scattering theory of matrix Schrödinger operators, see for example [3, 5, 4, 94]. Although. star graphs are simple quantum graphs but they are considered as elementary building block of a generic graph and represent a correct model for a scattering process in the

existence of a vertex. Schrödinger operator on a star graph subject to certain self-adjoint vertex conditions are useful in designing nanotubes for microscopic electronic devices and elementary gates in quantum computing. For a discussion on these aspects we refer to [55, 57] and references therein. For direct and inverse scattering theory on star graphs we refer the reader to [18, 33, 40], see also the recent article [36].

For Schrödinger operators on star graphs with finitely many edges of infinite length satisfying the Kirchhoff conditions ((3.1.3) with $a = 0$) at the vertex, the results on spectral shift function and Levinson's theorem were obtained by Demirel in [18]. Results of similar kind for the Schrödinger operators on the half-line as well as on the whole real line we refer to [97, 19], also see [5] and [94] for more general matrix-valued Schrödinger operators. Moreover, we discuss the perturbation determinant and Levinon's formula for one dimensional Schrödinger operator with properly connecting generalized point interaction in [102].

The chapter is organized as follows. In Section 2, we present the derivation of an expression that relates the trace of the difference of the perturbed and unperturbed resolvents in terms of a Wronskian. This allows us to derive an explicit expression for the perturbation determinants. In Section 3, we derive Levinson's formulas for Schrödinger operators with permutation invarient vertex conditions.

3.2 A trace formula and perturbation determinant for Star Graphs

In this section, our main purpose is to derive trace formulas and explicit expressions for perturbation determinants for star graphs. The trace formulas express the traces of resolvent difference of the above defined perturbed and unperturbed operators using Jost solutions. More precisely, If we denote the resolvent $(H_{V,\Gamma}-z)^{-1}$ of the perturbed operator $H_{V,\Gamma}$ by $R_{V,\Gamma}(z)$ and the resolvent $(H_{0,\Gamma} - z)^{-1}$ of unperturbed operator $H_{0,\Gamma}$ by $R_{0,\Gamma}(z)$ then we shall derive an expression for $\mathrm{Tr}(R_{V,\Gamma}(z) - R_{0,\Gamma}(z)))$ in terms of Jost solutions f_j on the edges e_j. For this purpose, we use the Krein's formula [6], see also [24] and [18].

Under condition (3.1.2) the differential equation

$$-u_j'' + V_j u = \kappa^2 u, \quad j = 1, 2, \cdots, n$$

has two particular solutions, namely, the Jost solution and the regular solution. The Jost solution f_j is characterized by the condition $f_j(x, \kappa) \sim e^{i\kappa x}$, as $x \to \infty$ and the regular

solution φ_j by the conditions

$$\varphi_j(0,\kappa) = 0, \quad \varphi_j'(0,\kappa) = 1.$$

We first consider the decoupled Schrödinger operator by imposing Dirichlet condition at the vertex. We denote the decoupled operator by $H^D_{V,\Gamma}$ which is the direct sum of Dirichlet Schrödinger operators $H^D_{e_j}$ on each edge, i.e. $H^D_{V,\Gamma} = \bigoplus_{j=1}^{n} H^D_{e_j}$ and its resolvent by $R^D_{V,\Gamma}(z) = (H^D_{V,\Gamma} - z)^{-1}$. The krein's formula [6] allows us to express the kernel of $R_{V,\Gamma}(z)$ in terms of kernel of $R^D_{V,\Gamma}(z)$. In particular, the formula states that if $\rho(H_{V,\Gamma})$ and $\rho(H^D_{V,\Gamma})$ are resolvent sets of $H_{V,\Gamma}$ and $H^D_{V,\Gamma}$ respectively, then for any κ, such that $\mathrm{Im}(\kappa) > 0$ and $z = \kappa^2 \in \rho(H_{V,\Gamma}) \cap \rho(H^D_{V,\Gamma})$ the kernel of matrix integral operator $R_{V,\Gamma}(z)$ is given by

$$R_{j,l}(x,y;z) := R^D_{j,l}(x,y;z) + \lambda_{j,l} f_j(x,\kappa) f_l(y,\kappa) \tag{3.2.1}$$

where $R^D_{j,l}(x,y;z)$ is kernel of the matrix integral operator $R^D_{V,\Gamma}(z)$. It is known (see e.g. [18]), that the resolvent of the operator $H^D_{e_j}$ is an integral operator with symmetric kernel

$$R^D_{e_j}(x,y;z) = \frac{\varphi_j(x,\kappa) f_j(y,\kappa)}{w_j(\kappa)}, \quad x \le y, \quad \kappa = \sqrt{z} \tag{3.2.2}$$

therefore, the resolvent $R^D_{V,\Gamma}(z)$ is a matrix valued integral operator with kernel that is given by

$$R^D_{j,l}(x,y;z) = \delta_{j,l} R^D_{e_j}(x,y;z) \qquad j,l = 1,\dots n. \tag{3.2.3}$$

The following theorem provides the explicit values of the coefficients $\lambda_{j,l}$ for the Schrödinger operators $H^{\delta_a}_{V,\Gamma}$, $H^{\delta'_b}_{V,\Gamma}$, $H^{\hat{\delta}_d}_{V,\Gamma}$ and $H^{\hat{\delta}'_c}_{V,\Gamma}$.

Theorem 3.2.1. *Let $\psi(x) := \int R(x,y;z)u(y)dy$ and $u = (u_1(x),\dots,u_n(x))^T \in L_2(\Gamma)$.*

1. *If $\psi(x)$ satisfies $H^{\delta_a}_{V,\Gamma}\psi = \kappa^2\psi + u$ then $\lambda_{j,l}$ in (3.2.1) are given by*

$$\lambda_{j,l} = ((a - K(\kappa)) f_j(0,\kappa) f_l(0,\kappa))^{-1}.$$

2. *If $\psi(x)$ satisfies $H^{\delta'_b}_{V,\Gamma}\psi = \kappa^2\psi + u$ then $\lambda_{j,l}$ in (3.2.1) are given by*

$$\lambda_{j,l} = ((M(\kappa) - b) f_j'(0,\kappa) f_l'(0,\kappa))^{-1} - \delta_{j,l}(f_j'(0,\kappa) f_l(0,\kappa))^{-1}.$$

3. If $\psi(x)$ satisfies $H_{V,\Gamma}^{\hat{\delta}_d}\psi = \kappa^2\psi + u$ then $\lambda_{j,l}$ in (3.2.1) are given by

$$\lambda_{j,l} = \left(d\delta_{j,l} - \left(\left(1 - d\frac{f_l'(0,\kappa)}{f_l(0,\kappa)} \right) J(\kappa) \right)^{-1} \right) \left(\left(1 - d\frac{f_j'(0,\kappa)}{f_j(0,\kappa)} \right) f_j(0,\kappa) f_l(0,\kappa) \right)^{-1}.$$

4. If $\psi(x)$ satisfies $H_{V,\Gamma}^{\hat{\delta}'_c}\psi = \kappa^2\psi + u$ then $\lambda_{j,l}$ in (3.2.1) are given by

$$\lambda_{j,l} = \left(\left(1 - c\frac{f_j(0,\kappa)}{f_j'(0,\kappa)} \right) \left(1 - c\frac{f_l(0,\kappa)}{f_l'(0,\kappa)} \right) P(\kappa) f_j'(0,\kappa) f_l'(0,\kappa) \right)^{-1} - \delta_{j,l} \left(f_j'(0,\kappa) f_l(0,\kappa) \left(1 - c\frac{f_j(0,\kappa)}{f_j'(0,\kappa)} \right) \right)^{-1}.$$

Here $K(\kappa) = \sum_{j=1}^{n} \frac{f_j'(0,\kappa)}{f_j(0,\kappa)}$, $M(\kappa) = \sum_{j=1}^{n} \frac{f_j(0,\kappa)}{f_j'(0,\kappa)}$, $J(\kappa) = \sum_{j=1}^{n} \frac{f_j'(0,\kappa)}{f_j(0,\kappa)} \left(1 - d\frac{f_j'(0,\kappa)}{f_j(0,\kappa)} \right)^{-1}$ *and* $P(\kappa) = \sum_{j=1}^{n} \frac{f_j(0,\kappa)}{f_j'(0,\kappa)} \left(1 - c\frac{f_j(0,\kappa)}{f_j'(0,\kappa)} \right)^{-1}$.

Proof. For simplicity, let us denote

$$R_{j,l}(x,y;z) = R_{j,l}, \quad \varphi_j(x,\kappa) = \varphi_j(x), \quad f_j(y,\kappa) = f_j(y) \quad \text{and} \quad w_j(\kappa) = w_j.$$

By substituting (3.2.2) and (3.2.3) in (3.2.1) and expressing it into a matrix form we get

$$\begin{bmatrix} R_{1,1} & R_{1,2} & \cdots & R_{1,n} \\ R_{2,1} & R_{2,2} & \cdots & R_{2,n} \\ \vdots & \vdots & \ddots & \vdots \\ R_{n,1} & R_{n,2} & \cdots & R_{n,n} \end{bmatrix} =$$

$$\begin{bmatrix} \frac{\varphi_1(x)f_1(y) + w_1\lambda_{1,1}f_1(x)f_1(y)}{w_1} & \lambda_{1,2}f_1(x)f_2(y) & \cdots & \lambda_{1,n}f_1(x)f_n(y) \\ \lambda_{2,1}f_2(x)f_1(y) & \frac{\varphi_2(x)f_2(y) + w_2\lambda_{2,2}f_2(x)f_2(y)}{w_2} & \cdots & \lambda_{2,n}f_2(x)f_n(y) \\ \vdots & \vdots & \ddots & \vdots \\ \lambda_{n,1}f_n(x)f_1(y) & \lambda_{n,2}f_n(x)f_2(y) & \cdots & \frac{\varphi_n(x)f_n(y) + w_n\lambda_{n,n}f_n(x)f_n(y)}{w_n} \end{bmatrix}.$$

Now multiplying u from right and using the definition of ψ, we get

$$\begin{bmatrix} \psi_1(x) \\ \psi_2(x) \\ \vdots \\ \psi_n(x) \end{bmatrix} = \begin{bmatrix} \int_{\mathbb{R}^+} \{ \frac{\varphi_1(x)f_1(y)}{w_1} u_1(y) + \sum_{i=1}^{n} \lambda_{1,i} f_1(x) f_i(y) u_i(y) \} dy \\ \int_{\mathbb{R}^+} \{ \frac{\varphi_2(x)f_2(y)}{w_2} u_2(y) + \sum_{i=1}^{n} \lambda_{2,i} f_2(x) f_i(y) u_i(y) \} dy \\ \vdots \\ \int_{\mathbb{R}^+} \{ \frac{\varphi_n(x)f_n(y)}{w_n} u_n(y) + \sum_{i=1}^{n} \lambda_{n,i} f_n(x) f_i(y) u_i(y) \} dy \end{bmatrix},$$

which is equivalent to following system of n equations

$$\psi_j(x) = \int\limits_{\mathbb{R}^+} \left\{ \frac{\varphi_j(x) f_j(y)}{w_j} u_j(y) + \sum_{i=1}^{n} \lambda_{j,i} f_j(x) f_i(y) f_i(y) \right\} dy, \quad j = 1, \ldots, n. \tag{3.2.4}$$

1. In order to determine $\lambda_{i,j}$ uniquely, we use both sub-conditions of (3.1.3). The continuity condition i.e. $(\psi_k(0) = \psi_j(0))$ along with Dirichlet condition on φ imply

$$\int\limits_{\mathbb{R}^+} \left\{ \sum_{i=1}^{n} \lambda_{k,i} f_k(0) f_i(y) u_i(y) \right\} dy = \int\limits_{\mathbb{R}^+} \left\{ \sum_{i=1}^{n} \lambda_{j,i} f_j(0) f_i(y) u_i(y) \right\} dy. \tag{3.2.5}$$

   Applying Dirichlet condition on φ and δ-condition on ψ which is given by (3.2.4), we get the following equation

$$\int\limits_{\mathbb{R}^+} \left(\sum_{i=1}^{n} \left(\frac{1}{f_i(0)} + \sum_{j=1}^{n} f_j'(0) \lambda_{j,i} \right) u_i(y) f_i(y) \right) dy = \int\limits_{\mathbb{R}^+} \left(\sum_{i=1}^{n} a f_k(0) \lambda_{k,i} u_i(y) f_i(y) \right) dy. \tag{3.2.6}$$

   Comparing the coefficients of $u_i(y) f_i(y)$ in (3.2.5) and (3.2.6) yields

$$\lambda_{k,i} f_k(0) = \lambda_{j,i} f_j(0) \tag{3.2.7}$$

   and

$$\frac{1}{f_i(0)} + \sum_{j=1}^{n} f_j'(0) \lambda_{j,i} = a f_k(0) \lambda_{k,i}. \tag{3.2.8}$$

   Substituting $\lambda_{j,i}$ from (3.2.7) to (3.2.8), we obtain

$$\lambda_{k,i} = \frac{1}{\left(a - \sum\limits_{j=1}^{n} \frac{f_j'(0)}{f_j(0)} \right) f_k(0) f_i(0)}.$$

2. Applying the condition $\psi_k'(0) = \psi_j'(0)$ on ψ which is give by (3.2.4) and Dirichlet conditions on φ, we get

$$\int\limits_{\mathbb{R}^+} \left\{ \sum_{i=1}^{n} \left(\frac{\delta_{k,i}}{f_i(0)} + f_k'(0) \lambda_{k,i} \right) f_i(y) u_i(y) \right\} dy = \int\limits_{\mathbb{R}^+} \left\{ \sum_{i=1}^{n} \left(\frac{\delta_{j,i}}{f_i(0)} + f_j'(0) \lambda_{j,i} \right) f_i(y) u_i(y) \right\} dy \tag{3.2.9}$$

and Dirichlet condition on φ and δ'-condition on ψ, we obtain

$$\int\limits_{\mathbb{R}^+} \left\{ \sum_{i=1}^{n} \left(\sum_{j=1}^{n} f_j(0)\lambda_{j,i} \right) f_i(y)u_i(y) \right\} dy = \int\limits_{\mathbb{R}^+} \left\{ \sum_{i=1}^{n} b \left(\frac{\delta_{k,i}}{f_i(0)} + f_k'(0)\lambda_{k,i} \right) f_i(y)u_i(y) \right\} dy. \tag{3.2.10}$$

Comparing the coefficients of $u_i(y)f_i(y)$ in (3.2.9) and (3.2.10), we obtain the following two equations

$$\frac{\delta_{k,i}}{f_i(0)} + f_k'(0)\lambda_{k,i} = \frac{\delta_{j,i}}{f_i(0)} + f_j'(0)\lambda_{j,i} \tag{3.2.11}$$

and

$$\sum_{j=1}^{n} f_j(0)\lambda_{j,i} = b \left(\frac{\delta_{k,i}}{f_i(0)} + f_k'(0)\lambda_{k,i} \right). \tag{3.2.12}$$

Substituting $\lambda_{j,i}$ from (3.2.11) to (3.2.12), we get

$$M(\kappa) \left(\frac{\delta_{k,i}}{f_i(0)} + f_k'(0)\lambda_{k,i} \right) - \frac{1}{f_i'(0)} = b \left(\frac{\delta_{k,i}}{f_i(0)} + f_k'(0)\lambda_{k,i} \right),$$

which yields

$$\lambda_{k,i} = \frac{1}{(M(\kappa) - b)f_k'(0)f_i'(0)} - \frac{\delta_{k,i}}{f_k'(0)f_i(0)}.$$

3. In order to determine $\lambda_{i,j}$ uniquely for $\hat{\delta_d}$ conditions we use both sub-conditions of (3.1.5) to the function ψ_j given by (3.2.4). Using condition $(\psi_j(0) - \psi_k(0) = d(\psi_j'(0) - \psi_k'(0))$ along with Dirichlet condition on φ we obtain

$$\int\limits_{\mathbb{R}^+} \left\{ \sum_{i=1}^{n} (\lambda_{j,i}f_j(0) - \lambda_{k,i}f_k(0))f_i(y)u_i(y) \right\} dy =$$

$$d \int\limits_{\mathbb{R}^+} \left\{ \sum_{i=1}^{n} \left(\frac{\delta_{j,i}}{f_i(0)} + \lambda_{j,i}f_j'(0) - \frac{\delta_{k,i}}{f_i(0)} - \lambda_{k,i}f_k'(0) \right) f_i(y)u_i(y) \right\} dy. \tag{3.2.13}$$

Now Dirichlet condition on φ and second sub-condition of (3.1.5) on ψ yields the following equation

$$\int\limits_{\mathbb{R}^+} \left(\sum_{i=1}^{n} \left(\frac{1}{f_i(0)} + \sum_{j=1}^{n} f_j'(0)\lambda_{j,i} \right) u_i(y)f_i(y) \right) dy = 0. \tag{3.2.14}$$

As before, comparing coefficients of $u_i(y)f_i(y)$ in (3.2.13) and (3.2.14), we obtain the following set of two equations

$$\lambda_{j,i}f_j(0) - \lambda_{k,i}f_k(0)) = d\left(\frac{\delta_{j,i}}{f_i(0)} + \lambda_{j,i}f_j'(0) - \frac{\delta_{k,i}}{f_i(0)} - \lambda_{k,i}f_k'(0)\right) \tag{3.2.15}$$

and

$$\frac{1}{f_i(0)} + \sum_{j=1}^{n} f_j'(0)\lambda_{j,i} = 0. \tag{3.2.16}$$

After substituting $\lambda_{j,i}$ from (3.2.15) to (3.2.16) and simplifying, we arrive at the desired result

$$\lambda_{j,l} = \left(d\delta_{j,l} - \frac{1}{\left(1 - d\frac{f_l'(0,\kappa)}{f_l(0,\kappa)}\right)J(\kappa)}\right)\frac{1}{\left(1 - d\frac{f_j'(0,\kappa)}{f_j(0,\kappa)}\right)f_j(0,\kappa)f_l(0,\kappa)}.$$

4. Once again considering ψ_j given by (3.2.4) and applying the condition $(\psi_j'(0) - \psi_k'(0) = c(\psi_j(0) - \psi_k(0)))$ on ψ and Dirichlet condition on φ, we get

$$\int_{\mathbb{R}^+}\left\{\sum_{i=1}^{n}\left(\frac{\delta_{j,i}}{f_i(0)} + f_j'(0)\lambda_{j,i} - \frac{\delta_{k,i}}{f_i(0)} - f_k'(0)\lambda_{k,i}\right)f_i(y)u_i(y)\right\}dy = c\int_{\mathbb{R}^+}\left\{\sum_{i=1}^{n}\left(f_j(0)\lambda_{j,i} - f_k(0)\lambda_{k,i}\right)f_i(y)u_i(y)\right\}dy. \tag{3.2.17}$$

Dirichlet condition on φ and second sub-condition of (3.1.6) on ψ yields

$$\int_{\mathbb{R}^+}\left\{\sum_{i=1}^{n}\left(\sum_{j=1}^{n} f_j(0)\lambda_{j,i}\right)f_i(y)u_i(y)\right\}dy = 0. \tag{3.2.18}$$

Now comparing coefficients of $u_i(y)f_i(y)$ in (3.2.17) and (3.2.18), we obtain the following two equations

$$\frac{\delta_{j,i}}{f_i(0)} + f_j'(0)\lambda_{j,i} - \frac{\delta_{k,i}}{f_i(0)} - f_k'(0)\lambda_{k,i} = c\left(f_j(0)\lambda_{j,i} - f_k(0)\lambda_{k,i}\right) \tag{3.2.19}$$

and

$$\sum_{j=1}^{n} f_j(0)\lambda_{j,i} = 0. \tag{3.2.20}$$

Substituting $\lambda_{j,i}$ from (3.2.19) into (3.2.20), we get

$$\sum_{j=1}^{n} f_j(0)\frac{(f_k'(0)-cf_k(0))\lambda_{k,i}+(\delta_{k,i}-\delta_{j,i})(f_i(0))^{-1}}{f_j'(0)-cf_j(0)}=0.$$

After some simplifications, we arrive at

$$\lambda_{k,i}=\frac{1}{\left(1-c\frac{f_k(0)}{f_k'(0)}\right)\left(1-c\frac{f_i(0)}{f_i'(0)}\right)P(\kappa)f_k'(0)f_i'(0)}-\frac{\delta_{k,i}}{f_k'(0)f_i(0)\left(1-c\frac{f_k(0)}{f_k'(0)}\right)}.$$

□

We can now write (3.2.1) for δ-conditions using (3.2.3) as

$$R^{\delta_a}_{j,l}(x,y;z):=\delta_{j,l}R^D_j(x,y;z)+\frac{f_j(x,\kappa)f_l(y,\kappa)}{(a-K(\kappa))f_j(0,\kappa)f_l(0,\kappa)}. \tag{3.2.21}$$

For unperturbed operator i.e. when $V_j(x)\equiv 0$, we may let

$$f_j(x,\kappa)=e^{ix_j\kappa}\Rightarrow K(\kappa)=in\kappa$$

hence

$$R^{\delta_a}_{(0),j,l}(x,y;z):=\delta_{j,l}R^D_{(0),j}(x,y;z)+\frac{e^{i(x_j+y_l)\kappa}}{a-in\kappa}. \tag{3.2.22}$$

Equation (3.2.1) for δ'-conditions (3.1.4) after substituting equation (3.2.3), becomes

$$\begin{aligned}R^{\delta_b'}_{j,l}(x,y;z):=&\delta_{j,l}R^D_j(x,y;z)\\&+\left(\frac{1}{(M(\kappa)-b)f_j'(0,\kappa)f_l'(0,\kappa)}-\frac{\delta_{j,l}}{f_j'(0,\kappa)f_l(0,\kappa)}\right)f_j(x,\kappa)f_l(y,\kappa).\end{aligned} \tag{3.2.23}$$

For unperturbed operator, we have

$$M(\kappa)=\frac{n}{i\kappa}$$

therefore

$$R^{\delta_b'}_{(0),j,l}(x,y;z):=\delta_{j,l}R^D_{(0),j}(x,y;z)+\left(\frac{1}{(n-b\kappa i)\kappa i}-\frac{\delta_{j,l}}{\kappa i}\right)e^{i(x_j+y_l)\kappa}. \tag{3.2.24}$$

Similarly,

$$R^{\hat{\delta}_d}_{j,l}(x,y;z) := \delta_{j,l} R^D_j(x,y;z) \tag{3.2.25}$$

$$+ \left(d\delta_{j,l} - \frac{1}{\left(1 - d\frac{f_l'(0,\kappa)}{f_l(0,\kappa)}\right) J(\kappa)} \right) \frac{f_j(x,\kappa) f_l(y,\kappa)}{\left(1 - d\frac{f_j'(0,\kappa)}{f_j(0,\kappa)}\right) f_j(0,\kappa) f_l(0,\kappa)}, \tag{3.2.26}$$

and for the unperturbed operator, we have

$$J(\kappa) = n\left(\frac{i\kappa}{1 - di\kappa}\right),$$

and hence

$$R^{\hat{\delta}_d}_{(0),j,l}(x,y;z) := \delta_{j,l} R^D_{(0),j}(x,y;z) + \left(d\delta_{j,l} - \frac{1}{in\kappa} \right) \frac{e^{i(x_j+y_l)\kappa}}{1 - id\kappa}. \tag{3.2.27}$$

Finally for $\hat{\delta}'_c$ conditions, equation (3.2.1), after substituting equation (3.2.3), becomes

$$R^{\hat{\delta}'_c}_{j,l}(x,y;z) := \delta_{j,l} R^D_j(x,y;z) +$$
$$\left(\frac{f_j(x,\kappa) f_l(y,\kappa)}{\left(1 - c\frac{f_j(0,\kappa)}{f_j'(0,\kappa)}\right)\left(1 - c\frac{f_l(0,\kappa)}{f_l'(0,\kappa)}\right) P(\kappa) f_j'(0,\kappa) f_l'(0,\kappa)} - \frac{\delta_{j,l} f_j(x,\kappa) f_l(y,\kappa)}{f_j'(0,\kappa) f_l(0,\kappa)\left(1 - c\frac{f_j(0,\kappa)}{f_j'(0,\kappa)}\right)} \right). \tag{3.2.28}$$

For the corresponding unperturbed operator

$$P(\kappa) = \frac{n}{i\kappa - c}$$

and hence

$$R^{\hat{\delta}'_c}_{(0),j,l}(x,y;z) := \delta_{j,l} R^D_{(0),j}(x,y;z) + \left(\frac{1}{n} - \delta_{j,l} \right) \frac{e^{i(x_j+y_l)\kappa}}{i\kappa - c}. \tag{3.2.29}$$

Remark 3.2.2. *The operators considered in this chapter can be seen as particular cases of a more general matrix valued Schrödinger operator considered in [94] on the half-line when potential is a diagonal matrix. The fact that the resolvent differences of perturbed and unperturbed operators belong to trace class follow from Lemma 9.1 of [94].*

The following theorem gives the traces of resolvent differences of perturbed and unperturbed operators.

Theorem 3.2.3. *If Γ is a star graph and the potential function V satisfy condition* (3.1.2) *then*

1. *the trace of the resolvent difference of Schrödinger operators $H^{\delta_a}_{V,\Gamma}$ and $H^{\delta_a}_{0,\Gamma}$ is given by*

$$Tr(R^{\delta_a}_{V,\Gamma}(z) - R^{\delta_a}_{0,\Gamma}(z)) = -\frac{1}{2\kappa}\left(\frac{d}{d\kappa}\ln\left(\frac{(K(\kappa)-a)}{\kappa+\frac{a}{n}i}\prod_{j=1}^{n} w_j(\kappa)\right)\right),$$

2. *the trace of the resolvent difference of operators $H^{\delta'_b}_{V,\Gamma}$ and $H^{\delta'_b}_{0,\Gamma}$ is given by*

$$Tr(R^{\delta'_b}_{V,\Gamma}(z) - R^{\delta'_b}_{0,\Gamma}(z)) = -\frac{1}{2\kappa}\left(\frac{d}{d\kappa}\left(\ln\left(\frac{(M(\kappa)-b)}{(b\kappa i-n)\kappa^{n-1}}\prod_{j=1}^{n} f'_j(0,\kappa)\right)\right)\right),$$

3. *the trace of the resolvent difference of operators $H^{\hat{\delta}_d}_{V,\Gamma}$ and $H^{\hat{\delta}_d}_{0,\Gamma}$ is given by*

$$Tr(R^{\hat{\delta}_d}_{V,\Gamma}(z) - R^{\hat{\delta}_d}_{0,\Gamma}(z)) = -\frac{1}{2\kappa}\left(\frac{d}{d\kappa}\ln\left(\frac{(J(\kappa)}{(i+d\kappa)^{n-1}\kappa}\prod_{j=1}^{n}(w_j(\kappa)-df'_j(0,\kappa))\right)\right),$$

4. *the trace of the resolvent difference of operators $H^{\hat{\delta}'_c}_{V,\Gamma}$ and $H^{\hat{\delta}'_c}_{0,\Gamma}$ is given by*

$$Tr(R^{\hat{\delta}'_c}_{V,\Gamma}(z) - R^{\hat{\delta}'_c}_{0,\Gamma}(z)) = -\frac{1}{2\kappa}\left(\frac{d}{d\kappa}\left(\ln\left(P(\kappa)(\kappa+ic)^{1-n}\prod_{j=1}^{n}\left(f'_j(0,\kappa)-cf_j(0,\kappa)\right)\right)\right)\right).$$

Here the functions $K(\kappa)$, $M(\kappa)$, $J(\kappa)$ and $P(\kappa)$ are given in Theorem (3.2.1).

Proof. 1. Consider

$$\mathrm{Tr}(R^{\delta_a}_{V,\Gamma}(z) - R^{\delta_a}_{0,\Gamma}(z)) = \sum_{j=1}^{n}\int_{e_j}\left(R_{j,j}(x,x,z) - R_{(0),j,j}(x,x,z)\right)dx.$$

Using (3.2.21) and (3.2.22)

$$\begin{aligned}\mathrm{Tr}(R^{\delta_a}_{V,\Gamma}(z) - R^{\delta_a}_{0,\Gamma}(z)) = &\sum_{j=1}^{n}\int_{e_j}\left(R^D_j(x,x,z) - R^D_{(0),j}(x,x,z)\right)dx\\ &+\sum_{j=1}^{n}\int_{e_j}\left(\frac{f_j^2(x,\kappa)}{(a-K(\kappa))f_j^2(0,\kappa)}+\frac{e^{2ix\kappa}}{in\kappa-a}\right)dx. \qquad (3.2.30)\end{aligned}$$

The first integral on the right hand side of (3.2.30) is given by, (see references [18] and [97])

$$\sum_{j=1}^{n}\int_{e_j}\left(R_j^D(x,x,z)-R_{(0),j}^D(x,x,z)\right)dx=-\frac{1}{2\kappa}\sum_{j=1}^{n}\frac{\dot{w}_j(\kappa)}{w_j(\kappa)}. \tag{3.2.31}$$

To compute the second term in (3.2.30), we make use of the following identity which is holds for two arbitrary solutions $u_j(x,\kappa)$ and $v_j(x,\kappa)$ of $H_{e_j}^D\psi_j=\kappa^2\psi_j$

$$u_j(x,\kappa)v_j(x,\kappa)=\frac{(u_j'(x,\kappa)\dot{v}_j(x,\kappa)-u_j(x,\kappa)\dot{v}_j'(x,\kappa))'}{2\kappa}. \tag{3.2.32}$$

Let $u_j=v_j=f_j$, we get

$$\sum_{j=1}^{n}\int_{e_j}\frac{f_j^2(x,\kappa)}{(a-K(\kappa))f_j^2(0,\kappa)}dx=\sum_{j=1}^{n}\frac{[f_j'(x,\kappa)\dot{f}_j(x,\kappa)-f_j(x,\kappa)\dot{f}_j'(x,\kappa)]_0^\infty}{2\kappa(a-K(\kappa))f_j^2(0,\kappa)}.$$

For the case of compactly supported potential V_j, the Jost solution $f_j(x,\kappa)$ is equal to $e^{i\kappa x}$. Letting $x\to\infty$, we obtain

$$f_j'(x,\kappa)\dot{f}_j(x,\kappa)-f_j(x,\kappa)\dot{f}_j'(x,\kappa)=ie^{2\kappa xi}.$$

As $\mathrm{Im}(\kappa)>0$, so $x\to\infty$ implies $ie^{2\kappa xi}\to 0$. Hence we are left with

$$\sum_{j=1}^{n}\int_{e_j}\frac{f_j^2(x,\kappa)}{(a-K(\kappa))f_j^2(0,\kappa)}dx=\sum_{j=1}^{n}\frac{f_j(0,\kappa)\dot{f}_j'(0,\kappa)-f_j'(0,\kappa)\dot{f}_j(0,\kappa)}{2\kappa(a-K(\kappa))f_j^2(0,\kappa)}=-\frac{\dot{K}(\kappa)}{2\kappa(K(\kappa)-a)}. \tag{3.2.33}$$

By a density argument the above result can be extended to all potentials satisfying (3.1.2), see Proposition 4.5.3 of [97]. It only remains to compute the last integral appearing in (3.2.30)

$$\sum_{j=1}^{n}\int_{e_j}\left(\frac{e^{2ix\kappa}}{in\kappa-a}\right)dx=\frac{1}{2\kappa(\kappa+\frac{a}{n}i)}. \tag{3.2.34}$$

Substituting values from (3.2.31), (3.2.33) and (3.2.34) in (3.2.30), we get

$$\begin{aligned}\mathrm{Tr}(R_{V,\Gamma}^{\delta_a}(z)-R_{0,\Gamma}^{\delta_a}(z))&=-\frac{1}{2\kappa}\left(\sum_{j=1}^{n}\frac{\dot{w}_j(\kappa)}{w_j(\kappa)}+\frac{\dot{K}(\kappa)}{K(\kappa)-a}-\frac{1}{(\kappa+\frac{a}{n}i)}\right)\\&=-\frac{1}{2\kappa}\left(\sum_{j=1}^{n}\frac{d}{d\kappa}\ln(w_j(\kappa))+\frac{d}{d\kappa}\ln(K(\kappa)-a)-\frac{d}{d\kappa}\ln((\kappa+\frac{a}{n}i))\right)\\&=-\frac{1}{2\kappa}\left(\frac{d}{d\kappa}\ln\left(\frac{(K(\kappa)-a)}{\kappa+\frac{a}{n}i}\prod_{j=1}^{n}w_j(\kappa)\right)\right).\end{aligned}$$

2. The proof of this part uses the same argument as above. We only point out the differences arising due to the δ' vertex conditions. Using (3.2.23) and (3.2.24) we see that

$$\begin{aligned}\mathrm{Tr}(R^{\delta'_b}_{V,\Gamma}(z) - R^{\delta'_b}_{0,\Gamma}(z)) = &\sum_{j=1}^{n} \int_{e_j} \left(R^D_j(x,x,z) - R^D_{(0),j}(x,x,z) \right) dx \\ &+ \sum_{j=1}^{n} \int_{e_j} \left(\frac{1}{(M(\kappa)-b) f_j'^2(0,\kappa)} - \frac{1}{f_j'(0,\kappa) f_j(0,\kappa)} \right) f_j^2(x,\kappa) dx \\ &- \sum_{j=1}^{n} \int_{e_j} \left(\frac{1}{(n-b\kappa i)\kappa i} - \frac{1}{\kappa i} \right) e^{2ix\kappa} dx. \end{aligned} \tag{3.2.35}$$

To compute the second integral we use identity (3.2.32) and obtain

$$\begin{aligned}&\sum_{j=1}^{n} \int_{e_j} \left(\frac{1}{(M(\kappa)-b) f_j'^2(0,\kappa)} - \frac{1}{f_j'(0,\kappa) f_j(0,\kappa)} \right) f_j^2(x,\kappa) dx \\ &= \sum_{j=1}^{n} \left(\frac{1}{(M(\kappa)-b) f_j'^2(0,\kappa)} - \frac{1}{f_j'(0,\kappa) f_j(0,\kappa)} \right) \left(\frac{f_j(0,\kappa)\dot{f}_j'(0,\kappa) - f_j'(0,\kappa)\dot{f}_j(0,\kappa)}{2\kappa} \right) \\ &= \frac{1}{2\kappa} \left(\frac{\dot{M}(\kappa)}{b - M(\kappa)} + \sum_{j=1}^{n} \left(\frac{\dot{f}_j(0,\kappa)}{f_j(0,\kappa)} - \frac{\dot{f}_j'(0,\kappa)}{f_j'(0,\kappa)} \right) \right) \\ &= -\frac{1}{2\kappa} \left(\frac{d}{d\kappa} \ln(M(\kappa) - b) - \sum_{j=1}^{n} \frac{d}{d\kappa} \ln \left(\frac{f_j(0,\kappa)}{f_j'(0,\kappa)} \right) \right) \\ &= -\frac{1}{2\kappa} \frac{d}{d\kappa} \left(\ln \left((M(\kappa) - b) \prod_{j=1}^{n} \frac{f_j'(0,\kappa)}{f_j(0,\kappa)} \right) \right). \end{aligned} \tag{3.2.36}$$

The last integral on the right hand side of equation (3.2.35) becomes

$$\begin{aligned}\sum_{j=1}^{n} \int_{e_j} \left(\frac{1}{(n-b\kappa i)\kappa i} - \frac{1}{\kappa i} \right) e^{2ix\kappa} dx &= -\left(\frac{1}{(n-b\kappa i)\kappa i} - \frac{1}{\kappa i} \right) \left(\frac{n}{2\kappa i} \right) \\ &= \frac{1}{2\kappa} \left(\frac{n}{(n-b\kappa i)\kappa} - \frac{n}{\kappa} \right) \\ &= \frac{1}{2\kappa} \frac{d}{d\kappa} \left(\ln(\kappa) - \ln(b\kappa i - n) - \ln(\kappa^n) \right) \\ &= \frac{1}{2\kappa} \frac{d}{d\kappa} \left(\ln \left(\frac{1}{(b\kappa i - n)\kappa^{n-1}} \right) \right). \end{aligned} \tag{3.2.37}$$

Substituting the values from (3.2.31), (3.2.36) and (3.2.37) into (3.2.35), we get

$$\begin{aligned}
&\mathrm{Tr}(R^{\delta_b'}_{V,\Gamma}(z) - R^{\delta_b'}_{0,\Gamma}(z)) \\
&= -\frac{1}{2\kappa}\left(\frac{d}{d\kappa}\left(\ln\left(\prod_{j=1}^{n} w_j(\kappa)\right) + \ln\left((M(\kappa)-b)\prod_{j=1}^{n}\frac{f_j'(0,\kappa)}{f_j(0,\kappa)}\right) + \ln\left(\frac{1}{(b\kappa i - n)\kappa^{n-1}}\right)\right)\right) \\
&= -\frac{1}{2\kappa}\left(\frac{d}{d\kappa}\left(\ln\left(\frac{(M(\kappa)-b)}{(b\kappa i - n)\kappa^{n-1}}\prod_{j=1}^{n} f_j'(0,\kappa)\right)\right)\right).
\end{aligned}$$

3. The $R^{\hat{\delta}_d}_{V,\Gamma}(z) - R^{\hat{\delta}_d}_{0,\Gamma}(z)$ belongs to trace class and

$$\mathrm{Tr}(R^{\hat{\delta}_d}_{V,\Gamma}(z) - R^{\hat{\delta}_d}_{0,\Gamma}(z)) = \sum_{j=1}^{n}\int_{e_j}\left(R_{j,j}(x,x,z) - R_{(0),j,j}(x,x,z)\right)dx.$$

Using (3.2.25) and (3.2.27) we see that

$$\begin{aligned}
Tr(R^{\hat{\delta}_d}_{V,\Gamma}(z) - R^{\hat{\delta}_d}_{0,\Gamma}(z)) &= \sum_{j=1}^{n}\int_{e_j}\left(R^D_j(x,x,z) - R^D_{(0),j}(x,x,z)\right)dx \\
&\quad + \sum_{j=1}^{n}\int_{e_j}\left(\frac{d}{1-d\frac{f_j'(0,\kappa)}{f_j(0,\kappa)}} - \frac{1}{\left(1-d\frac{f_j'(0,\kappa)}{f_j(0,\kappa)}\right)^2 J(\kappa)}\right)\frac{f_j^2(x,\kappa)}{f_j^2(0,\kappa)}dx \\
&\quad - \sum_{j=1}^{n}\int_{e_j}\left(\frac{d}{1-id\kappa} - \frac{1}{in\kappa(1-id\kappa)}\right)e^{2ix\kappa}dx. \qquad (3.2.38)
\end{aligned}$$

Using identity (3.2.32) the second integral on the right hand side can be computed as

$$\begin{aligned}
&\sum_{j=1}^{n}\int_{e_j}\left(\frac{d}{1-d\frac{f_j'(0,\kappa)}{f_j(0,\kappa)}} - \frac{1}{\left(1-d\frac{f_j'(0,\kappa)}{f_j(0,\kappa)}\right)^2 J(\kappa)}\right)\frac{f_j^2(x,\kappa)}{f_j^2(0,\kappa)}dx \\
&= \sum_{j=1}^{n}\left(\frac{d}{1-d\frac{f_j'(0,\kappa)}{f_j(0,\kappa)}} - \frac{1}{\left(1-d\frac{f_j'(0,\kappa)}{f_j(0,\kappa)}\right)^2 J(\kappa)}\right)\frac{[f_j'(x,\kappa)\dot{f}_j(x,\kappa) - f_j(x,\kappa)\dot{f}_j'(x,\kappa)]_0^\infty}{2\kappa f_j^2(0,\kappa)}dx.
\end{aligned}$$

When $x \to \infty$

$$f_j'(x,\kappa)\dot{f}_j(x,\kappa) - f_j(x,\kappa)\dot{f}_j'(x,\kappa) = ie^{2\kappa x i}.$$

As $\mathrm{Im}(\kappa) > 0$, so $x \to \infty$ implies $ie^{2\kappa x i} \to 0$. Hence, we are left with

$$\sum_{j=1}^{n} \int_{e_j} \left(\frac{d}{1 - d\frac{f_j'(0,\kappa)}{f_j(0,\kappa)}} - \frac{1}{\left(1 - d\frac{f_j'(0,\kappa)}{f_j(0,\kappa)}\right)^2 J(\kappa)} \right) \frac{f_j^2(x,\kappa)}{f_j^2(0,\kappa)} dx$$
$$= \sum_{j=1}^{n} \left(\frac{d}{1 - d\frac{f_j'(0,\kappa)}{f_j(0,\kappa)}} - \frac{1}{\left(1 - d\frac{f_j'(0,\kappa)}{f_j(0,\kappa)}\right)^2 J(\kappa)} \right) \frac{f_j(0,\kappa)\dot{f}_j'(0,\kappa) - f_j'(0,\kappa)\dot{f}_j(0,\kappa)}{2\kappa f_j^2(0,\kappa)} dx.$$

Using

$$\frac{d}{d\kappa}\left(\frac{f_j'(0,\kappa)}{f_j(0,\kappa)}\right) = \frac{f_j(0,\kappa)\dot{f}_j'(0,\kappa) - f_j'(0,\kappa)\dot{f}_j(0,\kappa)}{f_j^2(0,\kappa)}$$

and after some simplification, it can be shown that the above integral is equal to

$$\frac{-1}{2\kappa}\left(\sum_{j=1}^{n} \frac{\frac{d}{d\kappa}\left(1 - d\frac{f_j'(0,\kappa)}{f_j(0,\kappa)}\right)}{1 - d\frac{f_j'(0,\kappa)}{f_j(0,\kappa)}} + \frac{\dot{J}(\kappa)}{J(\kappa)} \right). \tag{3.2.39}$$

Now it only remains to compute the last integral on the right hand side of (3.2.38). Using partial fraction on the second term, we get

$$\sum_{j=1}^{n} \int_{e_j} \left(\frac{d}{1 - id\kappa} - \frac{1}{in\kappa(1 - id\kappa)} \right) e^{2ix\kappa} dx$$
$$= \sum_{j=1}^{n} \int_{e_j} \left(\left(1 - \frac{1}{n}\right) \frac{d}{1 - id\kappa} - \frac{1}{in\kappa} \right) e^{2ix\kappa} dx$$
$$= \frac{-1}{2\kappa}\left((n-1)\frac{d}{i + d\kappa} + \frac{1}{\kappa} \right). \tag{3.2.40}$$

Using the values from (3.2.31), (3.2.39) and (3.2.40) into (3.2.38), we get

$$\mathrm{Tr}(R_{V,\Gamma}^{\hat{\delta}_d}(z) - R_{0,\Gamma}^{\hat{\delta}_d}(z))$$
$$= -\frac{1}{2\kappa}\left(\sum_{j=1}^{n} \frac{\dot{w}_j(\kappa)}{w_j(\kappa)} + \sum_{j=1}^{n} \frac{\frac{d}{d\kappa}\left(1 - d\frac{f_j'(0,\kappa)}{f_j(0,\kappa)}\right)}{1 - d\frac{f_j'(0,\kappa)}{f_j(0,\kappa)}} + \frac{\dot{J}(\kappa)}{J(\kappa)} - (n-1)\frac{d}{i + d\kappa} - \frac{1}{\kappa} \right)$$
$$= -\frac{1}{2\kappa}\left(\sum_{j=1}^{n} \frac{d}{d\kappa}\ln(w_j(\kappa)) + \sum_{j=1}^{n} \frac{d}{d\kappa}\ln\left(1 - d\frac{f_j'(0,\kappa)}{f_j(0,\kappa)}\right) + \frac{d}{d\kappa}\ln(J(\kappa)) - \frac{d}{d\kappa}\ln\left((i + d\kappa)^{n-1}\kappa\right) \right)$$
$$= -\frac{1}{2\kappa}\left(\frac{d}{d\kappa}\ln\left(\frac{(J(\kappa)}{(i + d\kappa)^{n-1}\kappa} \prod_{j=1}^{n} (w_j(\kappa) - df_j'(0,\kappa)) \right) \right).$$

4. Using (3.2.28) and (3.2.29)

$$\begin{aligned}\mathrm{Tr}(R^{\hat{\delta}'_c}_{V,\Gamma}(z) - R^{\hat{\delta}'_c}_{0,\Gamma}(z)) &= \sum_{j=1}^{n} \int_{e_j} \left(R^D_j(x,x,z) - R^D_{(0),j}(x,x,z) \right) dx \\ &+ \sum_{j=1}^{n} \int_{e_j} \left(\frac{f_j^2(x,\kappa)}{\left(1 - c\frac{f_j(0,\kappa)}{f'_j(0,\kappa)}\right)^2 P(\kappa) f'^2_j(0,\kappa)} - \frac{f_j^2(x,\kappa)}{f'_j(0,\kappa) f_j(0,\kappa) \left(1 - c\frac{f_j(0,\kappa)}{f'_j(0,\kappa)}\right)} \right) dx \\ &- \sum_{j=1}^{n} \int_{e_j} \left(\frac{1-n}{n(i\kappa - c)} \right) e^{2ix\kappa} dx. \end{aligned} \tag{3.2.41}$$

To compute the second integral, we use identity (3.2.32) with the same arguments as above and get

$$\begin{aligned}&\sum_{j=1}^{n} \int_{e_j} \left(\frac{f_j^2(x,\kappa)}{\left(1 - c\frac{f_j(0,\kappa)}{f'_j(0,\kappa)}\right)^2 P(\kappa) f'^2_j(0,\kappa)} - \frac{f_j^2(x,\kappa)}{f'_j(0,\kappa) f_j(0,\kappa) \left(1 - c\frac{f_j(0,\kappa)}{f'_j(0,\kappa)}\right)} \right) dx \\ &= \sum_{j=1}^{n} \int_{e_j} \frac{1}{2\kappa} \left(\frac{f_j(0,\kappa)\dot{f}'_j(0,\kappa) - f'_j(0,\kappa)\dot{f}_j(0,\kappa)}{\left(1 - c\frac{f_j(0,\kappa)}{f'_j(0,\kappa)}\right)^2 P(\kappa) f'^2_j(0,\kappa)} - \frac{f_j(0,\kappa)\dot{f}'_j(0,\kappa) - f'_j(0,\kappa)\dot{f}_j(0,\kappa)}{f'_j(0,\kappa) f_j(0,\kappa) \left(1 - c\frac{f_j(0,\kappa)}{f'_j(0,\kappa)}\right)} \right) dx \\ &= -\frac{1}{2\kappa} \left(\frac{\dot{P}(\kappa)}{P(\kappa)} + \sum_{j=1}^{n} \left(\frac{\dot{f}'_j(0,\kappa)}{f'_j(0,\kappa)} - \frac{\dot{f}_j(0,\kappa)}{f_j(0,\kappa)} \right) \left(1 - c\frac{f_j(0,\kappa)}{f'_j(0,\kappa)} \right)^{-1} \right) \\ &= -\frac{1}{2\kappa} \left(\frac{d}{d\kappa} \ln(P(\kappa)) + \sum_{j=1}^{n} \frac{d}{d\kappa} \left(\ln\left(\frac{f'_j(0,\kappa)}{f_j(0,\kappa)} \right) + \ln\left(1 - c\frac{f_j(0,\kappa)}{f'_j(0,\kappa)} \right) \right) \right) \\ &= -\frac{1}{2\kappa} \left(\frac{d}{d\kappa} \left(\ln(P(\kappa)) + \sum_{j=1}^{n} \ln\left(\frac{f'_j(0,\kappa)}{f_j(0,\kappa)} - c \right) \right) \right) \\ &= -\frac{1}{2\kappa} \frac{d}{d\kappa} \left(\ln\left((P(\kappa) \prod_{j=1}^{n} \left(\frac{f'_j(0,\kappa)}{f_j(0,\kappa)} - c \right) \right) \right) \right). \end{aligned} \tag{3.2.42}$$

The last integral in equation (3.2.41) becomes

$$\begin{aligned}\sum_{j=1}^{n}\int_{e_j}\left(\frac{1-n}{n(i\kappa-c)}\right)e^{2ix\kappa}dx &= -\left(\frac{1-n}{n(i\kappa-c)}\right)\left(\frac{n}{2\kappa i}\right)\\ &=\frac{1}{2\kappa}\left(\frac{1-n}{(\kappa+ic)}\right)\\ &=\frac{1}{2\kappa}\frac{d}{d\kappa}\left(\ln\left((\kappa+ic)^{1-n}\right)\right). \qquad (3.2.43)\end{aligned}$$

Substituting the values from (3.2.31), (3.2.42) and (3.2.43) into (3.2.41), we get

$$\begin{aligned}&\mathrm{Tr}(R_{V,\Gamma}^{\hat{\delta}_c'}(z)-R_{0,\Gamma}^{\hat{\delta}_c'}(z))\\ &=-\frac{1}{2\kappa}\left(\frac{d}{d\kappa}\left(\ln\left(\prod_{j=1}^{n}w_j(\kappa)\right)+\ln\left((P(\kappa)\prod_{j=1}^{n}\left(\frac{f_j'(0,\kappa)}{f_j(0,\kappa)}-c\right)\right)+\ln\left((\kappa+ic)^{1-n}\right)\right)\right)\\ &=-\frac{1}{2\kappa}\left(\frac{d}{d\kappa}\left(\ln\left(P(\kappa)(\kappa+ic)^{1-n}\prod_{j=1}^{n}\left(f_j'(0,\kappa)-cf_j(0,\kappa)\right)\right)\right)\right).\end{aligned}$$

□

The rest of this section is devoted to computing explicit expressions for the (modified) perturbation determinants, when the perturbed and unperturbed Schrödinger operators defined on star graphs are subject to vertex conditions (3.1.3), (3.1.4), (3.1.5) or (3.1.6). From ow on, we shall refer to the modified perturbation determinant simply as the perturbation determinant and is given by

$$D(z) := \det(\mathbb{I}+\sqrt{V}R_0(z)\sqrt{|V|}), \quad z\in\rho(H_0).$$

Here, H_0 denotes the unperturbed Schrödinger operator, R_0 is the corresponding resolvent operator and $\sqrt{V}=\mathrm{sgn}V\sqrt{|V|}$.

We first consider the pair $H_{V,\Gamma}^{\delta_a}$ and $H_{0,\Gamma}^{\delta_a}$ of perturbed and unperturbed Schrödinger operators, respectively, on the star graph Γ satisfying the vertex conditions (3.1.3). The second term on the right side of (3.2.1) with values of $\lambda_{j,l}$ given by Theorem (3.2.1) (1) is a finite rank operator and under the assumption (3.1.2) on the function V, the operator $\sqrt{|V|}(H_{0,\Gamma}^{\delta_a})^{-1/2}$ is Hilbert-Schmidt and hence $\sqrt{V}R_{0,\Gamma}^{\delta_a}\sqrt{|V|}$ belongs to trace class. The implication is that the perturbation determinant D^{δ_a} is well defined.

With simple computations, it can be easily verified that the trace of resolvents difference of perturbed and unperturbed Schrödinger operators, $H_{V,\Gamma}^{\delta_a}, H_{0,\Gamma}^{\delta_a}$, and the corresponding perturbation determinant D^{δ_a} satisfies the relation

$$\mathrm{Tr}(R_{0,\Gamma}^{\delta_a}(z)-R_{V,\Gamma}^{\delta_a}(z))=\frac{\frac{d}{dz}(D^{\delta_a}(z))}{D^{\delta_a}(z)}, \qquad z\in\rho(H_{V,\Gamma}^{\delta_a})\cap\rho(H_{0,\Gamma}^{\delta_a}).$$

To compute the perturbation determinant, we choose $\kappa = \sqrt{z}$ such that $\mathrm{Im}(z) > 0$, then it follows from Theorem 3.2.3 (1) that

$$\frac{\frac{d}{dz}(D^{\delta_a}(z))}{D^{\delta_a}(z)} = \frac{\frac{d}{dz}\left(\left(\sqrt{z}+\frac{\alpha}{n}i\right)^{-1}(K(\sqrt{z})-\alpha)\prod_{j=1}^{n} w_j(\sqrt{z})\right)}{\left(\sqrt{z}+\frac{\alpha}{n}i\right)^{-1}(K(\sqrt{z})-\alpha)\prod_{j=1}^{n} w_j(\sqrt{z})}.$$

From here, it follows that

$$D^{\delta_a}(z) = C_1\left(\sqrt{z}+\frac{\alpha}{n}i\right)^{-1}(K(\sqrt{z})-\alpha)\prod_{j=1}^{n} w_j(\sqrt{z}), \quad C_1 \in \mathbb{C}.$$

In order to find the value of the complex coefficient C_1, we use the following asymptotic of perturbation determinant

$$\lim_{|\mathrm{Im}(z)|\to\infty} D^{\delta_a}(z) = 1.$$

This asymptotic holds if $\sqrt{|V|R^{\delta_a}_{0,\Gamma}(z)}$ is Hilbert-Schmidt operator [97]. Moreover, we have for $|\sqrt{z}| \to \infty$

$$w_j(\sqrt{z}) = f_j(0,\sqrt{z}) = 1 + O(|\sqrt{z}|^{-1}) \tag{3.2.44}$$

and

$$K(\sqrt{z}) = n\sqrt{z}i + O(1). \tag{3.2.45}$$

Using these asymptotics, we find $C_1 = (ni)^{-1}$. This proves the following expression for the perturbation determinant D^{δ_a}

Corollary 3.2.4. *Let condition (3.1.2) holds. Then for $z \in \rho(H^{\delta_a}_{V,\Gamma})$ such that $Im(\sqrt{z}) > 0$ the perturbation determinant D^{δ_a} of $H^{\delta_a}_{V,\Gamma}$ with respect to $H^{\delta_a}_{0,\Gamma}$ is given by*

$$D^{\delta_a}(z) = \frac{(K(\sqrt{z})-\alpha)\prod_{j=1}^{n} w_j(\sqrt{z})}{(n\sqrt{z}i-\alpha)}. \tag{3.2.46}$$

For the perturbation determinant $D^{\delta'_b}$ of $H^{\delta'_b}_{V,\Gamma}$ with respect to $H^{\delta'_b}_{0,\Gamma}$, we obtain, from Theorem 3.2.3 (2)

$$\frac{\frac{d}{dz}(D^{\delta'_b}(z))}{D^{\delta'_b}(z)} = \frac{\frac{d}{dz}\left((b\sqrt{z}i-n)^{-1}(\sqrt{z})^{1-n}(M(\sqrt{z})-b)\prod_{j=1}^{n} f'_j(0,\sqrt{z})\right)}{(b\sqrt{z}i-n)^{-1}(\sqrt{z})^{1-n}(M(\sqrt{z})-b)\prod_{j=1}^{n} f'_j(0,\sqrt{z})}.$$

This implies

$$D^{\delta'_b}(z) = C_2(b\sqrt{z}i - n)^{-1}(\sqrt{z})^{1-n}(M(\sqrt{z}) - b)\prod_{j=1}^{n} f'_j(0,\sqrt{z}), \quad C_2 \in \mathbb{C}.$$

The asymptotic of $f'_j(0,\sqrt{z})$ as $|\sqrt{z}| \to \infty$ is

$$f'_j(0,\sqrt{z}) = \sqrt{z}i + O(|\sqrt{z}|^{-1}) \tag{3.2.47}$$

and hence

$$M(\sqrt{z}) = \frac{n}{\sqrt{z}i} + O(1) \quad \text{as} \quad |\sqrt{z}| \to \infty. \tag{3.2.48}$$

This yields $C_2 = \dfrac{1}{i^{n+1}} = e^{-(n+1)\frac{\pi}{2}i}$. This proves the following expression for the perturbation determinant $D^{\delta'_b}$

Corollary 3.2.5. *Let condition (3.1.2) holds. Then for $z \in \rho(H^{\delta'_b}_{V,\Gamma})$ such that $Im(\sqrt{z}) > 0$ the perturbation determinant of $H^{\delta'_b}_{V,\Gamma}$ with respect to $H^{\delta'_b}_{0,\Gamma}$ is given by*

$$D^{\delta'_b}(z) = \frac{(M(\sqrt{z}) - b)\prod_{j=1}^{n} f'_j(0,\sqrt{z})}{e^{(n+1)\frac{\pi}{2}i}\,(b\sqrt{z}i - n)\,(\sqrt{z})^{n-1}}. \tag{3.2.49}$$

To find perturbation determinant $D^{\hat{\delta}_d}$ of $H^{\hat{\delta}_d}_{V,\Gamma}$ with respect to $H^{\hat{\delta}_d}_{0,\Gamma}$ we use Theorem 3.2.3 (3) which gives

$$\frac{\frac{d}{dz}(D^{\hat{\delta}_d}(z))}{D^{\hat{\delta}_d}(z)} = \frac{\dfrac{d}{dz}\left(\dfrac{J(\sqrt{z})}{(i + d\sqrt{z})^{n-1}\sqrt{z}}\prod_{j=1}^{n}(w_j(\sqrt{z}) - df'_j(0,\sqrt{z}))\right)}{\dfrac{J(\sqrt{z})}{(i + d\sqrt{z})^{n-1}\sqrt{z}}\prod_{j=1}^{n}(w_j(\sqrt{z}) - df'_j(0,\sqrt{z}))}.$$

From here, it follows that

$$D^{\hat{\delta}_d}(z) = C_3\frac{J(\sqrt{z})}{(i + d\sqrt{z})^{n-1}\sqrt{z}}\prod_{j=1}^{n}(w_j(\sqrt{z}) - df'_j(0,\sqrt{z})), \quad C_3 \in \mathbb{C}.$$

Using (3.2.44) and (3.2.47) we obtain

$$J(\sqrt{z}) = n\left(\frac{i\sqrt{z}}{1 - di\sqrt{z}}\right) + O(1) \quad \text{as} \quad |\sqrt{z}| \to \infty. \tag{3.2.50}$$

This yields $C_3 = \dfrac{i^{n-1}}{ni}$ and completes the proof of the following corollary

Corollary 3.2.6. *Let condition* (3.1.2) *holds. Then for* $z \in \rho(H_{V,\Gamma}^{\hat{\delta}_d})$ *such that* $Im(\sqrt{z}) > 0$ *the perturbation determinant of* $H_{V,\Gamma}^{\hat{\delta}_d}$ *with respect to* $H_{0,\Gamma}^{\hat{\delta}_d}$ *is given by*

$$D^{\hat{\delta}_d}(z) = \frac{J(\sqrt{z})}{(1 - d\sqrt{z}i)^{n-1} n\sqrt{z}i} \prod_{j=1}^{n} (w_j(\sqrt{z}) - df_j'(0, \sqrt{z})). \tag{3.2.51}$$

Now we find the expression for the perturbation determinant when the Schrödinger operator is subject to vertex conditions (3.1.6). Theorem 3.2.3 (4) implies

$$\frac{\frac{d}{dz}(D^{\hat{\delta}'_c}(z))}{D^{\hat{\delta}'_c}(z)} = \frac{\frac{d}{dz}\left(\frac{P(\sqrt{z})}{(\sqrt{z}+ic)^{n-1}} \prod\limits_{j=1}^{n} \left(f_j'(0,\sqrt{z}) - cf_j(0,\sqrt{z})\right)\right)}{\frac{P(\sqrt{z})}{(\sqrt{z}+ic)^{n-1}} \prod\limits_{j=1}^{n} \left(f_j'(0,\sqrt{z}) - cf_j(0,\sqrt{z})\right)}.$$

This yields

$$D^{\hat{\delta}'_c}(z) = C_4 \frac{P(\sqrt{z}) \prod\limits_{j=1}^{n} \left(f_j'(0,\sqrt{z}) - cf_j(0,\sqrt{z})\right)}{(\sqrt{z}+ic)^{n-1}}, \quad C_4 \in \mathbb{C}.$$

Using (3.2.44) and (3.2.47) We obtain

$$P(\sqrt{z}) = \frac{n}{\sqrt{z}i - c} + O(1), \quad \text{as} \quad |\sqrt{z}| \to \infty. \tag{3.2.52}$$

Hence $C_4 = \dfrac{1}{ni^{n-1}}$ and we have the following result

Corollary 3.2.7. *Assume condition* (3.1.2) *holds. Then for* $z \in \rho(H_{V,\Gamma}^{\hat{\delta}'_c})$ *such that* $Im(\sqrt{z}) > 0$ *the perturbation determinant of* $H_{V,\Gamma}^{\hat{\delta}'_c}$ *with respect to* $H_{0,\Gamma}^{\hat{\delta}'_c}$ *can be expressed as*

$$D^{\hat{\delta}'_c}(z) = \frac{P(\sqrt{z}) \prod\limits_{j=1}^{n} \left(f_j'(0,\sqrt{z}) - cf_j(0,\sqrt{z})\right)}{n(\sqrt{z}i - c)^{n-1}}, \quad C_4 \in \mathbb{C}. \tag{3.2.53}$$

In what follows we briefly discuss the relationship between perturbation determinant and spectral shift function. Let H denotes any of the Schrödinger operators $H_{V,\Gamma}^{\delta_a}, H_{V,\Gamma}^{\delta'_b}, H_{V,\Gamma}^{\hat{\delta}_d}$ or $H_{V,\Gamma}^{\hat{\delta}'_c}$ and H_0 is the corresponding unperturbed operator. The resolvents of H and H_0 are denoted by $R(z)$ and $R_0(z)$, respectively. If the potential function V satisfies (3.1.2) then from the above discussion the difference $R(z) - R_0(z)$ is a trace class operator for $z \in \rho(H)$ and the spectral shift function $\xi(\lambda; H, H_0)$ for H and H_0 can be defined via the following trace formula

$$\mathrm{Tr}(f(H) - f(H_0)) := \int_{-\infty}^{\infty} \xi(\lambda; H, H_0) f'(\lambda)\, d\lambda \tag{3.2.54}$$

for any $f \in C_0^\infty(\mathbb{R})$.

Theorem 9.2 of [94] explicitly characterize the spectral shift function in the more general case of matrix valued Schrödinger operators with general self-adjoint conditions at the origin. On the negative real-line, it was shown that the function $\xi(\lambda) = 0$ for $\lambda < \lambda_1$ and $\xi(\lambda) = -\sum_{i=1}^{p} m_i$ for $\lambda_p < \lambda < \lambda_{p+1}$, where $\lambda_1 < \lambda_2 < ....$ are the negative eigenvalues and m_i are their corresponding multiplicities. On the positive real-line $\xi(\lambda) = -\frac{1}{2\pi} f(\sqrt{\lambda})$, where $f(\lambda)$ is the continuous branch of the argument of the determinant of scattering matrix. It was also proved that the trace formula (3.2.54) holds for a bigger class of functions satisfying $f'(\lambda) = O(\lambda^{-1/2-\epsilon})$, $f''(\lambda) = O(\lambda^{-1-\epsilon})$, $\epsilon > 0$, $\lambda \to \infty$ and

$$\int_{-\infty}^{\infty} |\xi(\lambda; H, H_0)|(1 + |\lambda|)^{-1/2-\epsilon}\, d\lambda < \infty, \quad \epsilon > 0.$$

One of the main ingredient in the proof of Theorem 9.2 of [94] is the following estimate (cf. inequality (9.2) of [94], see also (5.11) of [97])

$$||R(-t) - R_0(-t)||_1 \leq C_\epsilon t^{-\frac{3}{2}+\epsilon}, \quad \epsilon > 0, \quad t \to \infty. \tag{3.2.55}$$

The above estimates are non-trivial and we provide its explicit derivation in Appendix (B). The above estimate implies

$$\int_1^{\infty} t^{-m} ||R_V^{\mathcal{A}}(-t) - R_0^{\mathcal{A}}(-t)||_1 < \infty$$

which holds for all $m > -1/2$. Proposition (3.3) of [18] then implies

$$\xi(\lambda;\, H, H_0) = \pi^{-1} \lim_{\epsilon \to 0} \arg D(\lambda + i\epsilon),$$

where $\arg D(z) = \operatorname{Im} \ln D(z)$ is defined by the condition $\ln D(z) \to 0$ as $\operatorname{dist}\{z, \sigma(H_0)\} \to \infty$. Moreover,

$$\ln D(z) = \int_{-\infty}^{\infty} \xi(\lambda;\, H, H_0)(\lambda - z)^{-1}\, d\lambda, \quad z \in \rho(H_0) \cap \rho(H).$$

3.3 Levinson's Formula

In this section we prove zero order trace formulas for the operators $H_{V,\Gamma}^{\delta_a}$, $H_{V,\Gamma}^{\delta'_b}$, $H_{V,\Gamma}^{\hat{\delta}_d}$ and $H_{V,\Gamma}^{\hat{\delta}'_c}$. These trace formulas are called Levinson's formulas and they provide a relationships between the number of negative eigenvalues of operators and their associated phase shift functions. The phase shift function is denoted by η and is defined in terms of the perturbation determinant as:

$$D(k) = a(k)e^{i\eta(k)}, \quad a(k) = |D(k)|, \quad \eta(k) = \arg D(k), \quad k \in \mathbb{R},$$

where the function $a(k)$ is called the limit amplitude. The Levinson's formula derived in this section is closely related to the Levinson's formulas obtained in Theorem 9.3 of [5] and Theorem 9.3 of [94]. Levinson's formula of [5] relates the number of negative eigenvalues with the determinant of the scattering matrix and certain parameters that depend on the boundary conditions. Formula obtained in [94] relates the number of negative eigenvalues with the spectral shift function. The vertex conditions of this chapter can be expressed as a particular case of more general conditions considered in references [5] and [94] and therefore the Levinson's formulas obtained there also holds for the operator studied in this chapter. Higher order trace formulas for Schrödinger operator, on star shaped graph with most general form of self-adjoint vertex conditions, in terms of limit amplitude and phase shift, we refer the reader to [95] and[92].

We will need the following low-energy asymptotics of the perturbation determinant.

Lemma 3.3.1. *Let the potential V satisfies the condition*

$$\int_{e_j} (1+x)|V_j(x)|dx < \infty, \quad 1 \leq j \leq n. \tag{3.3.1}$$

Then we have the following asymptotes of the perturbation determinants:

1. *The perturbation determinant D^{δ_a} as $\kappa \to 0$, satisfy*

$$D^{\delta_a}(\kappa) = \begin{cases} C_1\kappa^{l-g_1}(1+o(1)) & w_j(0) \neq 0,\ \forall j = 1,\dots,n, \\ C_1\kappa^{m-1-g_1}(1+o(\kappa)) & w_j(0) = 0,\ j = 1,\dots,m,\ m \leq n, \end{cases}$$

   where, $C_1 \neq 0$ and $l = 0$ if $K(0) \neq a$ and $l = 1$ if $K(0) = a$ and g_1 is

$$g_1 = \begin{cases} 0 & a \neq 0, \\ 1 & a = 0. \end{cases}$$

2. *The perturbation determinant $D^{\delta'_b}$ as $\kappa \to 0$, satisfy*

$$D^{\delta'_b}(\kappa) = \begin{cases} C_2\kappa^{p-n}(1+o(1)) & f'_j(0,0) \neq 0, \forall j = 1,\dots,n \\ C_2\kappa^{m-n}(1+o(\kappa)) & f'_j(0,0) = 0,\ j = 1,\dots,m,\ m \leq n. \end{cases}$$

   where $C_2 \neq 0$ and $p = 1$, if $M(0) \neq b$ and $p = 2$ if $M(0) = b$.

3. *The perturbation determinant $D^{\hat{\delta}_d}$ as $\kappa \to 0$, satisfy*

$$D^{\hat{\delta}_d}(\kappa) = \begin{cases} C_3\kappa^{g_3}(1+o(1)) & f_j(0,0) - df'_j(0,0) \neq 0,\ \forall j = 1,\dots,n, \\ C_3\kappa^{m-2}(1+o(\kappa)) & f_j(0,0) - df'_j(0,0) = 0,\ j = 1,\dots,m,\ m \leq n. \end{cases}$$

where $C_3 \neq 0$ and g_3 is defined as

$$g_3 = \begin{cases} -1 & J(0) \neq 0, \\ 0 & J(0) = 0. \end{cases}$$

4. *The perturbation determinant $D^{\hat{\delta}'_c}$ as $\kappa \to 0$, satisfy*

$$D^{\hat{\delta}'_c}(\kappa) = \begin{cases} C_4 \kappa^{g_4}(1 + o(1)) & f'_j(0,0) - c f_j(0,0) \neq 0, \ \forall j = 1, \ldots, n, \\ C_4 \kappa^{m-1}(1 + o(\kappa)) & f'_j(0,0) - c f_j(0,0) = 0, \ j = 1, \ldots, m, \ m \leq n. \end{cases}$$

where $C_4 \neq 0$ and g_4 is defined as

$$g_4 = \begin{cases} 0 & P(0) \neq 0, \\ 1 & P(0) = 0. \end{cases}$$

Proof. 1. The expression for perturbation determinant is

$$D^{\delta_a}(\kappa) = \frac{(K(\kappa) - a) \prod_{j=1}^{n} w_j(\kappa)}{in\kappa - a}.$$

If $w_j(0) \neq 0$, $\forall j = 1, \ldots, n$, this implies that, either $K(0) - a = 0$ or $K(0) - a \neq 0$.
If $K(0) - a \neq 0$:
Then $D^{\delta_a}(\kappa)$ has no zeroes and we can let

$$\begin{aligned} &(K(0) - a) w_j(0) = C \neq 0 \\ &\Rightarrow \lim_{\kappa \to 0} D^{\delta_a}(\kappa) = \lim_{\kappa \to 0} \frac{C}{in\kappa - a} \\ &\Rightarrow \lim_{\kappa \to 0} D^{\delta_a}(\kappa)(in\kappa - a) = C \\ &\Rightarrow \lim_{\kappa \to 0} \frac{D^{\delta_a}(\kappa)(in\kappa - a) - C}{C} = 0 \\ &\Rightarrow D^{\delta_a}(\kappa)(in\kappa - a) - C = o(C) \\ &\Rightarrow D^{\delta_a}(\kappa) = C(in\kappa - a)^{-1}(1 + o(1)) \text{ where } C \neq 0. \end{aligned}$$

If $K(0) - a = 0$:
First, we find asymptotic expansion for $K(\kappa)$. From Theorem 2.3 (iii) [3], we know that

$$\frac{f'_j(0,\kappa)}{f_j(0,\kappa)} = \frac{f'_j(0,0)}{f_j(0,0)} - \frac{i\kappa}{f_j^2(0,0)} + o(\kappa).$$

Summing from 1 to n gives

$$\sum_{j=1}^{n} \frac{f_j'(0,\kappa)}{f_j(0,\kappa)} = \sum_{j=1}^{n} \frac{f_j'(0,0)}{f_j(0,0)} - i\kappa \sum_{j=1}^{n} \frac{1}{f_j^2(0,0)} + o(\kappa).$$

$$K(\kappa) = K(0) - i\kappa C_7 + o(\kappa) \text{ where } C_7 = \sum_{j=1}^{n} \frac{1}{f_j^2(0,0)} \neq 0.$$

Hence

$$D^{\delta_a}(\kappa) = \frac{-i\kappa C_8 + o(\kappa)}{in\kappa - a} \text{ where } C_8 = C_7 \prod_{j=1}^{n} w_j(0) \neq 0$$

$$\Rightarrow D^{\delta_a}(\kappa) = (in\kappa - a)^{-1} i C_8 \kappa (1 + o(1)).$$

If $w_j(0) = 0$ for $j = 1, \ldots, m$; $\quad m \leq n$. i.e. $f_1(0,0) = \ldots = f_m(0,0) = 0$ then

$$\begin{aligned} D^{\delta_a}(z) &= \frac{1}{in\kappa - a} \left(\left(\sum_{j=1}^{n} \frac{f_j'(0,\kappa)}{f_j(0,\kappa)} - a \right) \prod_{k=1}^{n} f_k(0,\kappa) \right) \\ &= \frac{1}{in\kappa - a} \left(\left(\sum_{j=1}^{m} \frac{f_j'(0,\kappa)}{f_j(0,\kappa)} + \sum_{j=m+1}^{n} \frac{f_j'(0,\kappa)}{f_j(0,\kappa)} - a \right) \prod_{k=1}^{n} f_k(0,\kappa) \right) \\ &= \frac{1}{in\kappa - a} \left(\sum_{j=1}^{m} \frac{f_j'(0,\kappa)}{f_j(0,\kappa)} \prod_{k=1}^{n} f_k(0,\kappa) + \left(\sum_{j=m+1}^{n} \frac{f_j'(0,\kappa)}{f_j(0,\kappa)} - a \right) \prod_{k=1}^{n} f_k(0,\kappa) \right). \end{aligned} \tag{3.3.2}$$

We first consider the first term on the right hand side of (3.3.2) i.e.

$$\sum_{j=1}^{m} \frac{f_j'(0,\kappa)}{f_j(0,\kappa)} \prod_{k=1}^{n} f_k(0,\kappa) = \sum_{j=1}^{m} f_j'(0,\kappa) \prod_{k=1 k\neq j}^{n} f_k(0,\kappa).$$

In order to find the asymptotic of the above term, we use the following asymptotic for $f_j(x,\kappa)$ $j = 1, \ldots, m$ (cf. [17])

$$f_j(0,\kappa) = \kappa \dot{f}_j(0,0) + o(\kappa)$$

which implies

$$\prod_{j=1}^{m} f_j(0,\kappa) = \kappa^m \prod_{j=1}^{m} \dot{f}_j(0,0) + o(\kappa^m).$$

Therefore

$$\sum_{j=1}^{m} f_j'(0,\kappa) \prod_{k=1 k\neq j}^{n} f_k(0,\kappa) = \sum_{j=1}^{m} \kappa^{m-1} f_j'(0,0) \prod_{k=1 k\neq j}^{m} \dot{f}_k(0,0) \prod_{k=m+1}^{n} f_k(0,0) + o(\kappa^m).$$

We multiply and divide the right hand side by $\dot{f}_j(0,0) f_j'(0,0)$ and obtain

$$\sum_{j=1}^{m} f_j'(0,\kappa) \prod_{k=1 k\neq j}^{n} f_k(0,\kappa) = \sum_{j=1}^{m} \kappa^{m-1} \frac{(f_j'(0,0))^2}{\dot{f}_j(0,0) f_j'(0,0)} \prod_{k=1}^{m} \dot{f}_k(0,0) \prod_{k=m+1}^{n} f_k(0,0) + o(\kappa^m).$$

We now use the following identity: If $f(0,0) = 0$, then

$$\dot{f}(0,0) f'(0,0) = -i.$$

This implies

$$\begin{aligned}\sum_{j=1}^{m} f_j'(0,\kappa) \prod_{k=1 k\neq j}^{n} f_k(0,\kappa) &= \sum_{j=1}^{m} \kappa^{m-1} i f_j'(0,0))^2 \prod_{k=1}^{m} \dot{f}_k(0,0) \prod_{k=m+1}^{n} f_k(0,0) + o(\kappa^m) \\ &= C_9 \kappa^{m-1} + o(\kappa^m) \text{ where } C_9 \neq 0.\end{aligned}$$

We now consider the second term on the right hand side of (3.3.2) i.e.

$$\begin{aligned}&\left(\sum_{j=m+1}^{n} \frac{f_j'(0,\kappa)}{f_j(0,\kappa)} - a \right) \prod_{k=1}^{n} f_k(0,\kappa) \\ &= \left(\sum_{j=m+1}^{n} \frac{f_j'(0,\kappa)}{f_j(0,\kappa)} - a \right) \left(\kappa^m \prod_{j=1}^{m} \dot{f}_j(0,0) + o(\kappa^m) \right) = o(\kappa^m).\end{aligned}$$

In view of above

$$\begin{aligned}D^{\delta_a}(\kappa) &= \frac{1}{in\kappa - a} \left(C_9 \kappa^{m-1} + o(\kappa^m) \right) \\ &= \frac{C_9 \kappa^{m-1}}{in\kappa - a} \left(1 + o(\kappa) \right) \quad \text{as} \quad \kappa \to 0.\end{aligned}$$

2. The expression for the perturbation determinant $D^{\delta_b'}$ is

$$D^{\delta_b'}(\kappa) = \frac{(M(\kappa) - b) \prod_{j=1}^{n} f_j'(0,\kappa)}{i^{n+1}(b\kappa i - n)\kappa^{n-1}}.$$

If $f_j'(0,0) \neq 0$, $\forall j = 1, \ldots, n$ then, either $M(0) - b = 0$ or $M(0) - b \neq 0$. In the case of $M(0) - b \neq 0$, $D^{\delta_b'}(\kappa)$ has no zeroes and we can let

$$
\begin{aligned}
&(M(0) - b) \prod_{j=1}^{n} f_j'(0,0) = C \neq 0. \\
&\Rightarrow \lim_{\kappa \to 0} D^{\delta_b'}(\kappa) = \lim_{\kappa \to 0} \frac{C}{i^{n+1}(b\kappa i - n)\kappa^{n-1}} \\
&\Rightarrow \lim_{\kappa \to 0} D^{\delta_b'}(\kappa) i^{n+1}(b\kappa i - n)\kappa^{n-1} = C \\
&\Rightarrow \lim_{\kappa \to 0} \frac{D^{\delta_b'}(\kappa) i^{n+1}(b\kappa i - n)\kappa^{n-1} - C}{C} = 0 \\
&\Rightarrow D^{\delta_b'}(\kappa) i^{n+1}(b\kappa i - n)\kappa^{n-1} - C = o(C) \\
&\Rightarrow D^{\delta_b'}(\kappa) = C i^{-(n+1)}(b\kappa i - n)^{-1}\kappa^{1-n}(1 + o(1)) \text{ where } C \neq 0.
\end{aligned}
$$

In the case of $M(0) - b = 0$, we first find the asymptotic expansion for $M(\kappa)$ for small κ. From Theorem 2.3 (iv) [3],

$$\frac{f_j(0,\kappa)}{f_j'(0,\kappa)} = \frac{f_j(0,0)}{f_j'(0,0)} + \frac{i\kappa}{f_j'^2(0,0)} + o(\kappa).$$

Summing from 1 to n we get

$$
\begin{aligned}
\sum_{j=1}^{n} \frac{f_j(0,\kappa)}{f_j'(0,\kappa)} &= \sum_{j=1}^{n} \frac{f_j(0,0)}{f_j'(0,0)} + i\kappa \sum_{j=1}^{n} \frac{1}{f_j'^2(0,0)} + o(\kappa). \\
M(\kappa) = M(0) + i\kappa C_{10} + o(\kappa) &\text{ where } C_{10} = \sum_{j=1}^{n} \frac{1}{f_j'^2(0,0)} \neq 0.
\end{aligned}
$$

Hence

$$D^{\delta_b'}(\kappa) = \frac{i\kappa C_{11} + o(\kappa)}{i^{n+1}(b\kappa i - n)\kappa^{n-1}} \text{ where } C_{11} = C_{10} \prod_{j=1}^{n} f_j'(0,0) \neq 0.$$

$$\Rightarrow D^{\delta_b'}(\kappa) = C_{11} i^{-(n+1)}(b\kappa i - n)^{-1}\kappa^{2-n}(1 + o(1)).$$

If $f_j'(0,0)=0$ for $j=1,\dots,m;\quad m\le n$. i.e. $f_1'(0,0)=\dots,=f_m'(0,0)=0$ then

$$\begin{aligned}
D^{\delta_b'}(\kappa) &= \frac{1}{i^{n+1}(b\kappa i-n)\kappa^{n-1}}\left(\left(\sum_{j=1}^{n}\frac{f_j(0,\kappa)}{f_j'(0,\kappa)}-b\right)\prod_{k=1}^{n}f_k'(0,\kappa)\right)\\
&= \frac{1}{i^{n+1}(b\kappa i-n)\kappa^{n-1}}\left(\left(\sum_{j=1}^{m}\frac{f_j(0,\kappa)}{f_j'(0,\kappa)}+\sum_{j=m+1}^{n}\frac{f_j(0,\kappa)}{f_j'(0,\kappa)}-b\right)\prod_{k=1}^{n}f_k'(0,\kappa)\right)\\
&= \frac{1}{i^{n+1}(b\kappa i-n)\kappa^{n-1}}\left(\sum_{j=1}^{m}\frac{f_j(0,\kappa)}{f_j'(0,\kappa)}\prod_{k=1}^{n}f_k'(0,\kappa)+\left(\sum_{j=m+1}^{n}\frac{f_j(0,\kappa)}{f_j'(0,\kappa)}-b\right)\prod_{k=1}^{n}f_k'(0,\kappa)\right).
\end{aligned}\tag{3.3.3}$$

We consider the first term on the right hand side of (3.3.3) i.e.

$$\sum_{j=1}^{m}\frac{f_j(0,\kappa)}{f_j'(0,\kappa)}\prod_{k=1}^{n}f_k'(0,\kappa)=\sum_{j=1}^{m}f_j(0,\kappa)\prod_{k=1k\neq j}^{n}f_k'(0,\kappa).$$

In order to find small energy asymptotic of the above term, we use the following asymptotic for $f_j(x,\kappa)$ $j=1,\dots,m$ (cf. [17])

$$f_j(x,\kappa)=f_j(x,0)+\kappa\dot{f}_j(x,0)+o(\kappa),\quad \kappa\to 0.$$

Taking derivative with respect to x, we get

$$f_j'(x,\kappa)=f_j'(x,0)+\kappa\dot{f}_j'(x,0)+o(\kappa).$$

Evaluating at $x=0$ yields

$$f_j'(0,\kappa)=\kappa\dot{f}_j'(0,0)+o(\kappa)$$

which further implies

$$\prod_{j=1}^{m}f_j'(0,\kappa)=\kappa^m\prod_{j=1}^{m}\dot{f}_j'(0,0)+o(\kappa^m).$$

Therefore

$$\sum_{j=1}^{m}f_j(0,\kappa)\prod_{k=1k\neq j}^{n}f_k'(0,\kappa)=\sum_{j=1}^{m}\kappa^{m-1}f_j(0,0)\prod_{k=1k\neq j}^{m}\dot{f}_k'(0,0)\prod_{k=m+1}^{n}f_k'(0,0)+o(\kappa^m).$$

We multiply and divide the right hand side of above by $\dot{f}_j'(0,0)f_j(0,0)$ and obtain

$$=\sum_{j=1}^{m}\kappa^{m-1}\frac{(f_j(0,0))^2}{\dot{f}_j'(0,0)f_j(0,0)}\prod_{k=1}^{m}\dot{f}_k'(0,0)\prod_{k=m+1}^{n}f_k'(0,0)+o(\kappa^m).$$

Now we use the following identity
If $f'(0,0) = 0$, then

$$\dot{f}'(0,0)f(0,0) = i.$$

The above expression now becomes

$$\begin{aligned}
&= \sum_{j=1}^{m} \kappa^{m-1}(-i)(f_j(0,0))^2 \prod_{k=1}^{m} \dot{f}'_k(0,0) \prod_{k=m+1}^{n} f'_k(0,0) + o(\kappa^m) \\
&= C_{12}\kappa^{m-1} + o(\kappa^m) \text{ where } C_{12} \neq 0.
\end{aligned}$$

We now consider the second term on the right hand side of (3.3.3) i.e.

$$\begin{aligned}
&\left(\sum_{j=m+1}^{n} \frac{f_j(0,\kappa)}{f'_j(0,\kappa)} - b \right) \prod_{k=1}^{n} f'_k(0,\kappa) \\
&= \left(\sum_{j=m+1}^{n} \frac{f_j(0,\kappa)}{f'_j(0,\kappa)} - b \right) \left(\kappa^m \prod_{j=1}^{m} \dot{f}'_j(0,0) + o(\kappa^m) \right) = o(\kappa^m), \quad \kappa \to 0.
\end{aligned}$$

In view of above

$$\begin{aligned}
D^{\delta'_b}(\kappa) &= \frac{1}{i^{n+1}(b\kappa i - n)\kappa^{n-1}} \left(C_{12}\kappa^{m-1} + o(\kappa^m) \right) \\
&= \frac{C_{13}\kappa^{m-n}}{(b\kappa i - n)} \left(1 + o(\kappa) \right)
\end{aligned}$$

3. The expression for the perturbation determinant $D^{\hat{\delta}_d}$ is

$$D^{\hat{\delta}_d}(\kappa) = \frac{J(\kappa) \prod_{j=1}^{n} \left(f_j(0,\kappa) - d f'_j(0,\kappa) \right)}{in\kappa(1 - d\kappa i)^{n-1}}.$$

If $f_j(0,0) - d f'_j(0,0) \neq 0$, $\forall j = 1, \ldots, n$ then either $J(0) = 0$ or $J(0) \neq 0$

Let us first consider the case when $J(0) \neq 0$: In this case, $D^{\hat{\delta}_d}(\kappa)$ has no zeroes and

we can let

$$
\begin{aligned}
&J(0)\prod_{j=1}^{n}(f_j(0,0)-df_j'(0,0))=C\neq 0.\\
&\Rightarrow \lim_{\kappa\to 0} D^{\hat{\delta}_d}(\kappa)=\lim_{\kappa\to 0}\frac{C}{in\kappa(1-d\kappa i)^{n-1}}\\
&\Rightarrow \lim_{\kappa\to 0} D^{\hat{\delta}_d}(\kappa)in\kappa(1-d\kappa i)^{n-1}=C\\
&\Rightarrow \lim_{\kappa\to 0}\frac{D^{\hat{\delta}_d}(\kappa)in\kappa(1-d\kappa i)^{n-1}-C}{C}=0\\
&\Rightarrow D^{\hat{\delta}_d}(\kappa)in\kappa(1-d\kappa i)^{n-1}-C=o(C)\\
&\Rightarrow D^{\hat{\delta}_d}(\kappa)=C(in\kappa)^{-1}(1-d\kappa i)^{1-n}(1+o(1)) \text{ where } C\neq 0.
\end{aligned}
$$

Let us now consider the case when $J(0)=0$. In this case, we first find low energy asymptotic expansion for $J(\kappa)$. For this, following asymptotic is obtained by adapting the proof of Theorem 2.3 of [3]

$$\frac{f_j'(0,\kappa)}{f_j(0,\kappa)-df_j'(0,\kappa)}=\frac{f_j'(0,0)}{f_j(0,0)-df_j'(0,0)}-\frac{i\kappa}{f_j(0,0)(f_j(0,0)-df_j'(0,0))}+o(\kappa).$$

Summing from 1 to n we get

$$\sum_{j=1}^{n}\frac{f_j'(0,\kappa)}{f_j(0,\kappa)-df_j'(0,\kappa)}=\sum_{j=1}^{n}\frac{f_j'(0,0)}{f_j(0,0)-df_j'(0,0)}-i\kappa\sum_{j=1}^{n}\frac{1}{f_j(0,0)(f_j(0,0)-df_j'(0,0))}+o(\kappa).$$

$$J(\kappa)=J(0)-i\kappa C_{14}+o(\kappa) \text{ where } C_{14}=\sum_{j=1}^{n}\frac{1}{f_j(0,0)(f_j(0,0)-df_j'(0,0))}\neq 0.$$

Hence

$$D^{\hat{\delta}_d}(\kappa)=\frac{-i\kappa C_{15}+o(\kappa)}{in\kappa(1-d\kappa i)^{n-1}} \text{ where } C_{15}=C_{14}\prod_{j=1}^{n}(f_j(0,0)-df_j'(0,0))\neq 0.$$

$$\Rightarrow D^{\hat{\delta}_d}(\kappa)=(1-d\kappa i)^{1-n}C_{15}(1+o(1)).$$

If $f_j(0,0) - df_j'(0,0) = 0$ for $j = 1, \ldots, m; \quad m \leq n$ then

$$D^{\hat{\delta}_d}(z) = \frac{\left(\sum_{j=1}^{n} \frac{f_j'(0,\kappa)}{f_j(0,\kappa) - df_j'(0,\kappa)} \prod_{k=1}^{n} \left(f_k(0,\kappa) - df_k'(0,\kappa)\right) \right)}{in\kappa(1 - d\kappa i)^{n-1}}$$

$$= \frac{\left(\left(\sum_{j=1}^{m} \frac{f_j'(0,\kappa)}{f_j(0,\kappa) - df_j'(0,\kappa)} + \sum_{j=m+1}^{n} \frac{f_j'(0,\kappa)}{f_j(0,\kappa) - df_j'(0,\kappa)} \right) \prod_{k=1}^{n} \left(f_k(0,\kappa) - df_k'(0,\kappa)\right) \right)}{in\kappa(1 - d\kappa i)^{n-1}}$$

$$= \frac{\left(\sum_{j=1}^{m} f_j'(0,\kappa) \prod_{k=1 k\neq j}^{n} \left(f_k(0,\kappa) - df_k'(0,\kappa)\right) + \sum_{j=m+1}^{n} f_j'(0,\kappa) \prod_{k=1 k\neq j}^{n} \left(f_k(0,\kappa) - df_k'(0,\kappa)\right) \right)}{in\kappa(1 - d\kappa i)^{n-1}}. \tag{3.3.4}$$

Now we consider the first term in the numerator of the right hand side of (3.3.4) i.e.

$$\sum_{j=1}^{m} f_j'(0,\kappa) \prod_{k=1 k\neq j}^{n} \left(f_k(0,\kappa) - df_k'(0,\kappa)\right).$$

In order to find the asymptotic of the above term, we use the following asymptotic for $f_j(x,\kappa)$ and $f_j'(x,\kappa)$ $j = 1, \ldots, m$ (cf. [17])

$$f_j(0,\kappa) = f_j(0,0) + \kappa \dot{f}_j(0,0) + o(\kappa),$$
$$f_j'(0,\kappa) = f_j'(0,0) + \kappa \dot{f}_j'(0,0) + o(\kappa).$$

This implies

$$f_j(0,\kappa) - df_j'(0,\kappa) = \kappa(\dot{f}_j(0,0) - d\dot{f}_j'(0,0)) + o(\kappa), \quad \text{and hence}$$
$$\prod_{j=1}^{m} (f_j(0,\kappa) - df_j'(0,\kappa)) = \kappa^m \prod_{j=1}^{m} (\dot{f}_j(0,0) - d\dot{f}_j'(0,0)) + o(\kappa^m).$$

Therefore

$$\sum_{j=1}^{m} f_j'(0,\kappa) \prod_{k=1 k\neq j}^{n} \left(f_k(0,\kappa) - df_k'(0,\kappa)\right)$$
$$= \sum_{j=1}^{m} \kappa^{m-1} f_j'(0,0) \prod_{k=1 k\neq j}^{m} (\dot{f}_k(0,0) - d\dot{f}_k'(0,0)) \prod_{k=m+1}^{n} \left(f_k(0,0) - df_k'(0,0)\right) + o(\kappa^m)$$

$$= C_{16}\kappa^{m-1} + o(\kappa^m) \text{ where } C_{16} \neq 0.$$

Now, we consider the second term in the numerator on the right hand side of (3.3.4) i.e.

$$\sum_{j=m+1}^{n} f_j'(0,\kappa) \prod_{k=1k\neq j}^{n} \left(f_k(0,\kappa) - df_k'(0,\kappa)\right)$$
$$= \left(\sum_{j=m+1}^{n} f_j'(0,\kappa)\right)\left(\kappa^m \prod_{j=1}^{m}(\dot{f}_j(0,0) - d\dot{f}_j'(0,0)) + o(\kappa^m)\right) = o(\kappa^m).$$

In view of above

$$D^{\hat{\delta}_d}(\kappa) = \frac{\left(C_{16}\kappa^{m-1} + o(\kappa^m)\right)}{in\kappa(1-d\kappa i)^{n-1}}$$
$$= \frac{C_{16}\kappa^{m-2}}{(1-d\kappa i)^{n-1}}\left(1 + o(\kappa)\right), \quad \kappa \to 0.$$

4. The expression for the perturbation determinant $D^{\hat{\delta}_c'}$ is

$$D^{\hat{\delta}_c'}(\kappa) = \frac{P(\kappa)\prod_{j=1}^{n}\left(f_j'(0,\kappa) - cf_j(0,\kappa)\right)}{n(\kappa i - c)^{n-1}}$$

If $f_j'(0,0) - cf_j(0,0) \neq 0$, $\forall j = 1,\ldots,n$ then either $P(0) = 0$ or $P(0) \neq 0$

Let us first consider the case when $P(0) \neq 0$. In this case, $D^{\hat{\delta}_c'}(\kappa)$ has no zeroes and we can let

$$P(0)\prod_{j=1}^{n}(f_j'(0,0) - cf_j'(0,0)) = C \neq 0$$
$$\Rightarrow \lim_{\kappa\to 0} D^{\hat{\delta}_c'}(\kappa) = \lim_{\kappa\to 0}\frac{C}{n(\kappa i - c)^{n-1}}$$
$$\Rightarrow \lim_{\kappa\to 0} D^{\hat{\delta}_c'}(\kappa)n(\kappa i - c)^{n-1} = C$$
$$\Rightarrow \lim_{\kappa\to 0}\frac{D^{\hat{\delta}_c'}(\kappa)n(\kappa i - c)^{n-1} - C}{C} = 0$$
$$\Rightarrow D^{\hat{\delta}_c'}(\kappa)n(\kappa i - c)^{n-1} - C = o(C)$$
$$\Rightarrow D^{\hat{\delta}_c'}(\kappa) = C(\kappa i - c)^{1-n}(1 + o(1)) \text{ where } C \neq 0.$$

On the other hand if $P(0) = 0$, we first find asymptotic expansion for $J(\kappa)$. For this, following asymptotic is obtained by adapting the proof of Theorem 2.3 of [3]

$$\frac{f_j(0,\kappa)}{f_j'(0,\kappa) - cf_j(0,\kappa)} = \frac{f_j(0,0)}{f_j'(0,0) - cf_j(0,0)} + \frac{i\kappa}{f_j'(0,0)(f_j'(0,0) - cf_j(0,0))} + o(\kappa).$$

Summing from 1 to n we get

$$\sum_{j=1}^{n} \frac{f_j(0,\kappa)}{f_j'(0,\kappa) - cf_j(0,\kappa)} = \sum_{j=1}^{n} \frac{f_j(0,0)}{f_j'(0,0) - cf_j(0,0)} + i\kappa \sum_{j=1}^{n} \frac{1}{f_j'(0,0)(f_j'(0,0) - cf_j(0,0))} + o(\kappa)$$

$$P(\kappa) = P(0) + i\kappa C_{17} + o(\kappa) \text{ where } C_{17} = \sum_{j=1}^{n} \frac{1}{f_j'(0,0) - cf_j(0,0)} \neq 0.$$

Hence

$$D^{\hat{\delta}_c'}(\kappa) = \frac{i\kappa C_{18} + o(\kappa)}{n(\kappa i - c)^{n-1}} \text{ where } C_{18} = C_{17} \prod_{j=1}^{n} (f_j'(0,0) - cf_j(0,0)) \neq 0.$$

$$\Rightarrow D^{\hat{\delta}_c'}(\kappa) = \kappa(\kappa i - c)^{1-n} C_{18}(1 + o(1)).$$

If $f_j'(0,0) - cf_j(0,0) = 0$ for $j = 1, \ldots, m; \quad m \leq n$ then

$$\begin{aligned} D^{\hat{\delta}_c'}(\kappa) &= \frac{\left(\sum_{j=1}^{n} \frac{f_j(0,\kappa)}{f_j'(0,\kappa) - cf_j(0,\kappa)} \prod_{k=1}^{n} (f_k'(0,\kappa) - cf_k(0,\kappa)) \right)}{n(\kappa i - c)^{n-1}} \\ &= \frac{\left(\left(\sum_{j=1}^{m} \frac{f_j(0,\kappa)}{f_j'(0,\kappa) - cf_j(0,\kappa)} + \sum_{j=m+1}^{n} \frac{f_j(0,\kappa)}{f_j'(0,\kappa) - cf_j(0,\kappa)} \right) \prod_{k=1}^{n} (f_k'(0,\kappa) - cf_k(0,\kappa)) \right)}{n(\kappa i - c)^{n-1}} \\ &= \frac{\left(\sum_{j=1}^{m} f_j(0,\kappa) \prod_{k=1 k \neq j}^{n} (f_k'(0,\kappa) - cf_k(0,\kappa)) + \sum_{j=m+1}^{n} f_j(0,\kappa) \prod_{k=1 k \neq j}^{n} (f_k'(0,\kappa) - cf_k(0,\kappa)) \right)}{n(\kappa i - c)^{n-1}}. \end{aligned} \tag{3.3.5}$$

Let us consider the first term in the numerator on the right hand side of (3.3.5) i.e.

$$\sum_{j=1}^{m} f_j(0,\kappa) \prod_{k=1 k \neq j}^{n} \left(f_k'(0,\kappa) - cf_k(0,\kappa) \right).$$

In order to find the asymptotic of the above term, we use the following asymptotic for $f_j(x,\kappa)$ and $f_j'(x,\kappa)$ $j = 1, \ldots, m$ (cf. [17])

$$\begin{aligned} f_j'(0,\kappa) &= f_j'(0,0) + \kappa \dot{f}_j'(0,0) + o(\kappa) \quad \text{and} \\ f_j(0,\kappa) &= f_j(0,0) + \kappa \dot{f}_j(0,0) + o(\kappa). \end{aligned}$$

This implies

$$f_j'(0,\kappa) - cf_j'(0,\kappa) = \kappa(\dot{f}_j'(0,0) - c\dot{f}_j(0,0)) + o(\kappa) \quad \text{and hence}$$
$$\prod_{j=1}^{m}(f_j'(0,\kappa) - cf_j(0,\kappa)) = \kappa^m \prod_{j=1}^{m}(\dot{f}_j'(0,0) - c\dot{f}_j(0,0)) + o(\kappa^m).$$

Therefore

$$\begin{aligned}
&\sum_{j=1}^{m} f_j'(0,\kappa) \prod_{k=1k\neq j}^{n} \left(f_k'(0,\kappa) - cf_k(0,\kappa)\right) \\
&= \sum_{j=1}^{m} \kappa^{m-1} f_j(0,0) \prod_{k=1k\neq j}^{m} (\dot{f}_k'(0,0) - c\dot{f}_k(0,0)) \prod_{k=m+1}^{n} \left(f_k'(0,0) - cf_k(0,0)\right) + o(\kappa^m) \\
&= C_{19}\kappa^{m-1} + o(\kappa^m) \text{ where } C_{19} \neq 0.
\end{aligned}$$

Now, we consider the second term in the numerator on the right hand side of (3.3.5) i.e.

$$\begin{aligned}
&\sum_{j=m+1}^{n} f_j(0,\kappa) \prod_{k=1k\neq j}^{n} \left(f_k'(0,\kappa) - cf_k(0,\kappa)\right) \\
&= \left(\sum_{j=m+1}^{n} f_j(0,\kappa)\right) \left(\kappa^m \prod_{j=1}^{m}(\dot{f}_j'(0,0) - c\dot{f}_j(0,0)) + o(\kappa^m)\right) = o(\kappa^m), \quad \kappa \to 0.
\end{aligned}$$

In view of above

$$\begin{aligned}
D^{\hat{\delta}_c'}(\kappa) &= \frac{\left(C_{19}\kappa^{m-1} + o(\kappa^m)\right)}{n(\kappa i - c)^{n-1}} \\
&= \frac{C_{19}\kappa^{m-1}}{n(\kappa i - c)^{n-1}} \left(1 + o(\kappa)\right), \quad \kappa \to 0.
\end{aligned}$$

□

Now as we have low energy asymptotics, so we can develop Levinson Theorem, which is as follows

Theorem 3.3.2 (Levinson's theorem)**.** *Let the potential function V satisfies* (3.3.1) *and let N denotes the number of negative eigenvalues counting multiplicities.*

1. *Then the following Levinson's formula holds for the number of negative eigenvalues of the operator $H_{V,\Gamma}^{\delta_a}$*

$$\eta^{\delta_a}(\infty) - \eta^{\delta_a}(0) = \begin{cases} \pi\left(N + \frac{l-g_1}{2}\right) & w_j(0) \neq 0,\ \forall j = 1, \ldots, n, \\ \pi\left(N + \frac{m-1-g_1}{2}\right) & w_j(0) = 0,\ j = 1, \ldots, m,\ m \leq n, \end{cases}$$

where l and g_1 are defined in Lemma 3.3.1 (1).

2. *Then the following Levinson's formula holds for the number of negative eigenvalues of the operator $H_{V,\Gamma}^{\delta'_b}$*

$$\eta^{\delta'_b}(\infty) - \eta^{\delta'_b}(0) = \begin{cases} \pi\left(N + \frac{p-n}{2}\right) & f'_j(0,0) \neq 0,\ \forall j = 1, \ldots, n, \\ \pi\left(N + \frac{m-n+1}{2}\right) & f'_j(0,0) = 0,\ j = 1, \ldots, m,\ m \leq n, \end{cases}$$

where p is defined in Lemma 3.3.1 (2).

3. *Then the following Levinson's formula holds for the number of negative eigenvalues of the operator $H_{V,\Gamma}^{\hat{\delta}_d}$*

$$\eta^{\hat{\delta}_d}(\infty) - \eta^{\hat{\delta}_d}(0) = \begin{cases} \pi\left(N + \dfrac{g_3}{2}\right) & f_j(0,0) - df'_j(0,0) \neq 0,\ \forall j = 1, \ldots, n, \\ \pi\left(N + \dfrac{m-2}{2}\right) & f_j(0,0) - df'_j(0,0) = 0,\ j = 1, \ldots, m,\ m \leq n, \end{cases}$$

where g_3 is defined as in Lemma 3.3.1 (3).

4. *Then the following Levinson's formula holds for the negative eigenvalues of the operator $H_{V,\Gamma}^{\hat{\delta}'_c}$*

$$\eta^{\hat{\delta}'_c}(\infty) - \eta^{\hat{\delta}'_c}(0) = \begin{cases} \pi\left(N + \frac{g_4}{2}\right) & f'_j(0,0) - cf_j(0,0) \neq 0,\ \forall j = 1, \ldots, n, \\ \pi\left(N + \frac{m-1}{2}\right) & f'_j(0,0) - cf_j(0,0) = 0,\ j = 1, \ldots, m,\ m \leq n, \end{cases}$$

where g_4 is defined as in Lemma 3.3.1 (4).

Proof. 1. The function $D^{\delta_a}(\kappa)$ has a zero of order r iff κ^2 is an eigenvlue of multiplicity r of the operator $H_{V,\Gamma}^{\delta_a}$ [5]. As $H_{V,\Gamma}^{\delta_a}$ can have only real eigenvalues therefore the zeros of $D^{\delta_a}(\kappa)$ lie on the positive imaginary axis.

Let us consider the counter clockwise contour $\Gamma_{R,\epsilon}$ consisting of two semicircles $C_R^+ = \{|\kappa| = R, \operatorname{Im}\kappa \geq 0\}$ and $C_\epsilon^+ = \{|\kappa| = \epsilon, \operatorname{Im}\kappa \geq 0\}$ and the intervals (ϵ, R) and $(-R, -\epsilon)$. R and ϵ are chosen such that all N negative eigenvalues lie inside contour $\Gamma_{R,\epsilon}$.

By applying the argument principle to $D^{\delta_a}(\kappa)$ and the contour $\Gamma_{R,\epsilon}$, we obtain,

$$\int_{\Gamma_{R,\epsilon}} \frac{\frac{d}{d\kappa} D^{\delta_a}(\kappa)}{D^{\delta_a}(\kappa)} d\kappa = 2\pi i N. \tag{3.3.6}$$

Note that

$$\lim_{\mathrm{Im}\,\kappa\to\infty} D^{\delta_a}(\kappa) = \lim_{\mathrm{Im}\kappa\to\infty} \frac{(K(\kappa)-a)\prod_{j=1}^{n} w_j(\kappa)}{n\kappa i - a} = 1 + O(|\kappa|^{-1}). \tag{3.3.7}$$

Therefore, the branch of the function $\ln D^{\delta_a}(\kappa)$ can be fixed by the condition $\ln D^{\delta_a}(\kappa) \to 0$ as $|\kappa| \to \infty$.

For $k \in \mathbb{R}$, we use the definition $D^{\delta_a}(k) = a^{\delta_a}(k)e^{i\eta^{\delta_a}(k)}$, where $a^{\delta_a}(k) = |D^{\delta_a}(k)|$ and $\eta^{\delta_a}(k) = \arg D^{\delta_a}(k)$. Now

$$\begin{aligned}\mathrm{var}_{\Gamma_{R,\epsilon}} \arg D^{\delta_a}(\kappa) =& \eta^{\delta_a}(R) - \eta^{\delta_a}(\epsilon) + \mathrm{var}_{C_R^+} \arg D^{\delta_a}(\kappa) + \\ & \{\eta^{\delta_a}(-\epsilon) - \eta^{\delta_a}(-R)\} + \mathrm{var}_{C_\epsilon^+} \arg D^{\delta_a}(\kappa).\end{aligned}$$

It follows from the representation of $D^{\delta_a}(k)$ that $\eta^{\delta_a}(-k) = -\eta^{\delta_a}(k)$. Hence,

$$\mathrm{var}_{\Gamma_{R,\epsilon}} \arg D^{\delta_a}(\kappa) = 2(\eta^{\delta_a}(R) - \eta^{\delta_a}(\epsilon)) + \mathrm{var}_{C_R^+} \arg D^{\delta_a}(\kappa) + \mathrm{var}_{C_\epsilon^+} \arg D^{\delta_a}(\kappa).$$

Equation (3.3.6) implies that

$$\mathrm{var}_{\Gamma_{R,\epsilon}} \arg D^{\delta_a}(\kappa) = 2\pi N.$$

Therefore

$$2\pi N = 2(\eta^{\delta_a}(R) - \eta^{\delta_a}(\epsilon)) + \mathrm{var}_{C_R^+} \arg D^{\delta_a}(\kappa) + \mathrm{var}_{C_\epsilon^+} \arg D^{\delta_a}(\kappa).$$

Letting $R \to \infty$ yields $\lim_{R\to\infty} \mathrm{var}_{C_R^+} \arg D^{\delta_a}(\kappa) = 0$ because of equation (3.3.7). We are left with

$$\eta^{\delta_a}(\infty) - \eta^{\delta_a}(\epsilon) = \pi N - \frac{1}{2}\mathrm{var}_{C_\epsilon^+} \arg D^{\delta_a}(\kappa).$$

Finally, we let $\epsilon \to 0$ and by Lemma 3.3.1 (1) we get

$$\lim_{\epsilon\to 0} \mathrm{var}_{C_\epsilon^+} \arg D^{\delta_a}(\kappa) = \begin{cases} -(l-g_1)\pi & w_j(0) \neq 0,\ \forall j = 1,\dots,n, \\ -(m-1-g_1)\pi & w_j(0) = 0,\ j = 1,\dots,m,\ m \leq n. \end{cases}$$

Thus,

$$\eta^{\delta_a}(\infty) - \eta^{\delta_a}(0) = \begin{cases} \pi\left(N + \frac{l-g_1}{2}\right) & w_j(0) \neq 0,\ \forall j = 1,\dots,n, \\ \pi\left(N + \frac{m-1-g_1}{2}\right) & w_j(0) = 0,\ j = 1,\dots,m,\ m \leq n. \end{cases}$$

2. We first observe that

$$\lim_{\mathrm{Im}\,\kappa\to\infty} D^{\delta_b'}(\kappa) = \lim_{\mathrm{Im}\,\kappa\to\infty} \frac{(M(\kappa)-b)\prod_{j=1}^{n} f_j'(0,\kappa)}{i^{n+1}(b\kappa i - n)\kappa^{n-1}} = 1 + O(|\kappa|^{-1}). \tag{3.3.8}$$

Following the same argument as above we let $\epsilon \to 0$, and by Lemma 3.3.1 (2),

$$\lim_{\epsilon\to 0} \mathrm{var}_{C_\epsilon^+} \arg D^{\delta_b'}(\kappa) = \begin{cases} -(p-n)\pi & f_j'(0,0) \neq 0, \forall j = 1,\dots,n \\ -(m-n)\pi & f_j'(0,0) = 0,\ j = 1,\dots,m,\ m \leq n. \end{cases}$$

Thus,

$$\eta^{\delta_b'}(\infty) - \eta^{\delta_b'}(0) = \begin{cases} \pi\left(N + \frac{p-n}{2}\right) & f_j'(0,0) \neq 0,\ \forall j = 1,\dots,n, \\ \pi\left(N + \frac{m-n}{2}\right) & f_j'(0,0) = 0,\ j = 1,\dots,m,\ m \leq n. \end{cases}$$

3. Note that

$$\lim_{\mathrm{Im}\,\kappa\to\infty} D^{\hat{\delta}_d}(\kappa) = \lim_{\mathrm{Im}\,\kappa\to\infty} \frac{J(\kappa)\prod_{j=1}^{n}(f_j(0,\kappa) - df_j'(0,\kappa))}{in\kappa(1-d\kappa i)^{n-1}} = 1 + O(|\kappa|^{-1}). \tag{3.3.9}$$

We follow the same argument as above. We let $\epsilon \to 0$ and by Lemma 3.3.1 (3) we get

$$\lim_{\epsilon\to 0} \mathrm{var}_{C_\epsilon^+} \arg D^{\hat{\delta}_d}(\kappa) = \begin{cases} -g_3\pi & f_j(0,0) - df_j'(0,0) \neq 0,\ \forall j = 1,\dots,n, \\ -(m-2)\pi & f_j(0,0) - df_j'(0,0) = 0,\ j = 1,\dots,m,\ m \leq n. \end{cases}$$

Thus,

$$\eta^{\hat{\delta}_d}(\infty) - \eta^{\hat{\delta}_d}(0) = \begin{cases} \pi\left(N + \dfrac{g_3}{2}\right) & f_j(0,0) - df_j'(0,0) \neq 0,\ \forall j = 1,\dots,n, \\ \pi\left(N + \dfrac{m-2}{2}\right) & f_j(0,0) - df_j'(0,0) = 0,\ j = 1,\dots,m,\ m \leq n. \end{cases}$$

4. By considering the explicit expression for $D^{\hat{\delta}_c'}$ we see that

$$\lim_{\mathrm{Im}\,\kappa\to\infty} D^{\hat{\delta}_c'}(\kappa) = \lim_{\mathrm{Im}\,\kappa\to\infty} \frac{P(\kappa)\prod_{j=1}^{n}\left(f_j'(0,\kappa) - cf_j(0,\kappa)\right)}{n(\kappa i - c)^{n-1}} = 1 + O(|\kappa|^{-1}). \tag{3.3.10}$$

Following a similar argument as in the proof or part 1, we let $\epsilon \to 0$, and by Lemma 3.3.1 (4),

$$\lim_{\epsilon\to 0} \mathrm{var}_{C_\epsilon^+} \arg D^{\hat{\delta}_c'}(\kappa) = \begin{cases} -g_4\pi & f_j'(0,0) - cf_j(0,0) \neq 0,\ \forall j = 1,\dots,n, \\ -(m-1)\pi & f_j'(0,0) - cf_j(0,0) = 0,\ j = 1,\dots,m,\ m \leq n. \end{cases}$$

Hence,

$$\eta^{\hat{\delta}'_c}(\infty) - \eta^{\hat{\delta}'_c}(0) = \begin{cases} \pi\left(N + \frac{g_4}{2}\right) & f'_j(0,0) - cf_j(0,0) \neq 0,\ \forall j = 1, \ldots, n, \\ \pi\left(N + \frac{m-1}{2}\right) & f'_j(0,0) - cf_j(0,0) = 0,\ j = 1, \ldots, m,\ m \leq n. \end{cases}$$

□

Chapter 4

Lieb-Thirring type inequalities

In this chapter, we consider fourth order differential operators on semi-axis with Robin type boundary condition at zero. Using the commutation method, Lieb-Thirring inequalities are derived for the negative eigenvalues of double multiplicity depending only on the potentials and boundary parameters. We construct reflectionless potentials and prove the sharpness of the inequality. The results of this chapter have been published in [103].

4.1 Introduction

Consider the fourth order differential operator in $L^2(\mathbb{R}^d)$

$$H = (\Delta)^2 + V, \quad V(x) \in \mathbb{R}, \quad x \in \mathbb{R}^d. \tag{4.1.1}$$

For suitable V this operator is bounded from below and the negative spectrum is discrete. Let us denote the negative eigenvalues of H by $\{\lambda_n(H)\}$. The inequalities

$$\sum_n |\lambda_n(H)|^\gamma \leq L_{4,\gamma,d} \int_{\mathbb{R}^d} V_-^{\gamma+\frac{d}{4}}\, dx \tag{4.1.2}$$

are commonly refereed to as Lieb-Thirring inequalities. This type of inequality was introduced by Lieb and Thirring for the Schrödinger operators in [75]. Here and in the following, the positive and negative parts of the function V are defined as $V_\pm = (|V| \pm V)/2$.

The inequality (4.1.2) holds if and only if, $\gamma > 0$, $d = 4$; $\gamma \geq 0$, $d > 4$ and $\gamma \geq 1 - \frac{d}{4}$, $d < 4$. Moreover, it is known that (4.1.2) fails for $\gamma = 0$ if $d = 4$ and for $0 \leq \gamma < 1 - \frac{d}{4}$ if $d < 4$ (see [28, 78]).

If $V \in L^{\gamma+\frac{d}{4}}(\mathbb{R}^d)$ then inequalities (4.1.2) are accompanied by the Weyl type asymptotic

formula [28]

$$\lim_{\alpha\to+\infty}\frac{1}{\alpha^{\gamma+\frac{d}{4}}}\mathrm{tr}\ \left((\Delta)^2+\alpha V\right)_-^\gamma = \lim_{\alpha\to+\infty}\frac{1}{\alpha^{\gamma+\frac{d}{4}}}\iint_{\mathbb{R}^d\times\mathbb{R}^d}\left(|\xi|^4+\alpha V\right)_-^\gamma\frac{dxd\xi}{(2\pi)^d}$$
$$= L^{cl}_{4,\gamma,d}\int_{\mathbb{R}^d}V_-^{\gamma+\frac{d}{4}}dx, \tag{4.1.3}$$

where the so-called classical constant $L^{cl}_{4,\gamma,d}$ is defined as

$$L^{cl}_{4,\gamma,d} = \frac{\Gamma(\gamma+1)\Gamma(\frac{d}{4}+1)}{2^d\pi^{d/2}\Gamma(\frac{d}{2}+1)\Gamma(\frac{d}{4}+\gamma+1)},\quad \gamma\geq 0. \tag{4.1.4}$$

Moreover, we consider the following Lieb-Thirring bound for the lowest negative eigenvalue $\lambda_1(H)$ of (4.1.1)

$$|\lambda_1(H)|^\gamma \leq L^0_{4,\gamma,d}\int_{\mathbb{R}^d}V_-^{\gamma+\frac{d}{4}}\,dx\,,\quad V\in L^{\gamma+\frac{d}{4}}(\mathbb{R}^d). \tag{4.1.5}$$

The value of $L^0_{4,\gamma,d}$ is explicitly known in the case when $\gamma = 1-\frac{d}{4}$ and $d<4$ (see [78]) and is given by

$$L^0_{4,\gamma,d} = \frac{\pi d}{4\sin(\pi d/4)}L^{cl}_{4,0,d} = \frac{4}{4-d}L^{cl}_{4,1-\frac{d}{4},d}. \tag{4.1.6}$$

From (4.1.3) and (4.1.5), it is easy to see that

$$\max(L^{cl}_{4,\gamma,d}, L^0_{4,\gamma,d}) \leq L_{4,\gamma,d}, \tag{4.1.7}$$

for all values of γ and d for which (4.1.2) holds.

In [44] Hoppe, Laptev and Östensson considered the one dimensional operator

$$\widetilde{\mathcal{H}}\varphi = \Big(\frac{d^4}{dx^4}+\frac{d}{dx}\Big(\widetilde{U}\frac{d}{dx}\Big)+\widetilde{V}(x)\Big)\varphi(x)$$

in $L^2(\mathbb{R})$. Under certain assumptions on the functions $\widetilde{U}$ and $\widetilde{V}$, they proved the following sharp Lieb-Thirring inequality

$$\sum_{j=1}^n|\lambda_j(\widetilde{\mathcal{H}})|^{7/4}\leq L^{cl}_{4,7/4,1}Q[\widetilde{U},\widetilde{V}]. \tag{4.1.8}$$

Here, $\{\lambda_j(\widetilde{\mathcal{H}})\}_{j=1}^n$ are the negative eigenvalues of double multiplicity of the operator $\widetilde{\mathcal{H}}$ and $Q[\widetilde{U},\widetilde{V}]$ is a non-linear functional involving $\widetilde{U}$ and $\widetilde{V}$. A precise definition of $Q[\widetilde{U},\widetilde{V}]$ will be given in (4.3.7). For eigenvalue bounds of biharmonic operators with complex potentials in dimensions three and below, we refer the reader to [46].

In this chapter, we consider the following self-adjoint fourth order differential operator acting in $L^2(\mathbb{R}_+)$

$$\mathcal{H}\varphi(x) = \Big(\frac{d^4}{dx^4} + \frac{d}{dx}\Big(U\frac{d}{dx}\Big) + V(x)\Big)\,\varphi(x), \quad \begin{cases} \varphi''(0) = \sigma_0\varphi(0) + \sigma_1\varphi'(0), \\ \varphi'''(0) = -\sigma_2\varphi(0) - \sigma_0\varphi'(0), \end{cases} \tag{4.1.9}$$

where U and V are smooth functions vanishing on the set $(b, +\infty)$ for some $b > 0$, in addition $U(0) = U'(0) = 0$ and σ_0, σ_1 and σ_2 are all real parameters. Our aim is to derive an analogue of (4.1.8) for the operator $\mathcal{H}$. Note that, the three parameter boundary conditions in (4.1.9) do not describe all possible conditions for which the operator $\mathcal{H}$ is self-adjoint. For all possible boundary conditions for which the operator $\mathcal{H}$ is self-adjoint, we refer the reader to [96], see also [38, 52] for other boundary condition questions.

In our work, we follow the argument of [44] and apply the well known commutation method, which relies on the idea of removing (or inserting) eigenvalues from the spectrum of differential operators. The main idea is to remove the negative eigenvalues from the spectrum of the operator $\mathcal{H}$ starting from the lowest eigenvalue, λ_1. In order to do so, we factorize the fourth order differential operator $\mathcal{H}$ into two second order operators, let us say A_1 and A_1^*, such that $A_1^*A_1 = \mathcal{H} - \lambda_1$. If we commute the two operators A_1 and A_1^*, we get a new operator $\mathcal{H}_1$, i.e., $A_1A_1^* = \mathcal{H}_1 - \lambda_1$. This new operator $\mathcal{H}_1$, with new potential functions U_1 and V_1 and possibly different boundary conditions, is isospectral to the original operator $\mathcal{H}$ except for the lowest eigenvalue λ_1, which does not belong to the spectrum of $\mathcal{H}_1$. Continuing in this manner, one can remove all the negative eigenvalues of the operator $\mathcal{H}$.

In the case of the Schrödinger operators, the commutation method was used in [88] to obtain the Schmincke inequality. Benguria and Loss in [8] applied this method to prove sharp Lieb-Thirring inequalities for whole line Schrödinger operators with matrix-valued potentials. Similar results were obtained in [26] (see also [77]) for matrix-valued Schrödinger operators defined on the semi-axis with the Robin boundary condition at 0. For applications of the commutation method to Jacobi operators, we refer to [87].

Our main contributions in this chapter are Theorem 4.3.1 and Theorem 4.3.2. In Section 4.2, we provide some auxiliary results that we will need to prove our main results in Section 4.3.

4.2 Some auxiliary results

Lemma 4.2.1. *Let $\lambda < 0$ denotes the lowest negative eigenvalue of the operator $\mathcal{H}$ and let $\varphi \in L^2(\mathbb{R}_+)$ be a solution of*

$$\mathcal{H}\varphi = \lambda\varphi. \tag{4.2.1}$$

φ is identically zero on $\mathbb{R}_+$ if for some $x_0 \in \mathbb{R}_+$, $\varphi(x_0) = \varphi'(x_0) = 0$.

Proof. Consider

$$\hat{\varphi}(x) = \begin{cases} -\varphi(x) & \text{if } x \le x_0, \\ \varphi(x) & \text{if } x > x_0, \end{cases}$$

which is linearly independent of φ and it is a minimizer of the closed quadratic form of $\mathcal{H}$. Indeed,

$$\begin{aligned} &\int_{\mathbb{R}_+} \left(|\hat{\varphi}''|^2 - U|\hat{\varphi}'|^2 + V|\hat{\varphi}|^2\right) dx + \sigma_2|\hat{\varphi}(0)|^2 + \sigma_1|\hat{\varphi}'(0)|^2 + 2\sigma_0 \mathrm{Re}\big(\hat{\varphi}(0)\overline{\hat{\varphi}}'(0)\big) \\ &\quad = \int_{\mathbb{R}_+} \left(|\varphi''|^2 - U|\varphi'|^2 + V|\varphi|^2\right) dx + \sigma_2|\varphi(0)|^2 + \sigma_1|\varphi'(0)|^2 + 2\sigma_0 \mathrm{Re}\big(\varphi(0)\overline{\varphi}'(0)\big) \\ &\quad = \lambda \int_{\mathbb{R}_+} |\varphi|^2\, dx = \lambda \int_{\mathbb{R}_+} |\hat{\varphi}|^2\, dx. \end{aligned}$$

Therefore, the function $\varphi_1 = \hat{\varphi} + \varphi$ is an eigenfunction of $\mathcal{H}$ with eigenvalue λ and hence, $\varphi_1 = \hat{\varphi} = \varphi \equiv 0$. □

We will need the following functions

$$W_{mn}(x) := \varphi_+^{(m)}(x)\varphi_-^{(n)}(x) - \varphi_+^{(n)}(x)\varphi_-^{(m)}(x), \quad m, n = 0, 1, 2, \cdots \tag{4.2.2}$$

We denote the wronskian of the functions φ_+ and φ_- by $W(x) = W_{01}(x)$.

Lemma 4.2.2. *Let $\lambda < 0$ be the lowest eigenvalue of double multiplicity and let φ_+ and φ_- be the corresponding linearly independent eigenfunctions of the operator $\mathcal{H}$. Then the wronskian $W(x) \neq 0$ for all $x \in \mathbb{R}_+$.*

Proof. We can write the wronskian as

$$W(x) = \det \begin{pmatrix} \varphi_+ & \varphi_- \\ \varphi_+' & \varphi_-' \end{pmatrix}.$$

Now let us assume that $W(x_0) = 0$ for some $x_0 \in \mathbb{R}_+$. Then the homogeneous system of linear equations

$$\begin{cases} \varphi_+(x_0)C_1 + \varphi_-(x_0)C_2 &= 0 \\ \varphi_+'(x_0)C_1 + \varphi_-'(x_0)C_2 &= 0. \end{cases}$$

in C_1 and C_2 has a non-trivial solution. Moreover, at x_0 the function $\varphi_1(x) = \varphi_+(x)C_1 + \varphi_-(x)C_2$ and its derivative are zero. By Lemma 4.2.1 $\varphi_1 \equiv 0$, which implies φ_+ and φ_- are linearly dependent, a contradiction. □

In view of the Lemma 4.2.2 the functions

$$F(x) := \frac{W'(x)}{W(x)} \quad \text{and} \quad G(x) := -\frac{W_{12}(x)}{W(x)}, \quad x \in \mathbb{R}_+ \tag{4.2.3}$$

are well defined, where, $W_{12}(x)$ is defined by (4.2.2) with $m = 1$ and $n = 2$.

Lemma 4.2.3. *Let $\lambda < 0$ be the lowest eigenvalue of double multiplicity and let φ_+ and φ_- be the corresponding linearly independent eigenfunctions of the operator $\mathcal{H}$. The functions $F(x)$ and $G(x)$ defined by* (4.2.3) *satisfy*

$$F'(x) + F^2(x) + 2G(x) = -U(x), \tag{4.2.4a}$$

$$G^2(x) - \big(F(x)G(x) + G'(x)\big)' = V(x) - \lambda \tag{4.2.4b}$$

and

$$F(0) = \sigma_1, \quad G(0) = \sigma_0, \tag{4.2.5a}$$

$$F(x) = -2k, \quad G(x) = -2k^2, \quad x > b, \tag{4.2.5b}$$

where $\lambda = -4k^4$, $k > 0$.

Proof. The linearly independent eigenfunctions φ_+ and φ_- corresponding to the ground state energy λ of the operator $\mathcal{H}$ satisfy

$$\varphi_+^{(4)} + \big(U\varphi_+'\big)' + V\varphi_+ = \lambda\varphi_+, \tag{4.2.6a}$$

$$\varphi_-^{(4)} + \big(U\varphi_-'\big)' + V\varphi_- = \lambda\varphi_-. \tag{4.2.6b}$$

We multiply (4.2.6a) by φ_- and (4.2.6b) by φ_+ and subtract. This yields

$$U' + \frac{W'}{W}U = \frac{W_{40}}{W}.$$

This is a first order linear differential equation in U which can be exactly solved. The solution is

$$UW = 2W_{12} - W'' + C.$$

Since U vanishes for $x > b$ and the functions W, W'' and W_{12} all vanish at infinity the constant of integration C must be equal to 0. This yields

$$UW = 2W_{12} - W''. \tag{4.2.7}$$

Further, using the definition of F and G, given by (4.2.3), it can be seen that

$$F' + F^2 = \frac{W''}{W}. \tag{4.2.8}$$

Using (4.2.7) and (4.2.8) along with the definition of G from (4.2.3), we arrive at (4.2.4a).

In order to prove (4.2.4b), we multiply (4.2.6a) by φ'_- and (4.2.6b) by φ'_+ and subtract. This leads to

$$(V - \lambda)\, W = W_{14} + UW_{12}. \tag{4.2.9}$$

It can be seen that $W_{14} = W''_{12} - W_{23}$ and $WW_{23} = W'_{12}W' - W_{12}W'' + W^2_{12}$. Moreover, from (4.2.7), one get $U = \frac{2W_{12} - W''}{W}$. Substituting these values into (4.2.9), we obtain

$$(V - \lambda) = \left(\frac{W_{12}}{W}\right)^2 - \left(\frac{W'_{12}W'}{W^2} - \frac{W''_{12}}{W}\right). \tag{4.2.10}$$

Finally, using the definition of F and G, given by (4.2.3), we see that the first term on the right hand side is equal to G^2 and the second term is equal to $(FG + G')'$. This yields (4.2.4b).

Applying the boundary conditions that are associated with the operator $\mathcal{H}$

$$\begin{cases} \varphi''(0) = \sigma_0\varphi(0) + \sigma_1\varphi'(0), \\ \varphi'''(0) = -\sigma_2\varphi(0) - \sigma_0\varphi'(0), \end{cases}$$

to the functions φ_+ and φ_-, we obtain

$$\begin{aligned} F(0) &= \frac{W'(0)}{W(0)} = \frac{\varphi_+(0)\varphi''_-(0) - \varphi''_+(0)\varphi_-(0)}{\varphi_+(0)\varphi'_-(0) - \varphi'_+(0)\varphi_-(0)} \\ &= \frac{\sigma_0\varphi_+(0)\varphi_-(0) + \sigma_1\varphi_+(0)\varphi'_-(0) - \sigma_0\varphi_+(0)\varphi_-(0) - \sigma_1\varphi'_+(0)\varphi_-(0)}{\varphi_+(0)\varphi'_-(0) - \varphi'_+(0)\varphi_-(0)} = \sigma_1. \end{aligned}$$

Moreover, as $U(0) = 0$, equation (4.2.7) gives

$$W_{12}(0) = \frac{W''(0)}{2}. \tag{4.2.11}$$

Hence,

$$\begin{aligned} G(0) &= -\frac{W_{12}(0)}{W(0)} = -\frac{W''(0)}{2W(0)} \\ &= -\frac{1}{2}\left(\frac{\varphi'_+(0)\varphi''_-(0) - \varphi''_+(0)\varphi'_-(0) + \varphi_+(0)\varphi'''_-(0) - \varphi'''_+(0)\varphi_-(0)}{\varphi_+(0)\varphi'_-(0) - \varphi'_+(0)\varphi_-(0)}\right) = \sigma_0. \end{aligned} \tag{4.2.12}$$

Now, for $x \in (b, +\infty)$, equations (4.2.6a) and (4.2.6b) have the following solutions

$$\varphi_\pm(x) = \beta_1^\pm e^{-kx}\cos(kx) + \beta_2^\pm e^{-kx}\sin(kx).$$

This yields

$$W(x) = ke^{-2kx}\left(\beta_1^+\beta_2^- - \beta_1^-\beta_2^+\right)$$

and

$$W_{12}(x) = 2k^3e^{-2kx}\left(\beta_1^+\beta_2^- - \beta_1^-\beta_2^+\right).$$

Therefore,

$$F(x) = -2k \quad \text{and} \quad G(x) = -2k^2, \quad \text{for} \quad x > b.$$

□

Remark 4.2.4. *We will need the following limiting values of derivatives of F and G:*

1. *Equation* (4.2.4a) *yields*

$$F'(0) = -2G(0) - F^2(0) = -2\sigma_0 - \sigma_1^2.$$

2. *Using* (4.2.3)*, we obtain*

$$\begin{aligned} G'(0) &= -\frac{W_{12}'(0)}{W(0)} + \frac{W_{12}(0)}{W(0)}\frac{W'(0)}{W(0)} \\ &= -\frac{W_{12}'(0)}{W(0)} - G(0)F(0) \\ &= \frac{\varphi_+'''(0)\varphi_-'(0) - \varphi_+'(0)\varphi_-'''(0)}{\varphi_+'(0)\varphi_-(0) - \varphi_+(0)\varphi_-'(0)} - \sigma_0\sigma_1 \\ &= -\sigma_2 - \sigma_0\sigma_1. \end{aligned}$$

3. *Moreover,*

$$F''(0) = -2\left(G'(0) + F(0)F'(0)\right) = 2\left(\sigma_1^3 + 3\sigma_0\sigma_1 + \sigma_2\right).$$

4. *All derivatives of F and G are equal to zero for $x \in (b, \infty)$.*

4.3 Main results and their proofs

Let $-\lambda_1 = -4k_1^4$, $k_1 > 0$ be the ground state energy of the operator $\mathcal{H}$ of double multiplicity and φ_+ and φ_- be the corresponding eigenfunctions and $F_1 = \frac{W'(x)}{W(x)}$ and $G_1(x) = -\frac{W_{12}(x)}{W(x)}$. Here, W and W_{12} are defined by (4.2.2). We consider the operator

$$A_1 = -\frac{d^2}{dx^2} + F_1(x)\frac{d}{dx} + G_1(x)$$

and its adjoint

$$A_1^* = -\frac{d^2}{dx^2} - F_1(x)\frac{d}{dx} + G_1(x) - F_1'(x)$$

in $L^2(\mathbb{R}_+)$. Using equations (4.2.4a) and (4.2.4b), we obtain the following factorization of the original operator $\mathcal{H}$

$$A_1^* A_1 = \mathcal{H} - \lambda_1.$$

Consider

$$A_1 A_1^* = \frac{d^4}{dx^4} + \frac{d}{dx}U_1(x)\frac{d}{dx} + V_1(x) - \lambda_1 := \mathcal{H}_1 - \lambda_1,$$

where

$$\begin{cases} U_1 = U + 4F_1', \\ V_1 = V + 2F_1 G_1' - F_1 F_1'' + F_1'''. \end{cases} \tag{4.3.1}$$

The non-zero eigenvalues of $A_1^* A_1$ and $A_1 A_1^*$ are the same. Although, the eigenfunctions φ of $A_1^* A_1$ satisfy

$$\begin{cases} \varphi''(0) = \sigma_0\varphi(0) + \sigma_1\varphi'(0), \\ \varphi'''(0) = -\sigma_2\varphi(0) - \sigma_0\varphi'(0), \end{cases} \tag{4.3.2}$$

the eigenfunctions of $A_1 A_1^*$ satisfy the Dirichlet conditions at origin.

clearly, if φ is an eigenfunction of $A_1^* A_1$ satisfying (4.3.2) then $\psi = A_1\varphi$ is an eigenfunction of $A_1 A_1^*$ and

$$\begin{aligned} \psi(0) = (A_1\varphi)(0) &= -\varphi''(0) + F_1(0)\varphi'(0) + G_1(0)\varphi(0) \\ &= -\sigma_0\varphi(0) - \sigma_1\varphi'(0) + \sigma_1\varphi'(0) + \sigma_0\varphi(0) = 0, \end{aligned}$$

$$\begin{aligned} \psi'(0) &= -\varphi'''(0) + F_1'(0)\varphi'(0) + F_1(0)\varphi''(0) + G_1'(0)\varphi(0) + G_1(0)\varphi'(0) \\ &= \sigma_2\varphi(0) + \sigma_0\varphi'(0) + \left(-2\sigma_0 - \sigma_1^2\right)\varphi'(0) + \sigma_1\left(\sigma_0\varphi(0) + \sigma_1\varphi'(0)\right) \\ &+ \left(-\sigma_0\sigma_1 - \sigma_2\right)\varphi(0) + \sigma_0\varphi'(0) = 0. \end{aligned}$$

We now verify that $0 \notin \text{spectrum}(A_1 A_1^*)$. Assume there exist $\psi \neq 0$ with $\psi(0) = \psi'(0) = 0$ and

$$A_1 A_1^* \psi = 0.$$

This implies

$$< A_1 A_1^* \psi, \psi >= ||A_1^* \psi|| = 0.$$

But, $A_1^*\psi = 0$ implies

$$\psi'' - 2k_1\psi' + 2k_1^2\psi = 0, \quad x > b.$$

This shows that either $\psi = 0$ or it does not belong to $L^2(\mathbb{R}_+)$. Here, we used the values of F_1 and G_1 and their derivatives outside the support of potentials U and V given by Lemma 4.2.3.

This proves the following result:

Theorem 4.3.1. *The negative eigenvalues of double multiplicity of the operator $\mathcal{H}$ as defined by* (4.1.9) *coincide with the negative eigenvalues of double multiplicity of the operator*

$$\mathcal{H}_1\psi = \left(\frac{d^4}{dx^4} + \frac{d}{dx}U_1(x)\frac{d}{dx} + V_1(x)\right)\psi = \lambda\psi, \quad \psi(0) = \psi'(0) = 0, \tag{4.3.5}$$

with an exception of the lowest negative eigenvalue of $\mathcal{H}$, which is not in the spectrum of $\mathcal{H}_1$. Here, U_1 and V_1 are given by (4.3.1).

It is important to note that the eigenfunctions of the operator $\mathcal{H}$ satisfy the Robin type boundary conditions at $x = 0$, whereas the eigenfunctions of the new operator $\mathcal{H}_1$ satisfy the Dirichlet type boundary conditions at $x = 0$. A similar result was shown for the Schrödinger operators on semi-axis in [26].

Now the spectral problem of the operator (4.1.9) is reduced to the operator (4.3.5). The negative eigenvalues of double multiplicity of the operator $\mathcal{H}_1$ are $\{\lambda_j\}_{j=2}^n$. We can extend U_1 and V_1 by zero on the negative semi-axis and (4.3.5) can be considered as a spectral problem on the whole real line. By the variational principle, if the Dirichlet problem on the semi-axis is extended to the whole-line, the eigenvalues may only decrease and we can make use of the following sharp Lieb-Thirring inequality for the one-dimensional operator (see [44, Theorem 4.1])

$$\sum_{j=2}^{n} |\lambda_j|^{7/4} \leq L^{cl}_{4,7/4,1} Q[U_1, V_1]. \tag{4.3.6}$$

The non-linear functional $Q[U_1, V_1]$ is defined as

$$Q[U_1, V_1] := \frac{1}{48}\int_{\mathbb{R}_+} \left(48V_1^2 + \frac{5}{4}U_1^4 - 12U_1^2V_1 - 40U_1''V_1 + \frac{13}{2}U_1^2U_1'' + 9U_1''^2\right) dx. \tag{4.3.7}$$

This functional was introduced in [44] and corresponds to one of the infinitely many conserved quantities associated with the system of PDEs

$$\begin{cases} U_t = 10U'' + 6UU' - 24V', \\ V_t = 3\left(U'''' + UU'' + U'U''\right) - 8V''' - 6UV'. \end{cases}$$

We refer the reader to [44, Section 3] for more details. The so-called classical constant $L^{cl}_{4,\gamma,d}$ is defined by (4.1.4). Its value for $\gamma = 7/4$ and $d = 1$ is

$$L^{cl}_{4,7/4,1} = \frac{21\sqrt{2}}{128}.$$

In proving inequality (4.3.6), it was assumed that $Q[U_j, V_j] \geq 0$, where, the functions U_j and V_j are the potentials obtained after removing the j^{th} negative eigenvalue of double multiplicity.

Let us now consider $\delta Q := Q[U_1, V_1] - Q[U, V]$. Using (4.2.4a), (4.2.4b) and (4.3.1) one can express δQ as

$$\delta Q = \int_{\mathbb{R}_+} \mathbb{Q}' dx,$$

where,

$$\begin{aligned}\mathbb{Q} = &\left[\frac{2F_1^3}{3} - 2F_1(F_1' - 2G_1) - \frac{4F_1''}{3}\right]|\lambda_1| + F_1''\left[\frac{5F_1'^2}{24} - \frac{G_1^2}{6}\right] + F_1'\left[\frac{G_1G_1'}{3} - \frac{F_1'G_1'}{6}\right] \\ &+ \frac{F_1^2}{168}\left[42(F_1^3(F_1' - 2G_1) - F_1(F_1' - 2G_1)^2) + 28F_1'(G_1' - 4F_1'') + 196F_1''G_1\right. \\ &\left.+49F_1^2F_1'' - 10F_1^5\right] + \frac{F_1}{168}\left[56(F_1''G_1' - G_1'^2) - 70F_1''^2 - 14(F_1' - 2G_1)^3\right]. \qquad (4.3.8)\end{aligned}$$

This implies

$$\delta Q = \mathbb{Q}(\infty) - \mathbb{Q}(0),$$

which, by using Lemma 4.2.3 and Remark 4.2.4 yields

$$\delta Q := Q[U_1, V_1] - Q[U, V] = -\frac{1}{2}\left(L^{cl}_{4,7/4,1}\right)^{-1}|\lambda_1|^{7/4} - \frac{8}{3}|\lambda_1|\sigma_2 + \Omega(\sigma_0, \sigma_1, \sigma_2), \quad (4.3.9)$$

where,

$$\begin{aligned}\Omega(\sigma_0, \sigma_1, \sigma_2) = &-\frac{4}{21}\sigma_1^7 + \frac{8}{3}\sigma_1\sigma_2^2 + \frac{4}{3}\sigma_1^4\sigma_2 - \frac{4}{3}\sigma_0\sigma_1^5 - \frac{16}{3}\sigma_0^2\sigma_1^3 \\ &- \frac{32}{3}\sigma_0^3\sigma_1 + \frac{16}{3}\sigma_0\sigma_1^2\sigma_2 - \frac{8}{3}\sigma_0^2\sigma_2. \qquad (4.3.10)\end{aligned}$$

The derivation of (4.3.9) is very similar to the whole line case (see [44, Section 4]). The main difference is that we calculate the integral on $\mathbb{R}_+$ and use the values of F_1 and G_1 and their derivatives at 0 and infinity, as given by Lemma 4.2.3 and Remark 4.2.4.

Finally, by substituting the value of $Q[U_1, V_1]$ from (4.3.9) into (4.3.6), we obtain

$$\frac{8}{3}|\lambda_1|\sigma_2 L^{cl}_{4,7/4,1} + \frac{1}{2}|\lambda_1|^{7/4} + \sum_{j=2}^{n}|\lambda_j|^{7/4} \leq L^{cl}_{4,7/4,1}\left(Q[U, V] + \Omega(\sigma_0, \sigma_1, \sigma_2)\right).$$

This proves the following:

Theorem 4.3.2. *Let $U, V \in C^\infty(\mathbb{R}_+)$ vanishing on the set $(b, +\infty)$ for some $b > 0$, $U(0) = 0$ and $\{\lambda_j\}_{j=1}^n$ be n negative eigenvalues of double multiplicity of the operator $\mathcal{H}$ defined by (4.1.9). Assume that $Q[U_j, V_j] \geq 0$, where U_j and V_j are the potentials*

associated with the operator $\mathcal{H}_j$ that one obtains after removing the first j eigenvalues of the original operator $\mathcal{H}$. Then the following inequality holds

$$\frac{8}{3}|\lambda_1|\sigma_2 L^{cl}_{4,7/4,1} + \frac{1}{2}|\lambda_1|^{7/4} + \sum_{j=2}^{n}|\lambda_j|^{7/4} \leq L^{cl}_{4,7/4,1}\left(Q[U,V] + \Omega(\sigma_0,\sigma_1,\sigma_2)\right), \quad (4.3.11)$$

where, $\Omega(\sigma_0,\sigma_1,\sigma_2)$ is given by (4.3.10).

Note that, we obtain an equality if U and V are reflectionless potentials.

Corollary 4.3.3. *Let $U, V \in C^\infty(\mathbb{R}_+)$ vanishing on the set $(b,+\infty)$ for some $b > 0$, $U(0) = 0$ and $Q[U_j, V_j] \geq 0$. If σ_0, σ_1 and σ_2 are chosen such that $\Omega(\sigma_0,\sigma_1,\sigma_2) \leq 0$, then the inequality* (4.3.11) *implies*

$$\frac{8}{3}|\lambda_1|\sigma_2 L^{cl}_{4,7/4,1} + \frac{1}{2}|\lambda_1|^{7/4} + \sum_{j=2}^{n}|\lambda_j|^{7/4} \leq L^{cl}_{4,7/4,1}Q[U,V]. \quad (4.3.12)$$

In particular, if $\sigma_0 = \sigma_1 = \sigma_2 = 0$, then (4.1.9) correspond to the Neumann problem and we get

$$\frac{1}{2}|\lambda_1|^{7/4} + \sum_{j=2}^{n}|\lambda_j|^{7/4} \leq L^{cl}_{4,7/4,1}Q[U,V].$$

4.4 Reflectionless potentials and sharpness of the spectral inequality

In this section, we construct potentials U_k and V_k such that the operator

$$\mathcal{H}\varphi(x) = \Big(\frac{d^4}{dx^4} + \frac{d}{dx}\Big(U_k\frac{d}{dx}\Big) + V_k(x)\Big)\varphi(x), \quad \begin{cases}\varphi''(0) = \sigma_0\varphi(0) + \sigma_1\varphi'(0),\\ \varphi'''(0) = -\sigma_2\varphi(0) - \sigma_0\varphi'(0),\end{cases}$$

has exactly one negative eigenvalue of double multiplicity $\lambda = -4k^4$ and demonstrate that, for such potentials, equality is attained in (4.3.11).

In other words, we would like to find U_k and V_k such that the factorization $A^*A = \mathcal{H} - \lambda$ implies $AA^* = \mathcal{H}_0 - \lambda$, where $\mathcal{H}_0 = \frac{d^4}{dx^4}$ subject to the Dirichlet boundary conditions at zero. Following [44], we set $U = 0$ in (4.2.7) and $V = 0$ in (4.2.10). After eliminating W_{12} one obtains

$$16k^4W^2 = 2\left(W^{(4)}W - W^{(3)}W'\right) + W''^2.$$

Let us take

$$\tilde{W} = 2 + \frac{3}{2}e^{2kx} + \frac{1}{6}e^{-2kx} + \frac{3}{5}\cos(2kx) + \frac{4}{5}\sin(2kx)$$

as its 'prototypical' solution. This gives

$$\tilde{F} = \frac{\tilde{W}'}{\tilde{W}} = \frac{k(3e^{2kx} - \frac{1}{3}e^{-2kx} + \frac{8}{5}\cos(2kx) - \frac{6}{5}\sin(2kx))}{2 + \frac{3}{2}e^{2kx} + \frac{1}{6}e^{-2kx} + \frac{3}{5}\cos(2kx) + \frac{4}{5}\sin(2kx)}.$$

Only sign of F changes by interchanging A^* and A, therefore,

$$F(x) = -\frac{k(3e^{2kx} - \frac{1}{3}e^{-2kx} + \frac{8}{5}\cos(2kx) - \frac{6}{5}\sin(2kx))}{2 + \frac{3}{2}e^{2kx} + \frac{1}{6}e^{-2kx} + \frac{3}{5}\cos(2kx) + \frac{4}{5}\sin(2kx)}.$$

The Wronskian W of the two ground states $\varphi_\pm$ of $\mathcal{H}$ is the inverse of $\tilde{W}$, i.e.,

$$W = \frac{1}{2 + \frac{3}{2}e^{2kx} + \frac{1}{6}e^{-2kx} + \frac{3}{5}\cos(2kx) + \frac{4}{5}\sin(2kx)}.$$

The functions F and G are now given by

$$\begin{aligned} F &= \frac{k}{9}(\Theta_1 W - 24), \\ G &= \frac{1}{2}(3F' - F^2) = \frac{k^2}{81}((\Theta_1 W - 24)^2 - 162W\Theta_2 + 486), \end{aligned}$$

where,

$$\begin{aligned} \Theta_1 &= 9e^{2kx} + 7e^{-2kx} + 30\sin(2kx) + 48, \\ \Theta_2 &= 9e^{2kx} + e^{-2kx} + 6. \end{aligned}$$

For reflectionless potentials, (4.3.1) becomes:

$$\begin{cases} U &= -4F', \\ V &= FF'' - 2FG' - F'''. \end{cases}$$

Substituting F, G and their derivatives in the above equations, we obtain the following reflectionless potentials

$$\begin{aligned} U_k =& \frac{4k^2}{81}(108W\Theta_2 - (W\Theta_1 - 24)^2 - 324), \\ V_k =& \frac{8k^4}{6561}(-27W\left(152\Theta_1^2 W + (384\Theta_2 W - 9\Theta_3 W - 2984)\Theta_1 + 162\Theta_2^2 W - 5580\Theta_2\right. \\ & \left. + 216\Theta_3 + 972\right) - \Theta_1^2 W^3(\Theta_1(\Theta_1 W - 96) - 216\Theta_2) - 591300), \end{aligned}$$

where,

$$\Theta_3 = \Theta_1 - 6\left(\Theta_2 - 18e^{2kx} - 6\right).$$

4.4.1 Sharpness of the spectral inequality

Calculating the values of F, G and their derivatives at zero, we obtain

$$F(0) = -k, \quad G(0) = -\frac{k^2}{2}, \quad F'(0) = F''(0) = G'(0) = 0. \tag{4.4.1}$$

This implies, using Lemma (4.2.3) and Remark (4.2.4),

$$\sigma_0 = -\frac{k^2}{2}, \quad \sigma_1 = -k, \quad \sigma_2 = -\frac{k^3}{2}. \tag{4.4.2}$$

As U_k and V_k are reflectionless, therefore, $U_1 = V_1 = 0$ and hence, $Q[U_1, V_1] = 0$. This implies

$$\delta Q = Q[U_1, V_1] - Q[U_k, V_k] = -Q[U_k, V_k] = \mathbb{Q}(0) - \mathbb{Q}(\infty).$$

Moreover, (4.3.6) implies $\sum_{j=2}^{n} |\lambda_j|^{7/4} = 0$. Using (4.3.8) and values from (4.4.1) and Lemma (4.2.3), we obtain

$$Q[U_k, V_k] = \frac{403}{21} k^7. \tag{4.4.3}$$

Similarly substituting (4.4.2) into (4.3.10), we get

$$\Omega(\sigma_0, \sigma_1, \sigma_2) = -\frac{k^7}{7}. \tag{4.4.4}$$

Finally (4.4.3), (4.4.4) and the values $\lambda_1 = \lambda = -4k^2$, $\sigma_2 = -k^3/2$ and $L^{cl}_{4,7/4,1} = 21\sqrt{2}/128$ yields the equality

$$\frac{8}{3}|\lambda_1|\sigma_2 L^{cl}_{4,7/4,1} + \frac{1}{2}|\lambda_1|^{7/4} + \sum_{j=2}^{n} |\lambda_j|^{7/4} = \frac{25k^7}{4\sqrt{2}} = L^{cl}_{4,7/4,1}\bigg(Q[U_k, V_k] + \Omega(\sigma_0, \sigma_1, \sigma_2)\bigg).$$

Chapter 5

NSA quantum star graphs

5.1 Introduction and Main Results

In this chapter, we consider the Schrödinger operators on a star shaped graph Γ

$$H_\Gamma \psi(x) = \left(-\frac{d^2}{dx^2} + V(x) \right) \psi(x), \quad x \in \Gamma \tag{5.1.1}$$

acting in $L^2(\Gamma)$. The star graph Γ can be imagined as a metric graph with a finite number n of edges of infinite length connected at a single vertex. We identify each edge by the interval $\mathbb{R}_+ = [0, \infty)$ and the common vertex by the set $\{0\}$. We assume that V is complex-valued.

The main results of this chapter are the following:

Theorem 5.1.1. *Consider the Schrödinger operators H_Γ with vertex conditions*

$$\psi_1(0) = \ldots = \psi_n(0) := \psi(0), \quad \sum_{j=1}^{n} \psi_j'(0) = 0, \tag{5.1.2}$$

where ψ_j is the restriction of ψ on the j^{th} edge. Then any eigenvalue $\lambda = |\lambda| e^{i\theta} \in \mathbb{C} \backslash [0, \infty)$ of H_Γ satisfies

$$|\lambda|^{\frac{1}{2}} \leq \frac{\sqrt{n^3 + G(\theta)}}{2n} \int_\Gamma |V(x)| \, dx.$$

Here,

$$G(\theta) = \sup_{y_j \geq 0} \left(\sum_{j=1}^{n} e^{-2y_j} \left((n-2)^2 e^{-2y_j} - 2n(n-2) \cos(2 \cot(\theta/2) y_j) + 4 \sum_{l=1, l \neq j}^{n} e^{-2y_l} \right) \right).$$

Proposition 5.1.2. *Let $n = 2$ and consider the Schrödinger operator H_Γ.*

1. *Then any eigenvalue $\lambda = k^2 \in \mathbb{C}\backslash[0,\infty)$ of H_Γ subject to δ interaction*

$$\psi_1(0) = \psi_2(0) := \psi(0), \quad \psi_1'(0) + \psi_2'(0) = \alpha\psi(0), \quad \alpha \geq 0$$

satisfies

$$\left| ik - \frac{\alpha}{2} \right| \leq \int_{\mathbb{R}^2_+} |V(x)|\, dx.$$

2. *Any eigenvalue $\lambda \in \mathbb{C}\backslash[0,\infty)$ of H_Γ subject to δ' interaction*

$$\psi_1'(0) = \psi_2'(0) := \psi'(0), \quad \psi_1(0) + \psi_2(0) = \beta\psi'(0), \quad \beta \geq 0$$

satisfies

$$\frac{|k\,(\beta\, k + 2i)|}{\sqrt{(|\beta\, k + i|)^2 + 1}} \leq \sqrt{2} \int_{\mathbb{R}^2_+} |V(x)|\, dx.$$

5.2 Auxilary results

The matching conditions at a vertex of degree n can be expressed in terms of two $n \times n$ matrices A and B as

$$A\psi(x) + B\psi'(x) = 0, \tag{5.2.1}$$

where $\psi = (\psi_1, \psi_2, \ldots, \psi_n)^T \in \bigoplus_{i=1}^n L^2(\mathbb{R}_+; \mathbb{C})$. The operator H_Γ, defined in (5.1.1) subject to vertex conditions (5.2.1), is self-adjoint if $\mathrm{Rank}(A, B) = n$ and $AB^* = BA^*$.

Lemma 5.2.1 ([18], Lemma 3.4)**.** *If the matching conditions* (5.2.1) *are such that $A+ikB$ is invertible for some $k \in \mathbb{C}$ then the resolvent $(H_\Gamma - k^2)^{-1}$ is an integral operator*

$$(H_\Gamma - k^2)^{-1}\psi(x) = \int_{\mathbb{R}^n_+} R_{A,B}(x, y; k)\psi(y)dy,$$

with resolvent kernel

$$R_{A,B}(x, y; k) = \frac{i}{2k}\left(\mathrm{diag}\{e^{ik|x_j - y_j|}\} + \mathrm{diag}\{e^{ikx_j}\}\Theta(k; A, B)\mathrm{diag}\{e^{iky_j}\}\right), \tag{5.2.2}$$

where $k \in \mathbb{C}$ such that $\mathrm{Im}\, k > 0$, $j = 1, \ldots, n$, $\Theta(k; A, B) = -(A + ikB)^{-1}(A - ikB)$ and $x = (x_1, x_2, \ldots, x_n)^T, y = (y_1, y_2, \ldots, y_n)^T \in \mathbb{R}^n_+$.

For the δ conditions

$$\psi_1(0) = \ldots = \psi_n(0) := \psi(0), \quad \sum_{j=1}^{n} \psi_j'(0) = \alpha\psi(0), \tag{5.2.3}$$

we can choose

$$A_1 = \begin{bmatrix} 1 & -1 & 0 & \cdots & 0 & 0 \\ 0 & 1 & -1 & \cdots & 0 & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & \cdots & 1 & -1 \\ -\alpha & 0 & 0 & \cdots & 0 & 0 \end{bmatrix} \quad \text{and} \quad B_1 = \begin{bmatrix} 0 & 0 & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & \cdots & 0 \\ 1 & 1 & \cdots & 1 \end{bmatrix}.$$

A_1+ikB_1 is invertible for complex $k \neq 0$ and the kernel of the integral operator $(H_\Gamma - k^2)^{-1}$ is given by

$$R_{A_1,B_1}(x,y;k) = \tag{5.2.4}$$

$$\frac{i}{2k} \begin{bmatrix} e^{ik|x_1-y_1|} - \frac{\phi_a(n-2)}{\phi_a(n)} e^{ik(x_1+y_1)} & \frac{2}{\phi_a(n)} e^{ik(x_1+y_2)} & \cdots & \frac{2}{\phi_a(n)} e^{ik(x_1+y_n)} \\ \frac{2}{\phi_a(n)} e^{ik(x_2+y_1)} & e^{ik|x_2-y_2|} - \frac{\phi_a(n-2)}{\phi_a(n)} e^{ik(x_2+y_2)} & \cdots & \frac{2}{\phi_a(n)} e^{ik(x_2+y_n)} \\ \cdots & \cdots & \cdots & \cdots \\ \frac{2}{\phi_a(n)} e^{ik(x_n+y_1)} & \frac{2}{\phi_a(n)} e^{ik(x_n+y_2)} & \cdots & e^{ik|x_n-y_n|} - \frac{\phi_a(n-2)}{\phi_a(n)} e^{ik(x_n+y_n)} \end{bmatrix}, \tag{5.2.5}$$

where $\phi_a(n) = n + \frac{\alpha}{k} i$.

Similarly for δ' vertex conditions

$$\psi_1'(0) = \ldots = \psi_n'(0) := \psi'(0), \quad \sum_{j=1}^{n} \psi_j(0) = \beta\psi'(0), \tag{5.2.6}$$

we can choose

$$A_2 = \begin{bmatrix} 0 & 0 & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & \cdots & 0 \\ 1 & 1 & \cdots & 1 \end{bmatrix} \quad \text{and} \quad B_2 = \begin{bmatrix} 1 & -1 & 0 & \cdots & 0 & 0 \\ 0 & 1 & -1 & \cdots & 0 & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & \cdots & 1 & -1 \\ -b & 0 & 0 & \cdots & 0 & 0 \end{bmatrix}.$$

A_2+ikB_2 is invertible for complex $k \neq 0$ and the kernel of the integral operator $(H_\Gamma - k^2)^{-1}$

is given by

$$R_{A_2,B_2}(x,y;k) = \tag{5.2.7}$$

$$\frac{i}{2k}\begin{bmatrix} e^{ik|x_1-y_1|}+\frac{\varphi_\beta(n-2)}{\varphi_\beta(n)}e^{ik(x_1+y_1)} & \frac{2}{\varphi_\beta(n)}e^{ik(x_1+y_2)} & \dots & \frac{2}{\varphi_\beta(n)}e^{ik(x_1+y_n)} \\ \frac{2}{\varphi_\beta(n)}e^{ik(x_2+y_1)} & e^{ik|x_2-y_2|}+\frac{\varphi_\beta(n-2)}{\varphi_\beta(n)}e^{ik(x_2+y_2)} & \dots & \frac{2}{\varphi_\beta(n)}e^{ik(x_2+y_n)} \\ \dots & \dots & \dots & \dots \\ \frac{2}{\varphi_\beta(n)}e^{ik(x_n+y_1)} & \frac{2}{\varphi_\beta(n)}e^{ik(x_n+y_2)} & \dots & e^{ik|x_n-y_n|}+\frac{\varphi_\beta(n-2)}{\varphi_\beta(n)}e^{ik(x_n+y_n)} \end{bmatrix}, \tag{5.2.8}$$

where $\varphi_\beta(n) = \beta k i - n$.

5.3 Proofs

Proof of Theorem 5.1.1. Consider

$$-\psi''(x) - V(x)\psi(x) = k^2\psi(x), \quad x \in \Gamma$$

with vertex conditions (5.2.3) at vertex $\{0\}$ with $\alpha = 0$ and $V = \operatorname{diag}\{v_i\}$, $i = 1, \cdots, n$ be a complex-valued matrix potential. Let $\lambda = k^2 \in \mathbb{C} \setminus [0,\infty)$ be an eigenvalue of H_Γ with $\operatorname{Im} k > 0$ and let $\psi = (\psi_1, \psi_2, \dots, \psi_n)^T$ be the corresponding eigenfunction. Then the Birman-Schwinger operator

$$\sqrt{V}\left(-\frac{d^2}{dx^2} - k^2\right)^{-1}\sqrt{|V|}, \qquad \sqrt{V} := (\operatorname{sgn} V)\sqrt{|V|},$$

has an eigenvalue 1. Therefore its Hilbert Schmidt norm is greater than or equal to 1. The resolvent kernel of this operator is

$$\sqrt{V(x)}R_{A_1,B_1}(x,y;k)\sqrt{|V(y)|} \quad \text{with} \quad \alpha = 0,$$

and therefore

$$\begin{aligned} 1 \le \left\|\sqrt{V}\left(-\frac{d^2}{dx^2}+k^2\right)^{-1}\sqrt{|V|}\right\|_2 &\le \left\|\sqrt{V}\right\|_2 \left\|\left(-\frac{d^2}{dx^2}-k^2\right)^{-1}\sqrt{|V|}\right\|_2 \\ &= \left\|\sqrt{V}\right\|_2 \left\|R_{A_1,B_1}\sqrt{|V|}\right\|_2 \\ &\le \left\|\sqrt{V}\right\|_2 \left\|\sqrt{|V|}\right\|_2 \sup|R_{A_1,B_1}|^2 \\ &= \|V\|_1^2 \sup|R_{A_1,B_1}|^2. \end{aligned}$$

Hence

$$1 \le \|V\|_1^2 \sup|R_{A_1,B_1}|^2. \tag{5.3.1}$$

To compute $|R_{A_1,B_1}|^2$, we vectorize the matrix R_{A_1,B_1} and compute $|R_{A_1,B_1}|^2 = \mathrm{vec}(R^*_{A_1,B_1}) \cdot \mathrm{vec}(R_{A_1,B_1})$. Here $*$ denotes complex conjugate transpose, and find

$$|R_{A_1,B_1}|^2 = \frac{1}{4|k|^2}\left(\sum_{j=1}^{n}\left(\left|e^{ik|x_j-y_j|} - \frac{n-2}{n}e^{ik(x_j+y_j)}\right|^2 + \sum_{l=1,l\neq j}^{n}\left|\frac{2}{n}e^{ik(x_j+y_l)}\right|^2\right)\right)$$

$$\sup|R_{A_1,B_1}|^2 = \frac{1}{4|k|^2}\sup_{x_j,y_j\geq 0}\left(\sum_{j=1}^{n}\left(\left|e^{ik|x_j-y_j|} - \frac{n-2}{n}e^{ik(x_j+y_j)}\right|^2 + \sum_{l=1,l\neq j}^{n}\left|\frac{2}{n}e^{ik(x_j+y_l)}\right|^2\right)\right)$$

Without loss of generality, we can let $x_j - y_j \geq 0$, and can take the supremum over the smaller set $x_j \geq y_j \geq 0$ for $j = 1, \cdots, n$. Then

$$\begin{aligned}\sup|R_{A_1,B_1}|^2 &= \frac{1}{4|k|^2}\sup_{x_j\geq y_j\geq 0}\left(\sum_{j=1}^{n}\left(\left|e^{ik(x_j-y_j)} - \frac{n-2}{n}e^{ik(x_j+y_j)}\right|^2 + \sum_{l=1,l\neq j}^{n}\left|\frac{2}{n}e^{ik(x_j+y_l)}\right|^2\right)\right)\\ &= \frac{1}{4|k|^2}\sup_{x_j\geq y_j\geq 0}\left(\sum_{j=1}^{n}e^{-2\mathrm{Im}\,kx_j}\left(\left|e^{-iky_j} - \frac{n-2}{n}e^{iky_j}\right|^2 + \sum_{l=1,l\neq j}^{n}\left|\frac{2}{n}e^{iky_l}\right|^2\right)\right).\end{aligned}$$

Since $\mathrm{Im}\,k > 0$, the supremum over x_j is achieved at $x_j = y_j$ for $j = 1, \cdots n$, and hence

$$\begin{aligned}\sup|R_{A_1,B_1}|^2 &= \frac{1}{4|k|^2}\sup_{y_j\geq 0}\left(\sum_{j=1}^{n}\left(\left|1 - \frac{n-2}{n}e^{2iky_j}\right|^2 + \sum_{l=1,l\neq j}^{n}\left|\frac{2}{n}e^{ik(y_j+y_l)}\right|^2\right)\right)\\ &= \frac{1}{4|nk|^2}\sup_{y_j\geq 0}\left(\sum_{j=1}^{n}\left(\left|n-(n-2)e^{2iky_j}\right|^2 + \sum_{l=1,l\neq j}^{n}\left|2e^{ik(y_j+y_l)}\right|^2\right)\right).\end{aligned}$$

In order to make the above expression more explicit, let $k = |k|e^{i\tilde{\theta}}$ with $0 < \tilde{\theta} < \pi$. Then

$$
\begin{aligned}
&\sup |R_{A_1,B_1}|^2 \\
&= \frac{1}{4|nk|^2} \sup_{y_j \geq 0} \left(\sum_{j=1}^{n} \left(\left| n - (n-2)e^{2(|k|(\cos(\tilde{\theta})i - \sin(\tilde{\theta}))y_j} \right|^2 \right.\right. \\
&\qquad \left.\left. + \sum_{l=1, l\neq j}^{n} \left| 2e^{(|k|(\cos(\tilde{\theta})i - \sin(\tilde{\theta}))(y_j + y_l)} \right|^2 \right) \right) \\
&= \frac{1}{4|nk|^2} \sup_{y_j \geq 0} \left(\sum_{j=1}^{n} \left(\left| ne^{-2i|k|\cos(\tilde{\theta})y_j)} - (n-2)e^{-2|k|\sin(\tilde{\theta})y_j} \right|^2 \right.\right. \\
&\qquad \left.\left. + \sum_{l=1, l\neq j}^{n} \left(2e^{-|k|\sin(\tilde{\theta})(y_j + y_l)} \right)^2 \right) \right) \\
&= \frac{1}{4|nk|^2} \sup_{y_j \geq 0} \left(\sum_{j=1}^{n} \left(\left| n \left(\cos(2|k|\cos(\tilde{\theta})y_j) - i\sin(2|k|\cos(\tilde{\theta})y_j) \right) - (n-2)e^{-2|k|\sin(\tilde{\theta})y_j} \right|^2 \right) \right. \\
&\qquad \left. + \sum_{j=1}^{n} \sum_{l=1, l\neq j}^{n} \left(2e^{-|k|\sin(\tilde{\theta})(y_j + y_l)} \right)^2 \right) \\
&= \frac{1}{4|nk|^2} \sup_{y_j \geq 0} \left(\sum_{j=1}^{n} \left(\left(n\cos(2|k|\cos(\tilde{\theta})y_j) - (n-2)e^{-2|k|\sin(\tilde{\theta})y_j} \right)^2 + n^2 \sin^2(2|k|(\cos(\tilde{\theta})y_j) \right) \right. \\
&\qquad \left. + \sum_{j=1}^{n} \sum_{l=1, l\neq j}^{n} \left(2e^{-|k|\sin(\tilde{\theta})(y_j + y_l)} \right)^2 \right) \\
&= \frac{1}{4|nk|^2} \left(n^3 + \sup_{y_j \geq 0} \left(\sum_{j=1}^{n} e^{-2|k|\sin(\tilde{\theta})y_j} \left((n-2)^2 e^{-2|k|\sin(\tilde{\theta})y_j} \right.\right.\right. \\
&\qquad \left.\left.\left. -2n(n-2)\cos(2|k|\cos(\tilde{\theta})y_j) + 4 \sum_{l=1, l\neq j}^{n} e^{-2|k|\sin(\tilde{\theta})y_l} \right) \right) \right).
\end{aligned}
$$

If we write $\lambda = |\lambda|e^{i\theta}$ with $0 < \theta < 2\pi$, then

$$
\begin{aligned}
\sup |R_{A_1,B_1}|^2 = \frac{1}{4|nk|^2} &\left(n^3 + \sup_{y_j \geq 0} \left(\sum_{j=1}^{n} e^{-2\sqrt{|\lambda|}\sin(\theta/2)y_j} \left((n-2)^2 e^{-2\sqrt{|\lambda|}\sin(\theta/2)y_j} \right.\right.\right. \\
&\left.\left.\left. -2n(n-2)\cos(2\sqrt{|\lambda|}\cos(\theta/2)y_j) + 4 \sum_{l=1, l\neq j}^{n} e^{-2\sqrt{|\lambda|}\sin(\theta/2)y_l} \right) \right) \right).
\end{aligned}
$$

Since $\sqrt{|\lambda|}\sin(\theta/2)y_j \geq 0$, by change of variables the above expression can be re-written as

$$\sup|R_{A_1,B_1}|^2 = \frac{1}{4|nk|^2}\left(n^3 + \sup_{y_j\geq 0}\left(\sum_{j=1}^{n} e^{-2y_j}\left((n-2)^2e^{-2y_j} - 2n(n-2)\cos(2\cot(\theta/2)y_j)\right.\right.\right.$$
$$\left.\left.\left. +4\sum_{l=1,l\neq j}^{n} e^{-2y_l}\right)\right)\right).$$

Substituting it in (5.3.1), we get the desired result. □

Proof of Proposition 5.1.2(1). For $n = 2$ and delta conditions at the vertex, $|R_{A_1,B_1}|^2$ is given as

$$|R_{A_1,B_1}|^2 = \frac{1}{|2ik-\alpha|^2}\left(\left|\frac{(2ik-\alpha)e^{ik|x_1-y_1|} + \alpha e^{ik(x_1+y_1)}}{2k}\right|^2 + \left|e^{ik(x_1+y_2)}\right|^2\right.$$
$$\left. + \left|e^{ik(x_2+y_1)}\right|^2 + \left|\frac{(2ik-\alpha)e^{ik|x_2-y_2|} + \alpha e^{ik(x_2+y_2)}}{2k}\right|^2\right).$$

$$\sup|R_{A_1,B_1}|^2 = \frac{1}{|2ik-\alpha|^2}\sup_{x_i,y_i\geq 0}\left(\left|\frac{(2ik-\alpha)e^{ik|x_1-y_1|} + \alpha e^{ik(x_1+y_1)}}{2k}\right|^2 + \left|e^{ik(x_1+y_2)}\right|^2\right.$$
$$\left. + \left|e^{ik(x_2+y_1)}\right|^2 + \left|\frac{(2ik-\alpha)e^{ik|x_2-y_2|} + \alpha e^{ik(x_2+y_2)}}{2k}\right|^2\right).$$

Without loss of generality, we can let $x_i - y_i \geq 0$, and can take the supremum over the smaller set $x_i \geq y_i \geq 0$ for $i = 1, 2$. Then

$$\sup|R_{A_1,B_1}|^2 = \frac{1}{|2ik-\alpha|^2}\sup_{x_i\geq y_i\geq 0}\left(\left|\frac{(2ik-\alpha)e^{ik(x_1-y_1)} + \alpha e^{ik(x_1+y_1)}}{2k}\right|^2 + \left|e^{ik(x_1+y_2)}\right|^2\right.$$
$$\left. + \left|e^{ik(x_2+y_1)}\right|^2 + \left|\frac{(2ik-\alpha)e^{ik(x_2-y_2)} + \alpha e^{ik(x_2+y_2)}}{2k}\right|^2\right)$$
$$= \frac{1}{|2ik-\alpha|^2}\sup_{x_i\geq y_i\geq 0}\left(e^{-2\mathrm{Im}\,kx_1}\left(\left|\frac{(2ik-\alpha)e^{-iky_1} + \alpha e^{iky_1}}{2k}\right|^2 + \left|e^{iky_2}\right|^2\right)\right.$$
$$\left. + e^{-2\mathrm{Im}\,kx_2}\left(\left|e^{iky_1}\right|^2 + \left|\frac{(2ik-\alpha)e^{-iky_2} + \alpha e^{iky_2}}{2k}\right|^2\right)\right).$$

Since $\operatorname{Im} k > 0$, the superemum over x_i is achieved at $x_i = y_i$ for $i = 1, 2$, and hence

$$\begin{aligned}
&\sup |R_{A_1,B_1}|^2 \\
&= \frac{1}{|2ik-\alpha|^2} \sup_{y_1,y_2\geq 0} \left(\left| \frac{(2ik-\alpha)+\alpha e^{2iky_1}}{2k} \right|^2 + 2\left| e^{ik(y_1+y_2)} \right|^2 + \left| \frac{(2ik-\alpha)+\alpha e^{2iky_2)}}{2k} \right|^2 \right) \\
&= \frac{1}{|2ik-\alpha|^2} \sup_{y_1,y_2\geq 0} \left(\left| \frac{(2ik-\alpha)+\alpha e^{2iky_1}}{2k} \right|^2 + 2e^{-2\operatorname{Im} k(y_1+y_2)} + \left| \frac{(2ik-\alpha)+\alpha e^{2iky_2)}}{2k} \right|^2 \right).
\end{aligned}$$

For $\alpha \geq 0$

$$\sup_{y_1,y_2\geq 0} \left(\left| \frac{(2ik-\alpha)+\alpha e^{2iky_1}}{2k} \right|^2 + 2e^{-2\operatorname{Im} k(y_1+y_2)} + \left| \frac{(2ik-\alpha)+\alpha e^{2iky_2)}}{2k} \right|^2 \right) \leq 4$$

and therefore

$$\sup |R_{A_1,B_1}|^2 \leq \frac{4}{|2ik-\alpha|^2}.$$

Substituting it in (5.3.1) and simplifying, we get the claimed result. □

Proof of Proposition 5.1.2(2). For $n = 2$ and δ' conditions at the vertex, $|R_{A_2,B_2}|^2$ is given as

$$\begin{aligned}
|R_{A_2,B_2}|^2 = \frac{1}{|k(\beta k+2i)|^2} \Bigg(&\frac{\left|(\beta k+2i)e^{ik|x_1-y_1|} + \beta k e^{ik(x_1+y_1)}\right|^2}{4} + \left| e^{ik(x_1+y_2)} \right|^2 \\
&+ \left| e^{ik(x_2+y_1)} \right|^2 + \left| \frac{\left|(\beta k+2i)e^{ik|x_2-y_2|} + \beta k e^{ik(x_2+y_2)}\right|^2}{4} \right| \Bigg).
\end{aligned}$$

$$\begin{aligned}
\sup |R_{A_2,B_2}|^2 = \frac{1}{|k(\beta k+2i)|^2} \sup_{x_i,y_i\geq 0} \Bigg(&\frac{\left|(\beta k+2i)e^{ik|x_1-y_1|} + \beta k e^{ik(x_1+y_1)}\right|^2}{4} + \left| e^{ik(x_1+y_2)} \right|^2 \\
&+ \left| e^{ik(x_2+y_1)} \right|^2 + \left| \frac{\left|(\beta k+2i)e^{ik|x_2-y_2|} + \beta k e^{ik(x_2+y_2)}\right|^2}{4} \right| \Bigg).
\end{aligned}$$

Without loss of generality, we can let $x_i - y_i \geq 0$, and can take the supremum over the

smaller set $x_i \geq y_i \geq 0$ for $i = 1, 2$. Then

$$\begin{aligned}\sup |R_{A_2,B_2}|^2 &= \frac{1}{|k(\beta k+2i)|^2} \sup_{x_i \geq y_i \geq 0} \left(\frac{\left|(\beta k+2i)e^{ik(x_1-y_1)} + \beta k e^{ik(x_1+y_1)}\right|^2}{4} + \left|e^{ik(x_1+y_2)}\right|^2 \right. \\ &\quad \left. + \left|e^{ik(x_2+y_1)}\right|^2 + \left|\frac{\left|(\beta k+2i)e^{ik(x_2-y_2)} + \beta k e^{ik(x_2+y_2)}\right|^2}{4}\right| \right) \\ &= \frac{1}{|k(\beta k+2i)|^2} \sup_{x_i \geq y_i \geq 0} \left(e^{-2\mathrm{Im}\, k x_1} \left(\frac{\left|(\beta k+2i)e^{-iky_1} + \beta k e^{iky_1}\right|^2}{4} + \left|e^{iky_2}\right|^2 \right) \right. \\ &\quad \left. + e^{-2\mathrm{Im}\, k x_2} \left(\left|e^{iky_1}\right|^2 + \left|\frac{\left|(\beta k+2i)e^{-iky_2} + \beta k e^{iky_2}\right|^2}{4}\right| \right) \right).\end{aligned}$$

Since $\mathrm{Im}\, k > 0$, the supremum over x_i is achieved at $x_i = y_i$ for $i = 1, 2$, and hence

$$\begin{aligned}&\sup |R_{A_2,B_2}|^2 \\ &= \frac{1}{|k(\beta k+2i)|^2} \sup_{y_i \geq 0} \left(\frac{\left|(\beta k+2i) + \beta k e^{2iky_1}\right|^2}{4} + 2\left|e^{ik(y_1+y_2)}\right|^2 + \left|\frac{\left|(\beta k+2i) + \beta k e^{2iky_2}\right|^2}{4}\right| \right).\end{aligned}$$

Since $\beta \geq 0$, therefore

$$\sup |R_{A_2,B_2}|^2 \leq \frac{2(|\beta k+i|^2+1)}{|k(\beta k+2i)|^2}.$$

substituting it in (5.3.1) and simplifying, we get the required result. □

Appendix A

Estimate on trace norm of resolvent difference for GPI

Here we'll provide and explicit derivation of the estimate

$$||R_V^{\mathcal{A}}(-t) - R_0^{\mathcal{A}}(-t)||_1 \leq C_\epsilon t^{-\frac{3}{2}+\epsilon}$$

for all $\epsilon > 0$ and large t. We will need the following lemma.

Lemma A.0.1 ([18], Lemma 3.4)**.** *Let $\mathcal{H}$ be a Hilbert space and $q, r \in \mathcal{H}$. Assume that $\mathcal{R} = (\cdot, q)q - (\cdot, r)r$ is an operator of rank two on $\mathcal{H}$. Then, the trace norm of $\mathcal{R}$ is given by*

$$||\mathcal{R}||_1 = \sqrt{(||q||^2 + ||r||^2)^2 - 4|(q,r)|^2}. \tag{A.0.1}$$

Moreover, if we let $r = q + s$ then,

$$(||q||^2 + ||r||^2)^2 - 4|(q,r)|^2 \leq 6||s||^2||q||^2 + 3||s||^4. \tag{A.0.2}$$

Lemma A.0.2. *Assume that the potential V satisfy condition* (2.1.2)*. Then the resolvents $R_V^{\mathcal{A}}$ of $H_V^{\mathcal{A}}$ and $R_0^{\mathcal{A}}$ of $H_0^{\mathcal{A}}$ satisfy, for all $\epsilon > 0$ and for large t,*

$$||R_V^{\mathcal{A}}(-t) - R_0^{\mathcal{A}}(-t)||_1 \leq C_\epsilon t^{-\frac{3}{2}+\epsilon}.$$

Proof. Let $\mathcal{R}_1 = R_V^{\mathcal{A}}(-t) - R_V^D(-t) + R_0^D(-t) - R_0^{\mathcal{A}}(-t)$ and $\mathcal{R}_2 = R_V^D(-t) - R_0^D(-t)$ then,

$$R_V^{\mathcal{A}}(-t) - R_0^{\mathcal{A}}(-t) = \mathcal{R}_1 + \mathcal{R}_2.$$

Hence

$$||R_V^{\mathcal{A}}(-t) - R_0^{\mathcal{A}}(-t)||_1 \leq ||\mathcal{R}_1||_1 + ||\mathcal{R}_2||_1. \tag{A.0.3}$$

Trace norm on $\mathcal{R}_2$ can be estimated as $||\mathcal{R}_2||_1 \leq ct^{-\frac{3}{2}+\epsilon}$ (c.f. Lemma 4.5.6. [97]). We only need to find estimate on the trace norm of rank two operator $\mathcal{R}_1$. By adding and subtracting the quantity

$$\frac{f_j^2(x_j, i\sqrt{t})}{L(i\sqrt{t})f_j^2(0, i\sqrt{t})} + \frac{e^{-2x_j\sqrt{t}}}{(d-a)\sqrt{t}+bt-c} \qquad j = 1, 2$$

in the diagonal of $\mathcal{R}_1$ we can re-write it as

$$\mathcal{R}_1 = \mathcal{S}_1 + \mathcal{S}_2,$$

where

$$\mathcal{S}_1 = \begin{bmatrix} \frac{(a-\sqrt{t}b+1)e^{-2x_1\sqrt{t}}}{(d-a)\sqrt{t}+bt-c} - \frac{\left(a+b\frac{f_2'(0,i\sqrt{t})}{f_2(0,i\sqrt{t})}+1\right)f_1^2(x_1,i\sqrt{t})}{L(i\sqrt{t})f_1^2(0,i\sqrt{t})} & 0 \\ 0 & \frac{(1-\sqrt{t}b-d)e^{-2x_2\sqrt{t}}}{(d-a)\sqrt{t}+bt-c} - \frac{\left(b\frac{f_1'(0,i\sqrt{t})}{f_1(0,i\sqrt{t})}-d+1\right)f_2^2(x_2,i\sqrt{t})}{L(i\sqrt{t})f_2^2(0,i\sqrt{t})} \end{bmatrix}$$

and

$$\mathcal{S}_2 = \left[\frac{f_j(x_j,i\sqrt{t})f_k(x_k,i\sqrt{t})}{L(i\sqrt{t})f_j(0,i\sqrt{t})f_k(0,i\sqrt{t})} - \frac{e^{-(x_j+x_k)\sqrt{t}}}{(d-a)\sqrt{t}+bt-c}\right] \qquad j, k = 1, 2.$$

Now, as $\mathcal{S}_1$ is a diagonal matrix and in order to apply definition of trace norm, we can let $\mathcal{S}_1 = I\mathcal{S}_1 I$, where I is second order identity matrix. This implies,

$$||\mathcal{S}_1||_1 = |\sigma_1| + |\sigma_2|$$

where

$$|\sigma_1| = \int_0^\infty \left| \frac{(a-\sqrt{t}b+1)e^{-2x_1\sqrt{t}}}{(d-a)\sqrt{t}+bt-c} - \frac{\left(a+b\frac{f_2'(0,i\sqrt{t})}{f_2(0,i\sqrt{t})}+1\right)f_1^2(x_1,i\sqrt{t})}{L(i\sqrt{t})f_1^2(0,i\sqrt{t})} \right| dx_1$$

and

$$|\sigma_2| = \int_0^\infty \left| \frac{(1-\sqrt{t}b-d)e^{-2x_2\sqrt{t}}}{(d-a)\sqrt{t}+bt-c} - \frac{\left(b\frac{f_1'(0,i\sqrt{t})}{f_1(0,i\sqrt{t})}-d+1\right)f_2^2(x_2,i\sqrt{t})}{L(i\sqrt{t})f_2^2(0,i\sqrt{t})} \right| dx_2.$$

For t large enough, these expressions can be simplified to

$$\begin{aligned} |\sigma_1| &= \left|\frac{(a-\sqrt{t}b+1)}{(d-a)\sqrt{t}+bt-c}\right| \int_0^\infty \left|e^{-2x_1\sqrt{t}} - f_1^2(x_1, i\sqrt{t})\right| dx_1 \\ &= \left|\frac{(a-\sqrt{t}b+1)}{(d-a)\sqrt{t}+bt-c}\right| \int_0^\infty \left|f_1(x_1, i\sqrt{t}) - e^{-x_1\sqrt{t}}\right| \left|f_1(x_1, i\sqrt{t}) + e^{-x_1\sqrt{t}}\right| dx_1 \end{aligned}$$

and

$$|\sigma_2| = \left|\frac{(1-\sqrt{t}b-d)}{(d-a)\sqrt{t}+bt-c}\right| \int_0^\infty \left|f_1(x_1, i\sqrt{t}) - e^{-x_1\sqrt{t}}\right| \left|f_1(x_1, i\sqrt{t}) + e^{-x_1\sqrt{t}}\right| dx_1.$$

To find estimates for $|\sigma_1|$ and $|\sigma_2|$ we use the following estimates for large t

$$\left|f_k(x_k, i\sqrt{t}) - e^{-\sqrt{t}x_k}\right| \leq \frac{m_1}{\sqrt{t}} e^{-\sqrt{t}x_k} \tag{A.0.4}$$

and

$$\left|f_k(x_k, i\sqrt{t}) + e^{-\sqrt{t}x_k})\right| \leq \left(\frac{m_2}{\sqrt{t}} + 2\right) e^{-\sqrt{t}x_k} \tag{A.0.5}$$

This yields the following bounds

$$|\sigma_1| \leq \left|\frac{(a-\sqrt{t}b+1)}{(d-a)\sqrt{t}+bt-c}\right| \frac{m_1(m_2+2\sqrt{t})}{2t^{3/2}} = |-m_1 t^{-3/2} + O(t^{-2})|,$$
$$|\sigma_2| \leq \left|\frac{(1-\sqrt{t}b-d)}{(d-a)\sqrt{t}+bt-c}\right| \frac{m_1(m_2+2\sqrt{t})}{2t^{3/2}} = |-m_1 t^{-3/2} + O(t^{-2})|.$$

Therefore

$$|\sigma_1| = |\sigma_2| = O(t^{-3/2})$$

and hence

$$||\mathcal{S}_1||_1 = O(t^{-3/2}).$$

To find estimate on norm of $\mathcal{S}_2$, we use Lemma (A.0.1). Clearly, $\mathcal{S}_2 = (\cdot, q)q - (\cdot, r)r$ is an operator of rank two, where

$$q_k(x_k) = \frac{-e^{-x_k\sqrt{t}}}{\sqrt{(d-a)\sqrt{t}+bt-c}} \quad \text{and} \quad r_k(x_k) = \frac{-f_k(x_k, i\sqrt{t})}{\sqrt{L(i\sqrt{t})f_k(0, i\sqrt{t})}}.$$

Let $s = r - q$, then

$$\begin{aligned} s_k(x_k) &= \frac{e^{-x_k\sqrt{t}}}{\sqrt{(d-a)\sqrt{t}+bt-c}} - \frac{f_k(x_k, i\sqrt{t})}{\sqrt{L(i\sqrt{t})f_k(0, i\sqrt{t})}} \\ &= -\left(\frac{f_k(x_k, \sqrt{t}i) - e^{-\sqrt{t}x_k}}{\sqrt{L(i\sqrt{t})f_k(0, i\sqrt{t})}} + \left(\frac{1}{\sqrt{L(i\sqrt{t})f_k(0, i\sqrt{t})}} - \frac{1}{\sqrt{(d-a)\sqrt{t}+bt-c}}\right) e^{-\sqrt{t}x_k}\right). \end{aligned}$$

To compute estimate on $||s||^2 = \sum_{k=1}^{2} \int_0^{\infty} |h_k(x_k)|^2 \, dx_k$, we use (2.2.13) and (A.0.4) and after some simplifications we obtain

$$||s||^2 \leq \frac{m_1^2}{\left((d-a)\sqrt{t} + bt - c\right) t^{3/2}}.$$

Similarly,

$$||q||^2 = \sum_{k=1}^{2} \int_0^{\infty} \left| \frac{-e^{-\sqrt{t}x_k}}{\sqrt{(d-a)\sqrt{t} + bt - c}} \right|^2 dx_k = \frac{1}{\left((d-a)\sqrt{t} + bt - c\right)\sqrt{t}}.$$

The estimate on the right hand side of inequality (A.0.2) is now given by

$$\begin{aligned} 6||s||^2||q||^2 + 3||s||^4 &\leq \frac{6m_1^2}{\left((d-a)\sqrt{t} + bt - c\right)^2 t^2} + \frac{3m_1^4}{\left((d-a)\sqrt{t} + bt - c\right)^2 t^3} \\ &= \frac{3m_1^4 + 6m_1^2 t}{\left((d-a)\sqrt{t} + bt - c\right)^2 t^3} \\ &= \frac{6m_1^2}{b^2 t^4} + \frac{12m_1^2(a-d)}{b^3 t^{\frac{9}{2}}} + O(t^{-5}) \\ &= O(t^{-4}). \end{aligned}$$

This implies

$$||\mathcal{S}_2||_1 = O(t^{-2})$$

and hence

$$||\mathcal{R}_1||_1 = O(t^{-\frac{3}{2}}).$$

□

Appendix B

Estimate on trace norm of resolvent difference for PI vertex conditions

In order to obtain estimates on the trace norm of resolvent difference of perturbed and unperturbed Schrödinger operators, we first introduce an auxilliary function $b_j(x,\kappa) = e^{-ix\kappa} f_j(x,\kappa)$, with asymptotics

$$b_j(x,\kappa) = 1 + o(1), \quad b_j'(x,\kappa) = o(1), \quad x \to \infty. \tag{B.0.1}$$

Note that the asymptotics

$$f_j(x,\kappa) = e^{ix\kappa}(1+o(1)), \quad f_j'(x,\kappa) = i\kappa e^{ix\kappa}(1+o(1)) \quad x \to \infty \tag{B.0.2}$$

are equivalent to (B.0.1). Similarly, the differential equation

$$(H+V)b_j(x,\kappa) = \kappa^2 b_j(x,\kappa)$$

is equivalent to

$$b_j(x,\kappa) = 1 + (2i\kappa)^{-1} \int_x^\infty e^{2i\kappa(y-x)} - V_j(y) b_j(y,\kappa) dy \tag{B.0.3}$$

considered for all bounded functions $b_j(x,\kappa)$. The method of successive approximations can be used to construct the solution of (B.0.3). Let $b_{0,j}(x,\kappa) = 1$, we get

$$b_{n+1,j}(x,\kappa) = (2i\kappa)^{-1} \int_x^\infty \left(e^{2i\kappa(y-x)} - 1 \right) - V_j(y) b_j(y,\kappa) dy.$$

By assumption (3.1.2), it follows successively that

$$|b_{n,j}(x,\kappa)| \leq \frac{\left(\int_x^\infty |V_j(y)|dy\right)^n}{n!|\kappa|^n}. \tag{B.0.4}$$

For a given $x \geq 0$, every $b_{n,j}(x,\kappa)$ is analytic in κ in the upper half plane Im $\kappa > 0$ and is continuous in κ upto the real axis, with exception $\kappa = 0$. It follows from (B.0.4) that the limit

$$b_j(x,\kappa) := \lim_{N\to\infty} b_j^{(N)}(x,\kappa), \quad \text{where} \quad b_j^{(N)}(x,\kappa) = \sum_{n=0}^{N} b_{n,j}(x,\kappa) \tag{B.0.5}$$

exists for all $x \geq 0$ uniformly with respect to κ for $|\kappa| \geq c > 0$ where $c \in \mathbb{R}^+$.

Lemma B.0.1. *Assume* (3.1.2) *holds for a fixed j and $\kappa \neq 0$, Im $\kappa > 0$, then the following estimate holds for the solution $f_j(x,\kappa)$ with asymptotics* (B.0.2)*,*

$$|f_j(x,\kappa) + e^{ix\kappa}| \leq e^{-Im\ \kappa x}\left(e^{|\kappa|^{-1}\int_x^\infty |V_j(y)|dy} + 1\right).$$

Moreover, when $|\kappa| \geq c > 0$, then

$$|f_j(x,\kappa) + e^{ix\kappa}| \leq e^{-Im\ \kappa x}\left(\frac{c\int_x^\infty |V_j(y)|dy}{|\kappa|} + 2\right).$$

Proof. From (B.0.5), we have

$$\begin{aligned}
f_j(x,\kappa) &= e^{ix\kappa}\lim_{N\to\infty}\sum_{n=0}^{N} b_{n,j}(x,\kappa)\\
f_j(x,\kappa) + e^{ix\kappa} &= e^{ix\kappa}\left(\lim_{N\to\infty}\sum_{n=0}^{N} b_{n,j}(x,\kappa) + 1\right)\\
|f_j(x,\kappa) + e^{ix\kappa}| &= \left|e^{ix\kappa}\right|\left|\lim_{N\to\infty}\sum_{n=0}^{N} b_{n,j}(x,\kappa) + 1\right|\\
&= e^{-\text{Im }\kappa x}\left|\lim_{N\to\infty}\sum_{n=0}^{N} b_{n,j}(x,\kappa) + 1\right|\\
&\leq e^{-\text{Im }\kappa x}\left(\lim_{N\to\infty}\sum_{n=0}^{N} |b_{n,j}(x,\kappa)| + 1\right)\\
&\leq e^{-\text{Im }\kappa x}\left(\lim_{N\to\infty}\sum_{n=0}^{N} \frac{\left(\int_x^\infty |V_j(y)|dy\right)^n}{n!|\kappa|^n} + 1\right)\\
&= e^{-\text{Im }\kappa x_j}\left(e^{|\kappa|^{-1}\int_x^\infty |V_j(y)|dy} + 1\right)\\
&= e^{-\text{Im }\kappa x}\left(e^{|\kappa|^{-1}\int_x^\infty |V_j(y)|dy} - 1\right) + 2e^{-\text{Im }\kappa x}\\
&\leq e^{-\text{Im }\kappa x}\left(\frac{c\int_x^\infty |V_j(y)|dy}{|\kappa|} + 2\right).
\end{aligned}$$

□

Lemma B.0.2 ([18], Lemma 3.4)**.** *If $q, r \in \mathcal{H}$, where $\mathcal{H}$ is a Hilbert space and $\mathcal{R} = (\cdot, q)q - (\cdot, r)r$ is a rank two operator on $\mathcal{H}$, then the trace norm of $\mathcal{R}$ is*

$$||\mathcal{R}||_1 = \sqrt{(||q||^2 + ||r||^2)^2 - 4|(q,r)|^2}. \tag{B.0.6}$$

Moreover, if we let $r = q + s$ then,

$$(||q||^2 + ||r||^2)^2 - 4|(q,r)|^2 \leq 6||s||^2||q||^2 + 3||s||^4. \tag{B.0.7}$$

Lemma B.0.3. *Let condition* (3.1.2) *holds and $H_{V,\Gamma}$ denotes any of the operators $H_{V,\Gamma}^{\delta_a}, H_{V,\Gamma}^{\hat{\delta}_d}$ or $H_{V,\Gamma}^{\hat{\delta}'_c}$ and $H_{0,\Gamma}$ is the corresponding unperturbed operator. Then, for all $\epsilon > 0$ and for large t the resolvents $R_{V,\Gamma}(z)$ of $H_{V,\Gamma}$ and $R_{0,\Gamma}(z)$ of $H_{0,\Gamma}$ satisfy*

$$||R_{V,\Gamma}(-t) - R_{0,\Gamma}(-t)||_1 \leq C_\epsilon t^{-\frac{3}{2}+\epsilon}. \tag{B.0.8}$$

Proof. 1. We first prove the estimate (B.0.8) for the resolvent difference of $R_{V,\Gamma}^{\delta_a}$ and $R_{0,\Gamma}^{\delta_a}$. Let $\mathcal{R}_1 = R_{V,\Gamma}^{\delta_a}(-t) - R_{V,\Gamma}^{D}(-t) + R_{0,\Gamma}^{D}(-t) - R_{0,\Gamma}^{\delta_a}(-t)$ and $\mathcal{R}_2 = R_{V,\Gamma}^{D}(-t) - R_{0,\Gamma}^{D}(-t)$ then,

$$R_{V,\Gamma}^{\delta_a}(-t) - R_{0,\Gamma}^{\delta_a}(-t) = \mathcal{R}_1 + \mathcal{R}_2.$$

Hence

$$||R_{V,\Gamma}^{\delta_a}(-t) - R_{0,\Gamma}^{\delta_a}(-t)||_1 \leq ||\mathcal{R}_1||_1 + ||\mathcal{R}_2||_1. \tag{B.0.9}$$

Trace norm on $\mathcal{R}_2$ can be estimated as $||\mathcal{R}_2||_1 \leq Ct^{-\frac{3}{2}+\epsilon}$ (See Lemma 4.5.6. [97]). Now it remains to find estimate for rank two operator $\mathcal{R}_1$. From (3.2.21) and (3.2.22), we have

$$R_{0,\Gamma}^{\delta_a}(-t) - R_{0,\Gamma}^{D}(-t) = \begin{bmatrix} q_1(x_1)q_1(x_1) & q_1(x_1)q_2(x_2) & \cdots & q_1(x_1)q_n(x_n) \\ q_2(x_2)q_1(x_1) & q_2(x_2)q_2(x_2) & \cdots & q_2(x_2)q_n(x_n) \\ \vdots & \vdots & \ddots & \vdots \\ q_n(x_n)q_1(x_1) & q_n(x_n)q_2(x_2) & \cdots & q_n(x_n)q_n(x_n) \end{bmatrix},$$

where,

$$q_k(x_k) = \frac{e^{-\sqrt{t}x_k}}{\sqrt{a + \sqrt{t}n}}.$$

Therefore,

$$R_{0,\Gamma}^{\delta_a}(-t) - R_{0,\Gamma}^{D}(-t) = (\cdot, q)q, \quad q = (q_1, q_2, \cdots, q_n)^T.$$

Similarly,

$$R^{\delta_a}_{V,\Gamma}(-t) - R^{D}_{V,\Gamma}(-t) = \begin{bmatrix} r_1(x_1)r_1(x_1) & r_1(x_1)r_2(x_2) & \cdots & r_1(x_1)r_n(x_n) \\ r_2(x_2)r_1(x_1) & r_2(x_2)r_2(x_2) & \cdots & r_2(x_2)r_n(x_n) \\ \vdots & \vdots & \ddots & \vdots \\ r_n(x_n)r_1(x_1) & r_n(x_n)r_2(x_2) & \cdots & r_n(x_n)r_n(x_n) \end{bmatrix},$$

where,

$$r_k(x_k) = \frac{f_k(x_k, i\sqrt{t})}{\sqrt{a - K(i\sqrt{t})} f_k(0, i\sqrt{t})}.$$

Therefore,

$$R^{\delta_a}_{V,\Gamma}(-t) - R^{D}_{V,\Gamma}(-t) = (\cdot, r)r, \quad r = (r_1, r_2, \cdots, r_n)^T.$$

In view of (B.0.6), we have

$$||\mathcal{R}_1||_1 = \sqrt{(||q||^2 + ||r||^2)^2 - 4|(q,r)|^2}.$$

In order to find bound on the trace norm of $\mathcal{R}_1$ we need an explicit expression for right side of (B.0.7). For this we let $s = r - q$, hence

$$\begin{aligned} s_k(x_k) =& \frac{f_k(x_k, i\sqrt{t})}{\sqrt{a - K(i\sqrt{t})} f_k(0, i\sqrt{t})} - \frac{e^{-\sqrt{t}x_k}}{\sqrt{a + \sqrt{t}n}} \\ =& \frac{f_k(x_k, i\sqrt{t}) - e^{-\sqrt{t}x_k}}{\sqrt{a - K(i\sqrt{t})} f_k(0, i\sqrt{t})} + \left(\frac{1}{\sqrt{a - K(i\sqrt{t})} f_k(0, i\sqrt{t})} - \frac{1}{\sqrt{a + \sqrt{t}n}} \right) e^{-\sqrt{t}x_k}. \end{aligned}$$

Further,

$$||s||^2 = \sum_{k=1}^{n} \int_0^{\infty} |h_k(x_k)|^2 \, dx_k.$$

To calculate $||s||^2$, we use (3.2.45) and the following estimate from Lemma 4.1.4,[97]

$$\left| f_k(x_k, i\sqrt{t}) - e^{-\sqrt{t}x_k} \right| \leq \frac{C_5}{\sqrt{t}} e^{-\sqrt{t}x_k}, \quad \text{as} \quad t \to \infty, \tag{B.0.10}$$

and get

$$||s||^2 \leq \frac{nC_5^2}{2t^{3/2}(a + \sqrt{t}n)}.$$

Similarly,

$$||q||^2 = \sum_{k=1}^{n} \int_0^{\infty} \left| \frac{e^{-\sqrt{t}x_k}}{\sqrt{a+\sqrt{t}n}} \right|^2 dx_k = \frac{n}{2\sqrt{t}(a+\sqrt{t}n)}.$$

The estimate on the right hand side of inequality (B.0.7) is now given by

$$\begin{aligned} 6||s||^2||q||^2 + 3||s||^4 &\leq \frac{3C_5^2 n^2}{2t^2(a+\sqrt{t}n)^2} + \frac{3C_5^4 n^2}{4t^3(a+\sqrt{t}n)^2} \\ &= \frac{3C_5^2 n^2 (C_5^2+2t)}{4(t^3a^2 + 2nat^{7/2} + n^2t^4)}. \end{aligned}$$

The asymptotic expansion of the above expression is given by

$$\begin{aligned} \frac{3C_5^2 n^2 (C_5^2+2t)}{4(t^3a^2 + 2nat^{7/2} + n^2t^4)} &= \frac{3C_5^2}{2t^3} - \frac{3C_5^2 a}{nt^{\frac{7}{2}}} + O(t^{-4}) \\ &= O(t^{-3}). \end{aligned}$$

This implies $||\mathcal{R}_1||_1 = O(t^{-\frac{3}{2}})$. Estimate on the trace norm of $\mathcal{R}_2$ and inequality (B.0.9) yields the required result.

2. We now prove the estimate (B.0.8) for the resolvent difference of $R_{V,\Gamma}^{\hat{\delta}_d}$ and $R_{0,\Gamma}^{\hat{\delta}_d}$ when $d \neq 0$. For $d = 0$ the operator $H_{V,\Gamma}^{\hat{\delta}_0}$ coincides with $H_{V,\Gamma}^{\delta_0}$, in this case, the estimate on the trace norm of the resolvent difference is already proved above.

Let $\mathcal{R}_1 = R_{V,\Gamma}^{\hat{\delta}_d}(-t) - R_{V,\Gamma}^{D}(-t) + R_{0,\Gamma}^{D}(-t) - R_{0,\Gamma}^{\hat{\delta}_d}(-t)$ and $\mathcal{R}_2 = R_{V,\Gamma}^{D}(-t) - R_{0,\Gamma}^{D}(-t)$ then,

$$R_{V,\Gamma}^{\hat{\delta}_d}(-t) - R_{0,\Gamma}^{\hat{\delta}_d}(-t) = \mathcal{R}_1 + \mathcal{R}_2.$$

Hence

$$||R_{V,\Gamma}^{\hat{\delta}_d}(-t) - R_{0,\Gamma}^{\hat{\delta}_d}(-t)||_1 \leq ||\mathcal{R}_1||_1 + ||\mathcal{R}_2||_1. \tag{B.0.11}$$

It remains only to find estimate for rank two operator $\mathcal{R}_1$. From (3.2.25) and (3.2.27), we have

$$\begin{aligned} &(R_{V,\Gamma}^{\hat{\delta}_d}(-t) - R_{V,\Gamma}^{D}(-t))_{j,l} = \\ &\left(d\delta_{j,l} - \frac{1}{\left(1 - d\frac{f_l'(0,i\sqrt{t})}{f_l(0,i\sqrt{t})}\right) J(i\sqrt{t})} \right) \frac{f_j(x_j, i\sqrt{t}) f_l(x_l, i\sqrt{t})}{\left(1 - d\frac{f_j'(0,i\sqrt{t})}{f_j(0,i\sqrt{t})}\right) f_j(0,i\sqrt{t}) f_l(0,i\sqrt{t})} \end{aligned}$$

and

$$(R^{\hat{\delta}_d}_{0,\Gamma}(-t) - R^{D}_{0,\Gamma}(-t))_{j,l} = \left(d\delta_{j,l} + \frac{1}{n\sqrt{t}}\right)\frac{e^{-(x_j+x_l)\sqrt{t}}}{1+d\sqrt{t}}.$$

Adding above two equations, we get

$$\mathcal{R}_1 = \mathcal{S}_1 + \mathcal{S}_2,$$

where,

$$(\mathcal{S}_1)_{j,l} = d\left(\frac{e^{-(x_j+x_l)\sqrt{t}}}{1+d\sqrt{t}} - \frac{f_j(x_j,i\sqrt{t})f_l(x_l,i\sqrt{t})}{\left(1-d\frac{f_j'(0,i\sqrt{t})}{f_j(0,i\sqrt{t})}\right)f_j(0,i\sqrt{t})f_l(0,i\sqrt{t})}\right)\delta_{j,l}$$

and

$$(\mathcal{S}_2)_{j,l} = \frac{e^{-(x_j+x_l)\sqrt{t}}}{n(\sqrt{t}+dt)} - \frac{f_j(x_j,i\sqrt{t})f_l(x_l,i\sqrt{t})}{J(i\sqrt{t})\left(1-d\frac{f_j'(0,i\sqrt{t})}{f_j(0,i\sqrt{t})}\right)f_j(0,i\sqrt{t})\left(1-d\frac{f_l'(0,i\sqrt{t})}{f_l(0,i\sqrt{t})}\right)f_l(0,i\sqrt{t})}.$$

Now, as $\mathcal{S}_1$ is a scalar matrix, therefore, to apply definition of trace norm, we let $\mathcal{S}_1 = I\mathcal{S}_1 I$, where I is identity matrix of order n. So

$$||\mathcal{S}_1||_1 = \sum_{j=1}^{n}||\sigma_j||$$

where,

$$||\sigma_j|| = \int_0^\infty \left| d\left(\frac{e^{-2\sqrt{t}x_j}}{1+d\sqrt{t}} - \frac{f_j^2(x_j,i\sqrt{t})}{\left(1-d\frac{f_j'(0,i\sqrt{t})}{f_j(0,i\sqrt{t})}\right)f_j^2(0,i\sqrt{t})}\right)\right| dx_j.$$

When $t\to\infty$, we have a simplified form i.e.

$$||\sigma_j|| = \left|\frac{d}{1+d\sqrt{t}}\right|\int_0^\infty \left|f_j^2(x_j,i\sqrt{t}) + e^{-2\sqrt{t}x_j}\right| dx_j.$$

Adding and subtracting $e^{-2x_j\sqrt{t}}$ on the right hand side above and by the triangle inequality, we obtain

$$||\sigma_j|| \le \frac{|d|}{|1+d\sqrt{t}|}\left(\int_0^\infty \left(\left|f_j(x_j,i\sqrt{t}) + e^{-\sqrt{t}x_j}\right|\left|f_j(x_j,i\sqrt{t}) - e^{-\sqrt{t}x_j}\right| + 2e^{-2\sqrt{t}x_j}\right)dx_j\right).$$

Using (B.0.10) and the following estimate from Lemma (B.0.1),

$$\left|f_j(x_j, i\sqrt{t}) + e^{-\sqrt{t}x_j})\right| \leq e^{-\sqrt{t}x_j}\left(\frac{C_6}{\sqrt{t}} + 2\right), \quad t \to \infty, \tag{B.0.12}$$

we have,

$$\begin{aligned}||\sigma_j|| &\leq \frac{|d|}{|1 + d\sqrt{t}|}\left(\frac{C_5}{\sqrt{t}}\left(\frac{C_6}{\sqrt{t}} + 2\right)\right)\int_0^\infty e^{-2\sqrt{t}x_j}dx_j \\ &= \frac{|d|C_5(C_6 + 2\sqrt{t})}{2t^{\frac{3}{2}}|1 + d\sqrt{t}|}.\end{aligned}$$

This implies

$$||\mathcal{S}_1||_1 \leq \frac{n|d|C_5(C_6 + 2\sqrt{t})}{2t^{\frac{3}{2}}|1 + d\sqrt{t}|}$$

and hence

$$||\mathcal{S}_1||_1 = O\left(t^{-\frac{3}{2}}\right).$$

To find estimate on the trace norm of $\mathcal{S}_2$, we use the same arguments as in the first part of proof. Clearly, $\mathcal{S}_2 = (\cdot, q)q - (\cdot, r)r$ is an operator of rank two, where,

$q_k(x_k) = \dfrac{e^{-\sqrt{t}x_k}}{\sqrt{n(dt + \sqrt{t})}}$ and $r_k(x_k) = \dfrac{f_k(x_k, \sqrt{t}i)}{\sqrt{-J(\sqrt{t}i)}\left(1 - d\frac{f_k'(0,i\sqrt{t})}{f_k(0,i\sqrt{t})}\right)}$.

Let $s = r - q$, then

$$\begin{aligned}s_k(x_k) &= \frac{f_k(x_k, \sqrt{t}i)}{\sqrt{-J(\sqrt{t}i)}\left(1 - d\frac{f_k'(0,i\sqrt{t})}{f_k(0,i\sqrt{t})}\right)} - \frac{e^{-\sqrt{t}x_k}}{\sqrt{n(dt + \sqrt{t})}} \\ &= \frac{f_k(x_k, \sqrt{t}i) - e^{-\sqrt{t}x_k}}{\sqrt{-J(\sqrt{t}i)}\left(1 - d\frac{f_k'(0,i\sqrt{t})}{f_k(0,i\sqrt{t})}\right)} + \left(\frac{e^{-\sqrt{t}x_k}}{\sqrt{-J(\sqrt{t}i)}\left(1 - d\frac{f_k'(0,i\sqrt{t})}{f_k(0,i\sqrt{t})}\right)} - \frac{e^{-\sqrt{t}x_k}}{\sqrt{n(dt + \sqrt{t})}}\right).\end{aligned}$$

As

$$||s||^2 = \sum_{k=1}^{n}\int_0^\infty |h_k(x_k)|^2\, dx_k$$

we use (3.2.45) and (B.0.10) and after some simplifications, we arrive at

$$||s||^2 \leq \frac{C_5^2}{2\left(1 + d\sqrt{t}\right)t^2}.$$

Similarly,

$$||q||^2 = \sum_{k=1}^{n} \int_0^{\infty} \left| \frac{e^{-\sqrt{t}x_k}}{\sqrt{n(dt+\sqrt{t})}} \right|^2 dx_k = \frac{1}{2(dt+\sqrt{t}))\sqrt{t}}.$$

The estimate on the right hand side of inequality (B.0.7) is now given by

$$\begin{aligned} 6||s||^2||q||^2 + 3||s||^4 &\leq \frac{3C_5^2}{2\left(d\sqrt{t}+1\right)t^{\frac{5}{2}}\left(dt+\sqrt{t}\right)} + \frac{3C_5^4}{4\left(d\sqrt{t}+1\right)^2 t^4} \\ &= \frac{3C_5^2(C_5^2+2t)}{4t^{\frac{7}{2}}\left(d\sqrt{t}+1\right)\left(dt+\sqrt{t}\right)}. \end{aligned} \tag{B.0.13}$$

The asymptotic expansion of the above expression is

$$\begin{aligned} \frac{3C_5^2(C_5^2+2t)}{4t^{\frac{7}{2}}\left(d\sqrt{t}+1\right)\left(dt+\sqrt{t}\right)} &= \frac{3C_5^2}{2d^2t^4} - \frac{3C_5^2}{d^3t^{\frac{9}{2}}} + O(t^{-5}) \\ &= O(t^{-4}). \end{aligned}$$

Therefore,

$$||\mathcal{S}_2||_1 = O(t^{-2}).$$

this implies

$$||\mathcal{R}_1||_1 = O(t^{-\frac{3}{2}}).$$

The above estimate on $\mathcal{R}_1$ and already obtained estimate on $\mathcal{R}_2$ yields the desired result.

3. We now prove the estimate (B.0.8) for the resolvent difference of $R_{V,\Gamma}^{\hat{\delta}'_c}$ and $R_{0,\Gamma}^{\hat{\delta}'_c}$ when $c \neq 0$. For $c = 0$ the operator $H_{V,\Gamma}^{\hat{\delta}'_0}$ coincides with $H_{V,\Gamma}^{\delta'_0}$, in this case, the estimate on the trace norm of the resolvent difference is proved in Lemma (B.0.4).

Let $\mathcal{R}_1 = R_{V,\Gamma}^{\hat{\delta}'_c}(-t) - R_{V,\Gamma}^{D}(-t) + R_{0,\Gamma}^{D}(-t) - R_{0,\Gamma}^{\hat{\delta}'_c}(-t)$ and $\mathcal{R}_2 = R_{V,\Gamma}^{D}(-t) - R_{0,\Gamma}^{D}(-t)$ then,

$$R_{V,\Gamma}^{\hat{\delta}'_c}(-t) - R_{0,\Gamma}^{\hat{\delta}'_c}(-t) = \mathcal{R}_1 + \mathcal{R}_2.$$

Hence

$$||R_{V,\Gamma}^{\hat{\delta}'_c}(-t) - R_{0,\Gamma}^{\hat{\delta}'_c}(-t)||_1 \leq ||\mathcal{R}_1||_1 + ||\mathcal{R}_2||_1. \tag{B.0.14}$$

It remains to find estimate for rank two operator $\mathcal{R}_1$. From (3.2.28) and (3.2.29), we have

$$(R^{\hat{\delta}'_c}_{V,\Gamma}(-t) - R^D_{V,\Gamma}(-t))_{j,l} =$$
$$\left(\frac{1}{\left(1 - c\frac{f_l(0,i\sqrt{t})}{f'_l(0,i\sqrt{t})}\right) P(i\sqrt{t}) f'_l(0,i\sqrt{t})} - \frac{\delta_{j,l}}{f_l(0,i\sqrt{t})} \right) \frac{f_j(x_j,i\sqrt{t}) f_l(x_l,i\sqrt{t})}{\left(1 - c\frac{f_j(0,i\sqrt{t})}{f'_j(0,i\sqrt{t})}\right) f'_j(0,i\sqrt{t})}$$

and

$$(R^{\hat{\delta}'_c}_{0,\Gamma}(-t) - R^D_{0,\Gamma}(-t))_{j,l} = \left(\delta_{j,l} - \frac{1}{n}\right) \frac{e^{-(x_j+x_l)\sqrt{t}}}{\sqrt{t}+c}.$$

Adding the above two equations, we get

$$\mathcal{R}_1 = \mathcal{S}_1 + \mathcal{S}_2$$

where,

$$(\mathcal{S}_1)_{j,l} = \left(\frac{e^{-(x_j+x_l)\sqrt{t}}}{\sqrt{t}+c} - \frac{f_j(x_j,i\sqrt{t}) f_l(x_l,i\sqrt{t})}{\left(1 - c\frac{f_j(0,i\sqrt{t})}{f'_j(0,i\sqrt{t})}\right) f_l(0,i\sqrt{t}) f'_j(0,i\sqrt{t})} \right) \delta_{j,l}$$

and

$$(\mathcal{S}_2)_{j,l} = \frac{f_j(x_j,i\sqrt{t}) f_l(x_l,i\sqrt{t})}{P(i\sqrt{t}) \left(1 - c\frac{f_j(0,i\sqrt{t})}{f'_j(0,i\sqrt{t})}\right) f'_j(0,i\sqrt{t}) \left(1 - c\frac{f_l(0,i\sqrt{t})}{f'_l(0,i\sqrt{t})}\right) f'_l(0,i\sqrt{t})} - \frac{e^{-(x_j+x_l)\sqrt{t}}}{n(\sqrt{t}+c)}.$$

Now, as $\mathcal{S}_1$ is a scalar matrix, therefore, to apply definition of trace norm, we can let $\mathcal{S}_1 = I\mathcal{S}_1 I$, where I is identity matrix of order n. So

$$||\mathcal{S}_1||_1 = \sum_{j=1}^{n} ||\sigma_j||,$$

where,

$$||\sigma_j|| = \int_0^\infty \left| \left(\frac{e^{-2\sqrt{t}x_j}}{\sqrt{t}+c} - \frac{f_j^2(x_j,i\sqrt{t})}{\left(1 - c\frac{f_j(0,i\sqrt{t})}{f'_j(0,i\sqrt{t})}\right) f_j(0,i\sqrt{t}) f'_j(0,i\sqrt{t})} \right) \right| dx_j.$$

When $t \to \infty$, we have a simplified form of the above expression:

$$||\sigma_j|| = \frac{1}{|\sqrt{t}+c|} \int_0^\infty \left| f_j^2(x_j,i\sqrt{t}) + e^{-2\sqrt{t}x_j} \right| dx_j.$$

Adding and subtracting $e^{-2x_j\sqrt{t}}$ on the right hand side of the above expression and by the triangle inequality, we obtain

$$||\sigma_j|| \leq \frac{1}{|\sqrt{t}+c|}\left(\int_0^\infty \left(\left|f_j(x_j,i\sqrt{t})+e^{-\sqrt{t}x_j}\right|\left|f_j(x_j,i\sqrt{t})-e^{-\sqrt{t}x_j}\right|+2e^{-2\sqrt{t}x_j}\right)dx_j\right).$$

Using (B.0.10) and (B.0.12), we have

$$\begin{aligned}||\sigma_j|| &\leq \frac{1}{|\sqrt{t}+c|}\left(\frac{C_5}{\sqrt{t}}\left(\frac{C_6}{\sqrt{t}}+2\right)\right)\int_0^\infty e^{-2\sqrt{t}x_j}dx_j\\ &= \frac{C_5(C_6+2\sqrt{t})}{2t^{\frac{3}{2}}|\sqrt{t}+c|}.\end{aligned}$$

This implies

$$||\mathcal{S}_1||_1 \leq \frac{nC_5(C_6+2\sqrt{t})}{2t^{\frac{3}{2}}|\sqrt{t}+c|}$$

and hence

$$||\mathcal{S}_1||_1 = O\left(t^{-\frac{3}{2}}\right).$$

To find estimate for $\mathcal{S}_2$, we use the same arguments as before. Clearly, $\mathcal{S}_2 = (\cdot,q)q - (\cdot,r)r$ is a rank two operator. Where,

$$q_k(x_k) = \frac{-e^{-\sqrt{t}x_k}}{\sqrt{n(\sqrt{t}+c)}} \quad \text{and} \quad r_k(x_k) = \frac{f_k(x_k,\sqrt{t}i)}{\sqrt{-P(\sqrt{t}i)}\left(1-c\frac{f_k(0,i\sqrt{t})}{f_k'(0,i\sqrt{t})}\right)f_k'(0,i\sqrt{t})}.$$

Let $s = r - q$, then

$$\begin{aligned}s_k(x_k) =& \frac{f_k(x_k,\sqrt{t}i)}{\sqrt{-P(\sqrt{t}i)}\left(1-c\frac{f_k(0,i\sqrt{t})}{f_k'(0,i\sqrt{t})}\right)f_k'(0,i\sqrt{t})} + \frac{e^{\sqrt{t}x_k}}{\sqrt{n(\sqrt{t}+c)}}\\ =& \frac{f_k(x_k,\sqrt{t}i)-e^{-\sqrt{t}x_k}}{\sqrt{-P(\sqrt{t}i)}\left(1-c\frac{f_k(0,i\sqrt{t})}{f_k'(0,i\sqrt{t})}\right)f_k'(0,i\sqrt{t})} +\\ & \left(\frac{e^{-\sqrt{t}x_k}}{\sqrt{-P(\sqrt{t}i)}\left(1-c\frac{f_k(0,i\sqrt{t})}{f_k'(0,i\sqrt{t})}\right)f_k'(0,i\sqrt{t})} + \frac{e^{\sqrt{t}x_k}}{\sqrt{n(\sqrt{t}+c)}}\right).\end{aligned}$$

As,

$$||s||^2 = \sum_{k=1}^n \int_0^\infty |h_k(x_k)|^2\,dx_k$$

therefore, we use (3.2.45) and (B.0.10) and after some simplifications we arrive at

$$||s||^2 \leq \frac{C_5^2}{2\left(\sqrt{t}+c\right)t^{\frac{3}{2}}}.$$

Similarly,

$$||q||^2 = \sum_{k=1}^{n} \int_0^{\infty} \left| \frac{-e^{-\sqrt{t}x_k}}{\sqrt{n(\sqrt{t}+c)}} \right|^2 dx_k = \frac{1}{2(\sqrt{t}+c))\sqrt{t}}.$$

Hence the right side of inequality (B.0.7) can be estimated as

$$\begin{aligned} 6||s||^2||q||^2 + 3||s||^4 &\leq \frac{3C_5^2}{2(\sqrt{t}+c)^2t^2} + \frac{3C_5^4}{4(\sqrt{t}+c)^2t^3} \\ &= \frac{3C_5^2(C_5^2+2t)}{4(\sqrt{t}+c)^2t^3}. \end{aligned} \tag{B.0.15}$$

The asymptotic expansion of the above expression is

$$\begin{aligned} \frac{3C_5^2(C_5^2+2t)}{4(\sqrt{t}+c)^2t^3} &= \frac{3C_5^2}{2t^3} - \frac{3C_5^2c}{t^{\frac{7}{2}}} + O(t^{-4}) \\ &= O(t^{-3}). \end{aligned}$$

Therefore,

$$||\mathcal{S}_2||_1 = O(t^{-\frac{3}{2}}).$$

This implies

$$||\mathcal{R}_1||_1 = O(t^{-\frac{3}{2}}).$$

The above estimate on $\mathcal{R}_1$ and already obtained estimate on $\mathcal{R}_2$ yields the desired estimate.

□

The following lemma provides the estimate on the trace norm of the difference of $R_{V,\Gamma}^{\delta_b'}$ and $R_{0,\Gamma}^{\delta_b'}$.

Lemma B.0.4. *Let condition* (3.1.2) *holds and* $H_{V,\Gamma}^{\delta_b'}$ *be the Schrödinger operator in* $L_2(\Gamma)$ *and* $H_{0,\Gamma}^{\delta_b'}$ *the corresponding unperturbed operator. Then, for all* $\epsilon > 0$ *and large* t *the resolvents* $R_{V,\Gamma}^{\delta_b'}(z)$ *and* $R_{0,\Gamma}^{\delta_b'}(z)$ *satisfy*

$$||R_{V,\Gamma}^{\delta_b'}(-t) - R_{0,\Gamma}^{\delta_b'}(-t)||_1 \leq C_\epsilon t^{-1+\epsilon}.$$

Proof. Let $\mathcal{R}_1 = R^{\delta'_b}_{V,\Gamma}(-t) - R^D_{V,\Gamma}(-t) + R^D_{0,\Gamma}(-t) - R^{\delta'_b}_{0,\Gamma}(-t)$ and $\mathcal{R}_2 = R^D_{V,\Gamma}(-t) - R^D_{0,\Gamma}(-t)$ then,

$$R^{\delta'_b}_{V,\Gamma}(-t) - R^{\delta'_b}_{0,\Gamma}(-t) = \mathcal{R}_1 + \mathcal{R}_2.$$

Hence

$$||R^{\delta'_b}_{V,\Gamma}(-t) - R^{\delta'_b}_{0,\Gamma}(-t)||_1 \leq ||\mathcal{R}_1||_1 + ||\mathcal{R}_2||_1. \tag{B.0.16}$$

It remains to find estimate for rank two operator $\mathcal{R}_1$. From (3.2.23) and (3.2.24), we have

$$(R^{\delta'_b}_{V,\Gamma}(-t) - R^D_{V,\Gamma}(-t))_{j,l} = \left(\frac{1}{(M(i\sqrt{t}) - b) f'_j(0, i\sqrt{t}) f'_l(0, i\sqrt{t})} - \frac{\delta_{j,l}}{f'_j(0, i\sqrt{t}) f_l(0, i\sqrt{t})} \right) f_j(x_j, i\sqrt{t}) f_l(x_l, i\sqrt{t})$$

and

$$(R^{\delta'_b}_{0,\Gamma}(-t) - R^D_{0,\Gamma}(-t))_{j,l} = \left(\frac{\delta_{j,l}}{\sqrt{t}} - \frac{1}{(n + b\sqrt{t})\sqrt{t}} \right) e^{-(x_j + x_l)\sqrt{t}}.$$

Adding the above two equations , we get

$$\mathcal{R}_1 = \mathcal{S}_1 + \mathcal{S}_2,$$

where,

$$(\mathcal{S}_1)_{j,l} = \left(\frac{e^{-(x_j + x_l)\sqrt{t}}}{\sqrt{t}} - \frac{f_j(x_j, i\sqrt{t}) f_l(x_l, i\sqrt{t})}{f'_j(0, i\sqrt{t}) f_l(0, i\sqrt{t})} \right) \delta_{j,l}$$

and

$$(\mathcal{S}_2)_{j,l} = \frac{f_j(x_j, i\sqrt{t}) f_l(x_l, i\sqrt{t})}{(M(i\sqrt{t}) - b) f'_j(0, i\sqrt{t}) f'_l(0, i\sqrt{t})} - \frac{e^{-(x_j + x_l)\sqrt{t}}}{(n + b\sqrt{t})\sqrt{t}}.$$

Now, as $\mathcal{S}_1$ is a scalar matrix, therefore, to apply definition of trace norm, we can let $\mathcal{S}_1 = I\mathcal{S}_1 I$, where I is identity matrix of order n. So

$$||\mathcal{S}_1||_1 = \sum_{i=1}^{n} ||\sigma_j||,$$

where,

$$||\sigma_j|| = \int_0^\infty \left| \frac{e^{-2x_j\sqrt{t}}}{\sqrt{t}} - \frac{f_j^2(x_j, i\sqrt{t})}{f'_j(0, i\sqrt{t}) f_j(0, i\sqrt{t})} \right| dx_j.$$

When $t \to \infty$, we obtain a simplified form of the above expression:

$$||\sigma_j|| = \frac{1}{\sqrt{t}} \int_0^\infty \left| f_j^2(x_j, i\sqrt{t}) + e^{-2\sqrt{t}x_j} \right| dx_j.$$

Adding and subtracting $e^{-2x_j\sqrt{t}}$ on the right hand side of the above equation and by the triangle inequality, we obtain

$$||\sigma_j|| \leq \frac{1}{\sqrt{t}} \left(\int_0^\infty \left(\left| f_j(x_j, i\sqrt{t}) + e^{-\sqrt{t}x_j} \right| \left| f_j(x_j, i\sqrt{t}) - e^{-\sqrt{t}x_j} \right| + 2e^{-2\sqrt{t}x_j} \right) dx_j \right).$$

Using (B.0.10) and (B.0.12), we get,

$$\begin{aligned} ||\sigma_j|| &\leq \left(\frac{C_5}{t} \left(\frac{C_6}{\sqrt{t}} + 2 \right) + 2 \right) \int_0^\infty e^{-2\sqrt{t}x_i} dx_i \\ &= \frac{C_5 \left(C_6 + 2\sqrt{t} \right)}{2t^2} + \frac{1}{t}. \end{aligned}$$

Hence

$$||\mathcal{S}_1||_1 = O\left(t^{-1}\right).$$

To find estimate for $\mathcal{S}_2$, we use the same arguments as in Lemma B.0.3. Clearly, $\mathcal{S}_2 = (\cdot, q)q - (\cdot, r)r$ is a rank two operator. Here,

$$q_k(x_k) = \frac{-e^{-\sqrt{t}x_k}}{\sqrt{(n + b\sqrt{t})\sqrt{t}}} \quad \text{and} \quad r_k(x_k) = \frac{f_k(x_k, \sqrt{t}i)}{\sqrt{b - M(\sqrt{t}i)} f_k'(0, \sqrt{t}i)}.$$

Let $s = r - q$, then

$$\begin{aligned} s_k(x_k) &= \frac{f_k(x_k, \sqrt{t}i)}{\sqrt{b - M(\sqrt{t}i)} f_k'(0, \sqrt{t}i)} + \frac{e^{-\sqrt{t}x_k}}{\sqrt{(n + b\sqrt{t})\sqrt{t}}} \\ &= \frac{f_k(x_k, \sqrt{t}i) - e^{-\sqrt{t}x_k}}{\sqrt{b - M(\sqrt{t}i)} f_k'(0, \sqrt{t}i)} + \left(\frac{1}{\sqrt{b - M(\sqrt{t}i)} f_k'(0, \sqrt{t}i)} + \frac{1}{\sqrt{(n + b\sqrt{t})\sqrt{t}}} \right) e^{-\sqrt{t}x_k}. \end{aligned}$$

As,

$$||s||^2 = \sum_{k=1}^n \int_0^\infty |h_k(x_k)|^2 \, dx_k,$$

we use (3.2.45) and (B.0.10) and after some simplifications, we obtain the following estimate

$$||s||^2 \leq \frac{nC_5^2}{2\left(n+b\sqrt{t}\right)t^2}.$$

Similarly,

$$||q||^2 = \sum_{k=1}^{n} \int_0^{\infty} \left| \frac{-e^{-\sqrt{t}x_k}}{\sqrt{(n+b\sqrt{t})\sqrt{t}}} \right|^2 dx_k = \frac{n}{2t(n+b\sqrt{t})}.$$

So, the estimate on the right hand side of inequality (B.0.7) is

$$\begin{aligned} 6||s||^2||q||^2 + 3||s||^4 &\leq \frac{3n^2C_5^2}{2t^3\left(n+b\sqrt{t}\right)^2} + \frac{3n^2C_5^4}{4t^4\left(n+b\sqrt{t}\right)^2} \\ &= \frac{3n^2C_5^2(C_5^2+2t)}{4t^4\left(n+b\sqrt{t}\right)^2}. \end{aligned} \tag{B.0.17}$$

For $b \neq 0$, the asymptotic expansion of the above expression is given by

$$\begin{aligned} \frac{3n^2C_5^2(C_5^2+2t)}{4t^4\left(n+b\sqrt{t}\right)^2} &= \frac{3n^2C_5^2}{2b^2t^4} - \frac{3n^3C_5^2}{b^3t^{\frac{9}{2}}} + O(t^{-5}) \\ &= O(t^{-4}). \end{aligned}$$

Therefore,

$$||\mathcal{S}_2||_1 = O(t^{-2}).$$

This implies, for $b \neq 0$,

$$||\mathcal{R}_1||_1 = O(t^{-1}).$$

When $b = 0$, the asymptotic expansion of (B.0.17) is given by

$$\begin{aligned} \frac{3C_5^2(C_5^2+2t)}{4t^4} &= \frac{3C_5^2}{2t^3} + \frac{3C_5^4}{4t^4} \\ &= O(t^{-3}). \end{aligned}$$

In this case,

$$||\mathcal{S}_2||_1 = O(t^{-\frac{3}{2}}).$$

This implies

$$||\mathcal{R}_1||_1 = O(t^{-1}).$$

The assertion of the lemma follows from the above estimate on $\mathcal{R}_1$ and estimate obtained on $\mathcal{R}_2$ in lemma (B.0.3). □

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