Spectral Theory of Quantum Graphs

Von der Fakultät Mathematik und Physik der Universität Stuttgart
zur Erlangung der Würde eines Doktors der Naturwissenschaften
(Dr. rer. nat.) genehmigte Abhandlung

vorgelegt von

Dipl.-Math. Semra Demirel

geboren in Brackenheim

Hauptberichter Prof. TeknD Timo Weidl

Mitberichter Prof. Dr. Pavel Exner
Prof. Dr. Guido Schneider

Prüfungsdatum 19. Juli 2012

Institut für Analysis, Dynamik und Modellierung
Universität Stuttgart

2012

Contents

Preface

Mathematical theory of differential operators on graphs is an important and rapidly developing area of modern mathematical physics. A *quantum graph* is a metric graph with second order self-adjoint differential operators acting on functions defined on the graph's one-dimensional edges. As a generalization of the one-dimensional Schrödinger operator, a quantum graph describes the propagation of a quantum particle along the edges of the corresponding graph. In recent decades such objects have been studied as simplified models in mathematics and sciencies, including physics, chemistry, nanotechnology, microelectronics and medicine.

Quantum mechanics on graphs has a long history in physics and physical chemistry [43,80], but recent progress in experimental solid state physics has renewed attention on them as idealized models in thin domains. The problem of quantum systems in high dimensions turns out to be difficult. Though there are analytic facts for the concrete computation of specific states, the reduction of the problem to numerically accessible problems is nontrivial. Quantum graphs however are because of their one-dimensional nature a considerably easier model problem. Though the explicit analysis is still nontrivial, it is often possible to make progress by using one-dimensional techniques. Because of this fact quantum graphs have attracted attention of many researchers. The question whether spectral properties of the Schrödinger operator on thin branching domains with Dirichlet or Neumann boundary conditions can be approximated by the properties of the Schrödinger operator on the graph turns out to be a highly non-trivial question.

There are plenty of applications in other areas like dynamical systems, photonic crystals, quantum wires, quantum chaos, Anderson localization, optics and number theory. However, we restrict ourselves to give an example of the first applications and one of the most recent ones only.

The first one goes back to the 1930s when Pauling studied the spectrum of free electrons in conjugated organic molecules like naphthalene, see Fig.1. In approximation the atoms are considered as vertices and the $\sigma-$electrons are taken to be the edges of a graph on which the free electrons are confined.

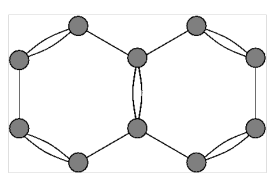

Figure 1. naphthalene

More recent applications of quantum graphs are in the field of nanotechnology where the understanding of mesoscopic systems, i.e. systems built with a width on the scale of nanometers, plays an important role. A thin quantum waveguide is considered here as a fattened graph where the edges are thin tubes. It was shown in [28,29,84] that under certain conditions the spectrum of the Laplace operator on this domain converges to the spectrum of the Laplace operator on the graph. Fig. 2 shows a remarkable nanostructure. A carbon nanotube is a cylindrical carbon molecule with a typical diameter of 1-2 nanometres, which is 80,000 times smaller than the thickness of a human hair. Not only are there potential applications of carbon nanotubes in nanotechnology as energy-saving transistors or wires, but they also can have the property of delivering medicine directly to a tumor.

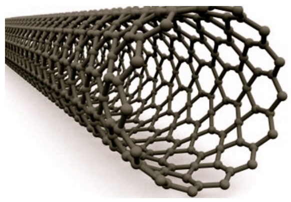

FIGURE 2. carbon nanotube

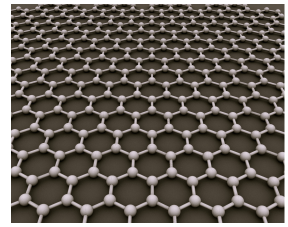

FIGURE 3. graphene

Carbon nano-structures are another example which recently have became very popular. Fig. 3 shows graphene, whose structure is a two-dimensional honeycomb lattice consisting of carbon atoms. It can also be considered as the limiting case of the family of flat polycyclic aromatic hydrocarbons, in which Naphthalene is the simplest example. Graphene can be rolled into a one-dimensional nanotube or stacked into three-dimensional graphite, which both are its lower-energy states. In 2010 the Nobel Prize in Physics was awarded to Andre Geim and Konstantin Novoselov for obtaining graphene by mechanical exfoliation of graphite. Since then graphene has attracted great interest because of its properties like being one of the strongest materials or having a remarkably high electron mobility. This makes it to an attractive object in the production of transistors.

Another fact is that new progress in nanotechnology also makes it possible to test predictions of quantum mechanics and to study various quantum effects from the theoretical and experimental points of view.

A large literature on the subject of quantum graphs has arisen, for which we refer to the bibliography given in [7, 12, 27, 54, 61–65, 88].

Fig. 1 is from http://en.wikipedia.org/wiki/Quantum_graph
Fig. 2,3 are from http://en.wikipedia.org/wiki/Graphene

Acknowledgements. First of all I would like to express my deep gratitude to my supervisor Timo Weidl. I had the fortune to visit his analysis lectures already from the very beginning of my studies in mathematics. Later, he introduced me to topics in spectral theory and mathematical phyiscs and shared many exciting mathematical problems and ideas with me. I'm grateful to him for his constant help concerning mathematical as well as personal matters.

I am indebted to my teacher and co-author Evans M. Harrell for the fruitful and very pleasent collaboration. I truly enjoyed working and discussing with him. I'm grateful to Ari Laptev and Dimitriĭ R. Yafaev for valuable comments. I further would like to thank my co-author Usman Muhammad for our collaboration on interesting problems.

Many thanks to Guido Schneider, to Pavel Exner, and to Michael Eisermann for their readiness to be member of my thesis committee.

I would like to thank my collegues and friends at the mathematics department of the University of Stuttgart for the very nice environment to work in.

Special thanks to my fiancé Rupert L. Frank for all his support and encouragement, and for filling life with meaning and joy. Sevgili anne'me ve sevgili baba'ma bana her daim vermiş oldukları destekleri ve güvenleri için içten teşekkür ederim. Ablam Sinem'e ve eniştem Yusuf'a evdeki sıcak ve neşeli ortam için teşekkürler. Ve tabii ki canım kardeşim Hami'ye varlığının vermiş olduğu eşsiz mutluluk için çok teşekkür ederim.

Abstract

We study some spectral problems for quantum graphs with a potential. On the one hand we analyze the quantitative dependence of bound states of $-d^2/dx^2 + V$ on the potential V. On the other hand we generalize certain basic identities from the one-dimensional scattering theory to quantum graphs.

The first paper is concerned with the study of the discrete negative spectra of quantum graphs. We use the method of trace identities (sum rules) to derive inequalities of Lieb-Thirring, Payne-Pólya-Weinberger, and Yang types, among others. We show that the sharp constants of these inequalities and even their forms depend on the topology of the graph. Conditions are identified under which the sharp constants are the same as for the classical inequalities; in particular, this is true in the case of trees. We also provide some counterexamples where the classical form of the inequalities is false.

The second paper deals with the scattering problem for the Schrödinger equation on the half-line with the Robin boundary condition at the origin. We derive an expression for the trace of the difference of the perturbed and unperturbed resolvent in terms of a Wronskian. This leads to a representation for the perturbation determinant and to trace identities of Buslaev-Faddeev type.

In the third paper we generalize results from the half-line case to the full graph case. More precisely, we consider the Schrödinger problem on a star shaped graph with n edges joined at a single vertex. A trace formula is derived for the difference of the perturbed and unperturbed resolvent in terms of a Wronskian. This leads to representations for the perturbation determinant and the spectral shift function, and to an analog of Levinson's formula.

Besides these three articles this thesis also contains some further results. The method of sum rules is applied to the modified Schrödinger operator with variable coefficients to obtain a Lieb-Thirring type inequality with optimal constant. Furthermore, Lieb-Thirring inequalities are studied for star shaped graphs by using variational arguments and the method of symmetry decomposition of the corresponding Hilbert space. In several cases this leads to optimal constants in the inequalities.

Zusammenfassung

Diese Arbeit beinhaltet Untersuchungen von Spektralproblemen für Quantengraphen mit Potential. Einerseits analysieren wir die quantitative Abhängigkeit der Eigenwerte von $-d^2/dx^2 + V$ vom Potential V. Andererseits verallgemeinern wir gewisse elementare Identitäten von der eindimensionalen Streutheorie auf Quantengraphen.

Im ersten Artikel wird das diskrete negative Spektrum von Quantengraphen analysiert. Dabei verwenden wir die Methode der Summenformeln, um Ungleichungen vom Lieb-Thirring-, Payne-Pólya-Weinberger- und Yang- Typ herzuleiten. Wir zeigen, dass die scharfen Konstanten für diese Ungleichungen, und sogar ihre Gestalt, von der Topologie des Graphen abhängen. Es werden Bedingungen angegeben, unter welchen die scharfen Konstanten mit den scharfen Konstanten für den klassischen Fall des Ganzraumes übereinstimmen. Insbesondere ist dies der Fall für metrische Bäume. Desweiteren konstruieren wir Gegenbeispiele, für welche die klassischen Konstanten falsch sind.

Der zweite Artikel befasst sich mit dem Streuproblem für den Schödingeroperator auf der Halbachse mit Robin-Randbedingung. Wir leiten einen Ausdruck für die Spur der Differenz von der gestörten und der ungestörten Resolvente her, welche eine Wronski-Determinante beinhaltet. Dies führt zu einer Darstellung der Störungsdeterminante und zu Spurformeln vom Buslaev-Faddeev-Typ.

Im dritten Artikel werden Resultate aus dem zweiten Artikel verallgemeinert auf sternförmige Quantengraphen, die aus n Halbachsen bestehen, welche in einem einzigen Knotenpunkt verbunden sind. Wir beweisen eine Spurformel für die Differenz der gestörten und der ungestörten Resolvente, welche eine Wronski-Determinante beinhaltet. Dies führt wiederum zu einer Darstellung der Störungsdeterminante und zu einem Analogon der Levinson-Formel.

Über diese drei Hauptteile hinaus beinhaltet diese Arbeit mehrere weitere Resultate. Mit der Methode der Summenformeln leiten wir für den modifizierten Schrödingeroperator mit variablen Koeffizienten eine Lieb-Thirring-Ungleichung mit einer optimalen Konstante her. Desweiteren werden mit Hilfe von Variationsargumenten und der Symmetriezerlegung des entsprechenden Hilbertraumes Lieb-Thirring Ungleichungen für den sternförmigen Graphen bewiesen. In zahlreichen Fällen erhalten wir dabei die optimale Konstante.

1. Introduction

1.1. **Quantum Graphs.** Quantum graphs describe wave propagation on a graph and are mostly important to model wave propagation in thin branching media such as thin waveguides, quantum wires, photonic crystals and vessels. In this section we shall give a more precise definition of quantum graphs. More details can be found in [65] .

A *graph* Γ consists of a finite or countably infinite set of vertices, denoted by $\mathcal{V} = \{v_i\}$, and a set of one-dimensional edges $E = \{e_i\}$ connecting the vertices. Each edge is identified with its endpoints (v_i, v_j). We denote by E_v the set of edges containing the vertex v. The number of edges emanating from the vertex v is called *degree* or *valence* d_v of v and is assumed to be finite and positive.

In this thesis we are not concerned with combinatorial objects, but with so-called *metric graphs.*

Definition 1.1. A *metric graph* is a graph Γ where each edge e is identified with an interval $[0, \ell_e]$. Denoting the coordinate on the interval by x_e, the vertex v_i corresponds to $x_e = 0$ and v_j to $x_e = \ell_e$ (or vice versa).

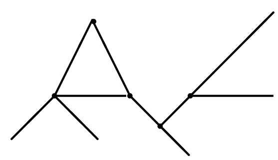

Figure 4. A metric graph

A graph Γ can be equipped with a natural metric in the following way. The length ℓ of a path formed by a sequence of edges $\{e_i\}_{i=1}^n$ is defined as $\ell := \sum_{i=1}^n \ell_i$, where the distance $\rho(v_i, v_j)$ of two vertices is defined as the shortest path between them. Similarly, the natural distance $\rho(x, y)$ for two arbitrary points on the graph is the shortest distance (measured along the graph) between them. Edges with one free end are called *leaves* and may be of finite or infinite length.

Unlike in the case of a discrete graph, the points of a metric graph are not only its vertices, but also all points on the edges. Thus, it is possible to define a natural Lebesgue measure on the graph as well as integration and differentiation along the edges of Γ. The following Definition states that the Hilbert space of the graph, denoted by $L_2(\Gamma)$, is defined as the orthogonal direct sum of spaces $L_2(e)$.

Definition 1.2. The space $L_2(\Gamma)$ on Γ consists of functions ψ that are in $L_2(e)$ for every edge e of Γ and fullfill the condition

$$\|\psi\|^2_{L_2(\Gamma)} = \sum_{e \in E} \|\psi\|^2_{L_2(e)} < \infty. \tag{1.1}$$

Definition 1.3. The Sobolev space $H^1(\Gamma)$ on Γ consists of functions ψ that are in $H^1(e)$ for every edge e of Γ and fullfill the condition

$$\sum_{e \in E} \|\psi\|^2_{H^1(e)} < \infty. \tag{1.2}$$

Further, ψ is continuous at each vertex $v \in \mathcal{V}$ and therefore on the whole graph Γ.

Of course, conditions (1.1) and (1.2) are needed for infinite graphs, i.e. graphs with infinitely many vertices, only.

A *quantum graph* is a metric graph with second order self-adjoint differential operators acting on functions defined on the graph's edges. In this thesis we will consider the Schrödinger operator H on Γ defined as follows. H acts on each edge of Γ on a function ψ as

$$H\psi = -\frac{d^2}{dx^2}\psi + \beta V\psi, \quad \beta > 0, \tag{1.3}$$

where V is the operator of multiplication by the real-valued function $V(x),\ x \in \Gamma$, satisfying appropriate regularity and decay conditions (to be specified later). The operator (1.3) is the stationary part of the Schrödinger equation, which describes the evolution of a particle on Γ with mass $1/2$ in the exterior electric potential βV. The wavefunction $\psi \in L_2(\Gamma)$ with $\int_\Gamma |\psi|^2\,dx$ describes the state of the particle. The value $|\psi(x)|^2$ is understood as the probability density of finding a particle at $x \in \Gamma$. The quadratic form of the Schrödinger operator (1.3) is given by

$$\int_\Gamma |\psi'|^2\,dx + \beta\int_\Gamma V|\psi|^2\,dx$$

and represents in the choice of mathematical units $\hbar = e = 1$ the total energy (kinetic and potential energy) of the system in the state ψ. We note that this definition is independent of the orientation of the graph's edges since ψ' appears only in the absolute value.

The domain of H is denoted by $D(H)$ and, provided V is sufficiently regular, consists of all functions ψ which belong to $H^2(e)$ for each edge e and satisfy

$$\sum_{e\in E} \|\psi\|^2_{H^2(e)} < \infty.$$

Further, ψ has to satisfy "appropriate" boundary conditions at each vertex v. There are different descriptions of all vertex conditions that give rise to self-adjoint operators H, see [32,44,61,65]. In what follows we will be concerned with the most common kind of boundary condition, the *Kirchhoff* condition coming from the theory of electric networks. This vertex condition states that ψ is continuous on Γ and fullfills at each vertex v the condition

$$\sum_{e\in E_v} \frac{d\psi}{dx_e}(v) = 0, \tag{1.4}$$

where the derivatives are taken in outgoing directions from v. Condition (1.4) means that at each vertex v the flux is conserved. In literature, this condition is also called as the *natural* boundary condition, as the domain of the quadratic form of H does only require the condition that a function is in the space $H^1(\Gamma)$ and thus continuous. Therefore, the Kirchhoff condition is sometimes also called "Neumann-Kirchhoff condition". Setting Dirichlet boundary condition at every vertex v gives rise to a disconnected graph with unrelated edges. In this case the Schrödinger operator decouples into the direct sum of Schrödinger operators on the edges. Similarly the operator decouples when Neumann boundary conditions are imposed at all vertices. Indeed, the topology of a quantum graph is encoded in the vertex conditions only.

1.2. **Weyl's law and Lieb Thirring inequalities in $\mathbb{R}^d$.** Since our goal will be to prove eigenvalue estimates for quantum graphs, we will first review related results on the euclidean space $\mathbb{R}^d$. In this section we give an overview of *Weyl's law* and the so called *Lieb-Thirring inequalities*. Let H be the Schrödinger operator on $L_2(\mathbb{R}^d)$ defined by

$$H = -\Delta + \beta V, \quad \beta > 0, \tag{1.5}$$

where the exterior potential V is a real-valued multiplication operator and goes to zero at infinity. Given a certain local regularity of V, the spectrum of H consists of a continuous spectrum on the positive semiaxis and a discrete spectrum consisting of negative eigenvalues which are denoted by $\{\lambda_j(\beta)\}_{j\in\mathbb{N}}$ in non-decreasing order and counting multiplicities. The continuous spectrum is usually associated with scattering states whereas the negative eigenvalues correspond to the energies at which a particle might be trapped by the potential well βV. There are only finitely many negative eigenvalues if V decays fast enough, otherwise there are countably many negative eigenvalues with zero as the only accumulation point. In the following, we consider the Riesz-means or moments of the negative eigenvalues of H,

$$R_\gamma(\beta V) := \mathrm{Tr}(-\Delta + \beta V)_-^\gamma = \sum_j |\lambda_j(\beta)|^\gamma, \quad \gamma \geq 0, \tag{1.6}$$

where $x_\pm := (|x| \pm x)/2$ denote the positive and negative part of numbers and operators, respectively. The special case $\gamma = 0$ corresponds to the function $N(-\Delta + \beta V) := \#\{j \in \mathbb{N} : \lambda_j < 0\}$ counting negative eigenvalues. In what follows, we will consider spectral estimates for (1.6).

Weyl's law. In 1911 Hermann Weyl discovered a connection between the frequencies of an oscillating membrane and the volume of the membrane, [95]. His result was highly important for further studies in mathematical physics and spectral analysis. The study of frequencies of an oscillating membrane corresponds in quantum mechanics to the study of the Dirichlet Laplacian $-\Delta_\Omega^D$ in a bounded domain Ω. Thereby, the frequencies are given by the discrete eigenvalues of the Dirichlet Laplacian and the membrane is described by Ω. Let us denote by $N_\Omega^D(\Lambda)$ the number of eigenvalues of $-\Delta_\Omega^D$ below Λ. Weyl's result states that for all bounded open domains the semiclassical limit

$$N_\Omega^D(\Lambda) = \frac{\Lambda^{d/2}\omega_d}{(2\pi)^d}\int_\Omega dx + o(\Lambda^{d/2}) \quad \text{as} \quad \Lambda \to +\infty, \tag{1.7}$$

holds. Here $\omega_d = \pi^{d/2}/\Gamma(1 + d/2)$ denotes the volume of the unit ball in $\mathbb{R}^d$. Weyl's law (1.7) can be generalized to the Schrödinger operator (1.5) and one obtains the asymptotic behaviour of $N(-\Delta + \beta V)$ in the strong coupling limit, i.e., when β tends to infinity,

$$N(-\Delta + \beta V) = \beta^{d/2}\frac{\omega_d}{(2\pi)^d}\int_{\mathbb{R}^d} V(x)_-^{d/2}\,dx + o(\beta^{d/2}), \quad \text{as} \quad \beta \to +\infty. \tag{1.8}$$

Asymptotics (1.8) was first proved by Birman for compactly supported potentials V in a compact domain with Dirichlet boundary condition, [10], and was later generalized in [9, 58, 74, 91]. For higher moments $\gamma > 0$ the analog asymptotics reads as

$$\mathrm{Tr}(-\Delta + \beta V)_-^\gamma = \beta^{\gamma+d/2}L_{\gamma,d}^{cl}\int_{\mathbb{R}^d} V(x)_-^{\gamma+d/2}\,dx + o(\beta^{\gamma+d/2}), \quad \text{as} \quad \beta \to +\infty, \tag{1.9}$$

with the semiclassical constant

$$L_{\gamma,d}^{cl} := \frac{\Gamma(\gamma+1)}{2^d \pi^{d/2} \Gamma(\gamma+1+d/2)}.$$

Note that the Schrödinger operator (1.5) is associated with the classical Hamiltonian function $H(x,\xi) = |\xi|^2 + \beta V(x)$ defined on the classical phase space $\mathbb{R}^d \times \mathbb{R}^d$. Therefore, the semiclassical asymptotics (1.9) and (1.8) are determined by the phase space volume of the Hamiltonian function, indeed

$$(2\pi)^{-d} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} H(x,\xi)_-^{\gamma}\, dx\, d\xi = \beta^{\gamma+d/2} L_{\gamma,d}^{cl} \int_{\mathbb{R}^d} V(x)_-^{\gamma+d/2}\, dx.$$

Thus, this can be interpreted as each quantum state occupying a volume of $(2\pi)^d$ in the classical phase space $\mathbb{R}^d \times \mathbb{R}^d$. This agrees with the Bohr-Sommerfeld quantization rule from early quantum mechanics, see also [30].

Lieb-Thirring inequalities. Sometimes, it is of interest not only to know the asymptotic behaviour of (1.6) but to have also uniform bounds for them. *Lieb-Thirring inequalities* provide an upper bound for the moments of the negative eigenvalues $\lambda_j(\beta)$ of the Schrödinger operator (1.5) in terms of integrals of V,

$$\sum_j |\lambda_j(\beta)|^{\gamma} \leq \beta^{\gamma+d/2} L_{\gamma,d} \int\limits_{\mathbb{R}^d} (V_-(x))^{\gamma+d/2}\, dx \tag{1.10}$$

for some constant $L_{\gamma,d} \geq L_{\gamma,d}^{cl}$ and $V \in L_{\gamma+d/2}(\mathbb{R}^d)$. This inequality holds true for various ranges of $\gamma \geq 0$ depending on the dimension d and was proved by Lieb and Thirring in the case $\gamma > \max\{0, 1-d/2\}$, see [72]. If $d \geq 3$, then (1.10) holds also in the endpoint case $\gamma = 0$ and is known as the Cwikel-Lieb-Rozenblyum inequality, [18, 71, 83]. The endpoint case $d = 1,\ \gamma = 1/2$ is due to Weidl, [94]. To summarize, inequality (1.10) is true in the following cases,

$$\begin{aligned} \gamma &\geq \frac{1}{2} \quad && \text{if} \quad d = 1, \\ \gamma &> 0 \quad && \text{if} \quad d = 2, \\ \gamma &\geq 0 \quad && \text{if} \quad d \geq 3. \end{aligned} \tag{1.11}$$

It is known that (1.10) fails in the cases $d = 2,\ \gamma = 0$ and $d = 1,\ 0 \leq \gamma < 1/2$. In the case $d = 1, 2$ and $\gamma = 0$ this is due to the fact that for $d = 1$ or $d = 2$ there exists at least one negative eigenvalue for any negative potential $V \neq 0$, [86]. Indeed, an inequality of the form (1.10) with $d = 1, 2$ and $\gamma = 0$ would imply that there is no negative eigenvalue if $\int_{\mathbb{R}^d} V_-^{d/2}\, dx < 1/L_{0,d}$. The failure of (1.10) in the case $d = 1,\ \gamma < 1/2$ follows for example from the behaviour of the lowest eigenvalue in the weak coupling limit $\beta \to 0$, [86]. Alternatively, one can consider a sequence of potentials V_n which converges to the delta function. Then, the right hand side in (1.10) converges to zero whereas the left hand side tends to a positive number.

Lieb-Thirring inequalities have great importance in applications. They were first used by Lieb and Thirring themselves in the study of the stability of matter. Also in the theory of Navier-Stokes equations they turned out to be useful for estimates on dimensions of attractors. Another application concerns the Weyl-type asymptotics, which were originally established for sufficiently regular potentials. With Lieb-Thirring estimates it was indeed possible to generalize these asymptotics to *all* potenials $V \in L_{\gamma+d/2}$ in the cases (1.11). Finally, we mention that Lieb-Thirring inequalities were considered in the study of the continuous spectrum of Schrödinger operators, see [19, 68]

While the question about the existence of uniform constants $L_{\gamma,d}$ for which (1.10) holds is answered completely, the sharp constants, i.e. the best possible constants in (1.10), are only known in the cases $d \geq 1,\ \gamma \geq 3/2$ and for $d = 1,\ \gamma = 1/2$, [53]. In 1976, Lieb and Thirring showed that $L_{\gamma,1} = L^{cl}_{\gamma,1}$ for all $\gamma \geq 3/2$, see [72]. This result was generalized to higher dimensions by Laptev and Weidl, [70].

Recently, a new proof of sharp Lieb-Thirring inequalities for $\gamma \geq 2$ and $d \geq 1$ has been given by Stubbe [90]. Remarkably, his proof shows that for $\gamma \geq 2$ the semiclassical limit is reached in a monotone way. His proof is based on general trace identities for operators [50] known as sum rules. Before presenting the idea of his proof, we give an overview of the analogs of Weyl's law and Lieb-Thirring inequalities for the case of quantum graphs.

1.3. **Weyl's law and Lieb Thirring inequalities for quantum graphs.** For quantum graphs an analog of Weyl's aymptotic formula (1.9) can be proved by the standard Dirichlet-Neumann bracketing techniques, see [77, 82]. The corresponding Weyl-type asymptotic formula states that

$$\operatorname{Tr}\left(-\frac{d^2}{dx^2} + \beta V\right)_-^{\gamma} = \beta^{\gamma+1/2} L^{cl}_{\gamma,1} \int_\Gamma (V_-(x))^{\gamma+1/2}\, dx + o(\beta^{\gamma+1/2}), \tag{1.12}$$

as $\beta \to +\infty$, with the semiclassical constant

$$L^{cl}_{\gamma,1} := \frac{\Gamma(\gamma+1)}{2\pi^{1/2}\Gamma(\gamma+3/2)}.$$

For the study of Lieb-Thirring inequalities for quantum graphs this means that we cannot expect an inequality with a constant better than $L^{cl}_{\gamma,1}$. In other words, if for a given quantum graph an inequality of this type holds with the semiclassical constant for the one-dimensional Schrödinger operator, then the inequality for the quantum graph is sharp. Moreover, the best possible constant L_γ for quantum graphs cannot be less than the best possible constant $L_{\gamma,1}$ for the one-dimensional Schrödinger operator. This can be seen easily by considering a metric graph which has at least one infinite edge. Shifting the potential $V \in L_{\gamma+1/2}(\Gamma)$ on the graph Γ to infinity, the spectrum of the quantum graph converges to the spectrum of the one-dimensional Schrödinger operator.

The papers [24, 31, 78, 89] contain inequalities about eigenvalues of Schrödinger operators on metric graphs. In [24, 31] the authors prove Lieb-Thirring inequalities for regular metric trees. A metric graph is called *regular* if the length of each edge and the branching number of each vertex depend only on the distance to the root. Their result states that in this case the Lieb-Thirring inequality

$$\sum_j (-\lambda_j)^\gamma \leq C_\gamma \int\limits_\Gamma (V_-(x))^{\gamma+1/2}\, dx$$

holds for all $\gamma \geq 1/2$.

Another result concerning the weak coupling for quantum graphs was obtained by Exner in [26]. If the graph consists of N semi-infinite edges joined at a single vertex and the corresponding quantum graph is given with Kirchhoff vertex condition, then an arbitrarily weak attractive potential produces a bound state. More precisely, under the assumption that $V_j \in L_2(\mathbb{R}_+, (1+|x|)dx)$, $1 \le j \le N$, the Schrödinger operator $H = -d^2/dx^2 + \beta V$ in $L_2(\Gamma)$ has for all sufficiently small $\beta > 0$, a single negative eigenvalue iff $\sum_{j=1}^N \int_0^\infty V_j(x)\, dx \le 0$. This generalizes the result of Simon [86] in the one-dimensional case.

1.4. **Sum rules of Harrell and Stubbe.** In [50] Harrell and Stubbe derived "sum rule" identities involving traces and commutators of certain self-adjoint operators H, including the Dirichlet Laplacian on bounded Euclidean domains and Schrödinger operators with discrete spectra. These "sum rules" lead to *universal* bounds on spectral gaps and on moments of eigenvalues, i.e. bounds which do not depend on the specific geometry of the domain or on details of the potential.

In the following these sum rules and the idea of the proof is presented. Let H be a self-adjoint operator with domain $D(H)$ on a Hilbert space $\mathcal{H}$ with scalar product $\langle \cdot, \cdot \rangle$. Suppose that H has nonempty point spectrum, and that $\mathcal{J}$ is a finite-dimensional subspace of $\mathcal{H}$ spanned by an orthonormal set $\{\phi_j\}$ of eigenfunctions of H. The discrete part of the spectrum of H is denoted by $J := \{\lambda_j : H\phi_j = \lambda_j \phi_j\}$. Further let P_A denote the spectral projector associated with H and a Borel set A. Assume that G is another self-adjoint operator with domain $D(G)$ and that $G(\mathcal{J}) \subseteq D(H) \subseteq D(G)$. Then for any z the following trace identity holds,

$$\sum_{\lambda_j \in J} (z-\lambda_j)^2 \langle [G,[H,G]]\phi_j, \phi_j \rangle - 2(z-\lambda_j) \langle [H,G]\phi_j, [H,G]\phi_j \rangle$$

$$= 2 \sum_{\lambda_j \in J} \int_{\kappa \in J^c} (z-\lambda_j)(z-\kappa)(\kappa-\lambda_j)\, dG_{j\kappa}^2, \tag{1.13}$$

where $dG_{j\kappa}^2 := |\langle G\phi_j, dP_\kappa G\phi_j \rangle|$.

This sum rule is an abstract version of what is known in quantum theory as the oscillator-strength sum rule of Thomas, Reiche, and Kuhn and the Bethe sum rule [8]. To prove (1.13), note that by a straightforward calculation, the self-adjoint operators H and G satisfy

$$\langle [G,[H,G]]\phi_j, \phi_j \rangle = 2 \langle (H-\lambda_j)G\phi_j, G\phi_j \rangle,$$

which by the spectral theorem equals $2\int (\kappa-\lambda_j) \langle dP_\kappa G\phi_j, G\phi_j \rangle$. Thus,

$$\langle [G,[H,G]]\phi_j, \phi_j \rangle = 2 \int (\kappa-\lambda_j)\, dG_{j\kappa}^2.$$

Multiplying the last equation by $(z-\lambda_j)^2$ and summing over $\lambda_j \in J$ leads to

$$\sum_{\lambda_j \in J} (z-\lambda_j)^2 \langle [G,[H,G]]\phi_j, \phi_j \rangle = 2 \sum_{\lambda_j \in J} \int (z-\lambda_j)^2 (\kappa-\lambda_j)\, dG_{j\kappa}^2. \tag{1.14}$$

Next, a direct computation shows that

$$\langle [H,G]\phi_j, [H,G]\phi_j \rangle = \int (\kappa-\lambda_j)^2\, dG_{j\kappa}^2,$$

which after multiplication by $-2(z-\lambda_j)$ and summing over $\lambda_j \in J$ turns into

$$-\sum_{\lambda_j \in J} 2(z-\lambda_j)\left\langle [H,G]\phi_j, [H,G]\phi_j \right\rangle = -2\sum_{\lambda_j \in J} \int (z-\lambda_j)(\kappa-\lambda_j)^2\, dG^2_{j\kappa}. \tag{1.15}$$

Combining (1.14) with (1.15) proves sum rule (1.13).

Sum rule (1.13) was generalized in [51] to non-self-adjoint operators G. Assume that H has purely discrete spectrum and fix a subset J of the spectrum. Under the assumption that G is a linear operator with adjoint G^* such that $G(D(H)) \subseteq D(H) \subseteq D(G)$ and $G^*(D(H)) \subseteq D(H) \subseteq D(G^*)$, it follows that

$$\begin{aligned}
&\frac{1}{2}\sum_{\lambda_j \in J} (z-\lambda_j)^2 \left(\langle [G^*,[H,G]]\phi_j,\phi_j\rangle + \langle [G,[H,G^*]]\phi_j,\phi_j\rangle\right)\\
&\qquad\qquad -(z-\lambda_j)\left(\|[H,G]\phi_j\|^2 + \|[H,G^*]\phi_j\|^2\right)\\
&= \sum_{\lambda_j \in J}\sum_{\lambda_k \notin J} (z-\lambda_j)(z-\lambda_k)(\lambda_k-\lambda_j)\left(|\langle G\phi_j,\phi_k\rangle|^2 + |\langle G^*\phi_j,\phi_k\rangle|^2\right).
\end{aligned} \tag{1.16}$$

Remark 1.4. Sum rule (1.16) can be extended to the case where continuous spectrum is allowed in J^c lying above the discrete spectrum J. This follows exactly as in the proof of (1.13).

Stubbe's monotonicity argument. In [90] Stubbe gave a new proof of sharp Lieb-Thirring inequalities for $\gamma \geq 2$ and $d \geq 1$. His proof is based on sum rules and provides also monotonicity with respect to coupling constants. The monotonicity fact has not been known so far and can be shown only for $\gamma \geq 2$, indeed the harmonic oscillator is a counterexample.

Let us consider the operator

$$H = -\hbar^2\Delta + V(x)$$

on $L_2(\mathbb{R}^d)$, where $\hbar$ is the Planck's constant. Rewriting (1.9) in terms of the Planck's constant, one obtains in the limit $\hbar \to 0$,

$$\mathrm{Tr}(-\hbar^2\Delta + V)^\gamma_- = \hbar^{-d} L^{cl}_{\gamma,d} \int_{\mathbb{R}^d} (V_-(x))^{\gamma+d/2}\, dx + o(\hbar^d).$$

In what follows, we set $\hbar^2 = \alpha$ and consider the Schrödinger operator

$$H(\alpha) = -\alpha\Delta + V(x), \quad \alpha > 0 \tag{1.17}$$

on $L_2(\mathbb{R}^d)$.

Without loss of generality we may assume that $V \in C_0^\infty$. Then, for any $\alpha > 0$, the spectrum of $H(\alpha)$ consists of a discrete spectrum J with at most a finite number of negative eigenvalues $\lambda_j(\alpha)$ lying below the continuous spectrum J^c on the positive semiaxis. The normalized eigenfunctions corresponding to the eigenvalues $\lambda_j(\alpha)$ are denoted by ϕ_j. Stubbe's Theorem states that under these assumptions, the mapping

$$\alpha \mapsto \alpha^{d/2} \sum_{\lambda_j(\alpha)<0} (-\lambda_j(\alpha))^2$$

is nonincreasing for all $\alpha > 0$ and consequently

$$\alpha^{d/2} \sum_{\lambda_j(\alpha)<0} (-\lambda_j(\alpha))^2 \le L^{cl}_{2,d} \int_{\mathbb{R}^d} (V_-(x))^{2+d/2}\, dx$$

for all $\alpha > 0$ and $\gamma = 2$. By the Aizenman-Lieb argument [1] analog inequalities hold for all $\gamma \ge 2$.

We now give the idea of his proof in a slightly different way as given in [90], namely by a direct application of (1.13). Obviously, because of the choice of J and J^c, it follows from (1.13) that

$$\sum_{\lambda_j \in J} (z-\lambda_j)^2 \langle [G,[H,G]]\phi_j, \phi_j\rangle - 2(z-\lambda_j)\langle [H,G]\phi_j, [H,G]\phi_j\rangle \le 0. \tag{1.18}$$

In order to present the main idea of the argument, we first ignore some technicalities and give the details later. Let $x_a,\ a = 1,\dots,d$ denote the cartesian coordinates in $\mathbb{R}^d$. Stubbe's idea was to choose G as the multiplication operator $G = x_a$. (The problem with this choice is that this G is not a bounded operator. We will find a way around this later.) For this choice of G, the first and second commutators are given by

$$[H,G] = -2\alpha \frac{\partial}{\partial x_a} \quad \text{and} \quad [G,[H,G]] = 2\alpha.$$

Inserting these in (1.18) and setting $z = 0$, we get

$$\sum_{\lambda_j \in J} (-\lambda_j(\alpha))^2 2\alpha \|\phi_j\|^2 - 2(-\lambda_j(\alpha)) 4\alpha^2 \|\frac{\partial \phi_j}{\partial x_a}\|^2 \le 0. \tag{1.19}$$

Dividing by 2 and summing over all coordinates in (1.19), the following inequality holds

$$\alpha d \sum_{\lambda_j \in J} (-\lambda_j(\alpha))^2 - 4\alpha^2 \sum_{\lambda_j \in J} (-\lambda_j(\alpha)) \|\nabla \phi_j\|^2 \le 0. \tag{1.20}$$

This important inequality is the point of departure of Stubbe's monotonicity argument:
For any $\alpha > 0$, the functions $\lambda_j(\alpha)$ are non-positive, continuous and increasing. $\lambda_j(\alpha)$ is continuously differentiable except at countably many values where $\lambda_j(\alpha)$ fails to be isolated or enters the continuum. By the Feynman-Hellman theorem,

$$\frac{d}{d\alpha}\lambda_j(\alpha) = \langle \phi_j, -\Delta\phi_j\rangle = \|\nabla\phi_j\|^2.$$

Thus, (1.20) can be rewritten as

$$\alpha\ d \sum_{\lambda_j(\alpha)<0} (-\lambda_j(\alpha))^2 + 2\alpha^2 \frac{d}{d\alpha} \sum_{\lambda_j(\alpha)<0} (-\lambda_j(\alpha))^2 \le 0.$$

For any $\alpha \in]\alpha_{N+1}, \alpha_N[$ the number of eigenvalues is constant, and therefore

$$\frac{d}{d\alpha}\left(\alpha^{d/2} \sum_{\lambda_j(\alpha)<0} (-\lambda_j(\alpha))^2 \right) \le 0.$$

This means that $\alpha^{d/2}\sum_{\lambda_j(\alpha)<0}\lambda_j^2(\alpha)$ is monotone decreasing in α. Hence, by Weyl's asymptotics,

$$\alpha^{d/2}\sum_{\lambda_j(\alpha)<0}\lambda_j^2(\alpha)\le\lim_{\alpha\to 0+}\alpha^{d/2}\sum_{\lambda_j(\alpha)<0}\lambda_j^2(\alpha)=L_{2,1}^{cl}\int\limits_{\mathbb{R}^d}(V_-(x))^{2+d/2}\,dx.$$

Remark 1.5. Strictly speaking, the Feynman-Hellman theorem only holds for nondegenerate eigenvalues. In the case of degenerate eigenvalues one has to take the right basis in the corresponding degeneracy space and to change the numbering if necessary, see e.g. [92].

As we explained the above approach is not completely rigorous since the assumption $G(D(H))\subseteq D(H)\subseteq D(G)$ is not satisfied. We now explain how to avoid this problem. (Our approach is different from Stubbe's who avoids the problem by considering the Dirichlet problem on a *bounded* domain.) The reader who is mostly interested in a non-technical overview may skip the remainder of this subsection. For the sake of simplicity we assume that $d=1$. We consider for a fixed $\varepsilon>0$ and $x\in\mathbb{R}$, the operator of multiplication by

$$G_\varepsilon(x):=\frac{x}{\sqrt{1+\varepsilon x^2}}. \tag{1.21}$$

Obviously, $\lim_{\varepsilon\to 0}G_\varepsilon(x)=x$. We show that G_ε fullfills the domain condition and further it satisfies, in the limit when $\varepsilon\to 0$, the desired inequality (1.19). To make the idea of the proof clear, let us first work under the simplifying assumption the *operator domain* is $H^2(\mathbb{R})$ (this is true, for instance, if $V\in L_2(\mathbb{R})$). Afterwards, we will present a proof which uses only the form domain of H.

Step one: The function G_ε is a bounded function for all $x\in\mathbb{R}$ with the asymptotics $\lim_{x\to-\infty}G_\varepsilon(x)=-1/\sqrt{\varepsilon}$ and $\lim_{x\to\infty}G_\varepsilon(x)=1/\sqrt{\varepsilon}$. If $V\in L_2(\mathbb{R})$, then $D(H)=H^2(\mathbb{R})$. Obviously, $D(H)\subseteq D(G_\varepsilon)$, as $D(G_\varepsilon)=L_2(\mathbb{R})$. We note that G_ε' and G_ε'' are uniformly bounded functions in $x\in\mathbb{R}$. Indeed,

$$G_\varepsilon'(x)=\frac{1}{(1+\varepsilon x^2)^{3/2}},$$

hence by substituting $t:=\sqrt{\varepsilon}x$, we have $G_\varepsilon'(x)=h(\sqrt{\varepsilon}x)$ with $h(t)=(1+t^2)^{-3/2}$. Thus, G_ε' is uniformly bounded by $|G_\varepsilon'(x)|\le 1$ for all $x\in\mathbb{R}$. For the second derivative we have

$$G_\varepsilon''(x)=-3\frac{\varepsilon x}{(1+\varepsilon x^2)^{5/2}}=\sqrt{\varepsilon}\tilde{h}(\sqrt{\varepsilon}x),$$

where $\tilde{h}(t)=-3t(1+t^2)^{-5/2},\ t:=\sqrt{\varepsilon}x$. Therefore, also G_ε'' is uniformly bounded in x by $|G_\varepsilon''(x)|\le\sqrt{\varepsilon}c,\ c>0$. Hence, by the chain rule (which is valid for Sobolev functions as well), $(G_\varepsilon\psi)'=G_\varepsilon'\psi+\psi'G_\varepsilon\in L_2$. This implies $G_\varepsilon(D(H))\subset D(H)$.

Step two: As the function G_ε fullfills the domain conditions for fixed $\varepsilon>0$, we can apply inequality (1.18) to G_ε,

$$\sum_{\lambda_j\in J}(z-\lambda_j)^2\,\langle[G_\varepsilon,[H,G_\varepsilon]]\phi_j,\phi_j\rangle-2(z-\lambda_j)\,\langle[H,G_\varepsilon]\phi_j,[H,G_\varepsilon]\phi_j\rangle\le 0. \tag{1.22}$$

It remains to show that the left-hand side tends for $\varepsilon\to 0$ to the desired inequality (1.19).

Step three: The first commutator is given by $[H,G_\varepsilon]=-2\alpha G_\varepsilon' d/dx-\alpha G_\varepsilon''$ and the second one by $[[H,G_\varepsilon],G_\varepsilon]=2\alpha(G_\varepsilon')^2$. Without loss of generality, we set $\alpha=1$. Then, for every

$\psi \in H^1(\mathbb{R})$,

$$\|[H, G_\varepsilon]\psi\|^2 = 4\|G'_\varepsilon \psi'\|^2 + \|G''_\varepsilon \psi\|^2 + 4\,\mathrm{Re}\left\langle G'_\varepsilon \psi', G''_\varepsilon \psi \right\rangle,$$

and for every $\psi \in L_2(\mathbb{R})$,

$$\langle [[H, G_\varepsilon], G_\varepsilon]\psi, \psi\rangle = 2\left\langle (G'_\varepsilon)^2 \psi, \psi \right\rangle.$$

Remember, that $G'_\varepsilon(x)$ is uniformly bounded and further $\lim_{\varepsilon\to 0} G'_\varepsilon = 1$ for all $x \in \mathbb{R}$. Hence, it follows by the dominated convergence that

$$\lim_{\varepsilon\to 0} \|G'_\varepsilon \psi'\|^2 = \|\psi'\|^2, \quad \lim_{\varepsilon\to 0} \left\langle (G'_\varepsilon)^2 \psi, \psi \right\rangle = \|\psi\|^2. \tag{1.23}$$

Similarly, it follows that

$$\lim_{\varepsilon\to 0} \|G''_\varepsilon \psi\|^2 = 0, \tag{1.24}$$

as G''_ε is uniformly bounded and $\lim_{\varepsilon\to 0} G''_\varepsilon = 0$ for all $x \in \mathbb{R}$. With (1.23) and (1.24) it follows by the Cauchy-Schwarz inequality that

$$\lim_{\varepsilon\to 0} \mathrm{Re}\left\langle G'_\varepsilon \psi', G''_\varepsilon \psi \right\rangle = 0. \tag{1.25}$$

Step four: Passing to the limit $\varepsilon \to 0$ in (1.22), we obtain in view of (1.23), (1.24) and (1.25) that the desired inequality

$$\sum_{\lambda_j \in J} (-\lambda_j)^2 2\|\phi_j\|^2 - 2(-\lambda_j)4\|\phi'_j\|^2 \le 0 \tag{1.26}$$

holds.

Next, let us check the domain condition by using only the form domain of H. That is, we assume that $d(H) = H^1(\mathbb{R})$. This is known to hold under rather weak conditions on V (e.g. $V \in L_p(\mathbb{R})$ for some $p \ge 1$). By the definition of H via its quadratic form we have

$$D(H) = \{\psi \in H^1(\mathbb{R}) : \ \exists f \in L_2(\mathbb{R})\ \forall \varphi \in H^1(\mathbb{R}) : \quad h[\varphi, \psi] = (\varphi, f)\}. \tag{1.27}$$

We also recall that for $\psi \in D(H)$ the f is unique and given by $f = H\psi$. To show that $G_\varepsilon(D(H)) \subseteq D(H)$, we set $\tilde{f} = G_\varepsilon f - 2G'_\varepsilon \psi' - G''_\varepsilon \psi \in L_2(\mathbb{R})$ and show that then $h[\varphi, G_\varepsilon \psi] = (\varphi, \tilde{f})$ holds for all $\varphi \in H^1(\mathbb{R})$. This will then imply that $G_\varepsilon \psi \in D(H)$ and $HG_\varepsilon \psi = \tilde{f}$. The identity $h[\varphi, G_\varepsilon \psi] = (\varphi, \tilde{f})$ is equivalent to

$$\int_{\mathbb{R}} \left(\overline{\varphi'}(G'_\varepsilon \psi + G_\varepsilon \psi') + V\overline{\varphi} G_\varepsilon \psi\right) dx = \int_{\mathbb{R}} \overline{\varphi}(G_\varepsilon f - 2G'_\varepsilon \psi' - G''_\varepsilon \psi)\, dx \tag{1.28}$$

Replacing $\overline{\varphi'} G_\varepsilon$ by $\overline{(G_\varepsilon \varphi)'} - G_\varepsilon \overline{\varphi}$, (1.28) is equivalent to

$$\int_{\mathbb{R}} \left(\overline{(G_\varepsilon \varphi)'}\psi' + V\overline{\varphi G_\varepsilon}\psi\right) dx + \int_{\mathbb{R}} \left(\overline{\varphi'} G'_\varepsilon \psi - G'_\varepsilon \overline{\varphi}\psi'\right) dx = \int_{\mathbb{R}} \overline{\varphi}(G_\varepsilon f - 2G'_\varepsilon \psi' - G''_\varepsilon \psi)\, dx.$$

It follows from (1.27) with $G_\varepsilon \varphi \in H^1(\mathbb{R})$ in place of φ that

$$\int_{\mathbb{R}} \left(\overline{(G_\varepsilon \varphi)'}\psi' + V\overline{\varphi G_\varepsilon}\psi\right) dx = \int_{\mathbb{R}} \overline{\varphi} G_\varepsilon f\, dx.$$

Hence, it remains to show that the identity

$$\int_{\mathbb{R}} \overline{\varphi'} G'_\varepsilon \psi\, dx = -\int_{\mathbb{R}} \overline{\varphi} G'_\varepsilon \psi'\, dx - \int_{\mathbb{R}} \overline{\varphi} G''_\varepsilon \psi\, dx \tag{1.29}$$

holds for all $\varphi \in H^1(\mathbb{R})$. This follows simply by integrating the first integral in the right-hand side in (1.29) by parts. This concludes our rigorous justification of inequality (1.19).

Up to now we were concerned with the discrete spectrum of Schrödinger operators. In the following, we turn our attention to the one-dimensional scattering theory, which is closely related to the theory of the continuous spectrum of the Schrödinger operator.

1.5. **Scattering on the real line and trace formulas of Buslaev-Faddeev type.** In this section, we present some results from the one-dimensional scattering theory. Details can be found in many textbooks. Our presentation here follows [20, 98]. First, we recall some results on solutions of the differential equation

$$-u'' + V(x)u = zu, \quad z = \zeta^2, \tag{1.30}$$

where $\zeta \in \mathbb{C}$ and $x \in \mathbb{R}$. Throughout this section we assume that the function V satisfies the assumption

$$\int_{-\infty}^{\infty} |V(x)|\, dx < \infty. \tag{1.31}$$

Then, the Schrödinger equation (1.30) has for all $\zeta \neq 0$ from the closed upper half-plane a unique solution $\theta_1(x,\zeta)$ satisfying as $x \to +\infty$ the conditions

$$\theta_1(x,\zeta) = e^{i\zeta x}(1+o(1)), \quad \theta_1'(x,\zeta) = i\zeta e^{i\zeta x}(1+o(1)) \tag{1.32}$$

and a unique solution $\theta_2(x,\zeta)$ satisfying as $x \to -\infty$ the conditions

$$\theta_2(x,\zeta) = e^{-i\zeta x}(1+o(1)), \quad \theta_2'(x,\zeta) = -i\zeta e^{-i\zeta x}(1+o(1)). \tag{1.33}$$

The solutions $\theta_1(x,\zeta)$ and $\theta_2(x,\zeta)$ are called *Jost solutions* and are for any fixed $x \in \mathbb{R}$ analytic in ζ up to the real axis, with a possible exception of the point $\zeta = 0$. The Wronskian

$$w(\zeta) = w\{\theta_2(\cdot,\zeta), \theta_1(\cdot,\zeta)\} = \theta_2'(\cdot,\zeta)\theta_1(\cdot,\zeta) - \theta_1'(\cdot,\zeta)\theta_2(\cdot,\zeta) \tag{1.34}$$

is analytic in the upper half-plane and is continuous up to the real axis, with a possible exception of the point $\zeta = 0$. An important fact is that complex zeros of $w(\zeta)$ are simple and lie on the imaginary axis. Moreover, $w(\zeta) = 0$ if and only if ζ^2 is an eigenvalue of the Schrödinger operator $H = -d^2/dx^2 + V$ on $L_2(\mathbb{R})$.
For $k > 0$, the Jost solutions have the property

$$\theta_j(x,-k) = \overline{\theta_j(x,k)}, \quad j = 1, 2,$$

and the solutions $\theta_1(\cdot,k), \theta_1(\cdot,-k)$ and $\theta_2(\cdot,k), \theta_2(\cdot,-k)$ are linearly independent as can be seen by the Wronskians,

$$w\{\theta_1(\cdot,k), \theta_1(\cdot,-k)\} = 2ik, \quad w\{\theta_2(\cdot,k), \theta_2(\cdot,-k)\} = -2ik.$$

Thus for $k > 0$,

$$\theta_2(x,k) = (2ik)^{-1}\left(w_0(k)\theta_1(x,k) - w(k)\theta_1(x,-k)\right), \tag{1.35}$$

where $w_0(k) = w\{\theta_2(\cdot,k), \theta_1(\cdot,-k)\}$. Similarly,

$$\theta_1(x,k) = (2ik)^{-1}\left(\overline{w_0(k)}\theta_2(x,k) - w(k)\theta_2(x,-k)\right). \tag{1.36}$$

From these representations, the following important property follows,

$$|w(k)|^2 = 4k^2 + |w_0(k)|^2. \tag{1.37}$$

We introduce the *Jost function*

$$m(\zeta) := -(2i\zeta)^{-1} w(\zeta),$$

which is analytic for $\operatorname{Im}\zeta > 0$ and is continuous up to the boundary, except the point $\zeta = 0$. We normalize the functions θ_1 and θ_2 to obtain

$$\psi_1(x,k) = m(k)^{-1}\theta_1(x,k), \quad \psi_2(x,k) = m(k)^{-1}\theta_2(x,k). \tag{1.38}$$

In a sense that can be made precise, these functions can be interpreted as "continuum eigenfunctions" of H. Because of (1.35) and (1.36) it follows that

$$\begin{aligned} \psi_1(x,k) &= e^{ikx} + s_{21}(k)e^{-ikx} + o(1), \quad x \to -\infty, \\ \psi_1(x,k) &= s_{11}(k)e^{ikx} + o(1), \quad x \to \infty \end{aligned} \tag{1.39}$$

and

$$\begin{aligned} \psi_2(x,k) &= e^{-ikx} + s_{12}(k)e^{ikx} + o(1), \quad x \to \infty, \\ \psi_2(x,k) &= s_{22}(k)e^{-ikx} + o(1), \quad x \to -\infty, \end{aligned} \tag{1.40}$$

where

$$s_{11}(k) = s_{22}(k) = -2ikw(k)^{-1}, \quad s_{12}(k) = -w_0(k)w(k)^{-1}, \quad s_{21}(k) = -\overline{w_0(k)}w(k)^{-1}.$$

The coefficients $s_{ij}(k)$ are determined uniquely by asymptotics (1.39) and (1.40). The scattering matrix is defined as follows,

$$s(k) := \begin{pmatrix} s_{11}(k) & s_{12}(k) \\ s_{21}(k) & s_{22}(k) \end{pmatrix} = -w(k)^{-1}\begin{pmatrix} 2ik & w_0(k) \\ \overline{w_0(k)} & 2ik \end{pmatrix}.$$

It follows from (1.37) that the scattering matrix is unitary.

In quantum mechanics the asymptotic relations (1.39) and (1.40) are interpreted as follows. The solution $\psi_1(x,k)$ describes a particle with energy k^2 coming from $-\infty$ and interacting with the potential $V(x)$. After interaction the reflected part $s_{21}(k)e^{-ikx}$ goes back to $-\infty$ and the transmitted part $s_{11}(k)e^{ikx}$ goes to $+\infty$. Similarly, the solution $\psi_2(x,k)$ describes a particle coming from $+\infty$ and interacting with $V(x)$. The coefficients $s_{11}(k)$ and $s_{22}(k)$ are called *transmission coefficients*, whereas $s_{12}(k)$ and $s_{21}(k)$ are called *reflection coefficients* to the right and to the left. The values $|s_{ij}(k)|^2$ are interpreted as the probabilities of the corresponding processes and fullfill $|s_{1j}(k)|^2 + |s_{2j}(k)|^2 = 1$ for $j = 1, 2$.

Next, let us state some results concerning the low-energy asymptotics. Under the assumption

$$\int_{-\infty}^{\infty} (1+|x|)|V(x)|\,dx < \infty \tag{1.41}$$

the Jost solutions $\theta_j(x,\zeta)$ and the Jost function $w(\zeta)$ are continuous as $\zeta \to 0$. The real solutions $\theta_j(x) := \theta_j(x,0)$ satisfy the equation $-u'' + Vu = 0$ and $w(0) = \overline{w(0)} = w\{\theta_2,\theta_1\}$. For $x \to \infty$, we have the asymptotics

$$\theta_1(x) = 1 + o(1), \quad \theta'(x) = o(x^{-1}). \tag{1.42}$$

In the following, we have to distinguish the generic case $w(0) \neq 0$ from the case $w(0) = 0$. Under assumption (1.41) and $w(0) \neq 0$ the scattering matrix $S(\lambda)$ has for $\lambda \to 0$, the finite limit

$$S(0) = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}.$$

This shows that the transmission coefficients $s_{11}(k)$ and $s_{22}(k)$ are equal to zero which means that for low energies a quantum particle cannot pass through a potential barrier or well $V(x)$ in the generic case.

Definition 1.6. Assume that (1.41) holds. If $w(0) = 0$, then one says that the Schrödinger operator H has a zero-energy resonance.

This means that H has a zero-energy resonance if and only if the solutions θ_1 and θ_2 of the homogenous Schrödinger equation are proportional, i.e.

$$\theta_1(x) = \alpha\theta_2(x), \quad \alpha > 0.$$

Thus, in view of (1.42) this implies that equation (1.30) has a bounded solution (which is not necessarily in $L_2(\mathbb{R})$). In this case we have,

$$w(\zeta) = -i(\alpha + \alpha^{-1})\zeta + o(|\zeta|), \quad |\zeta| \to 0$$

and

$$w_0(k) = -i(\alpha + \alpha^{-1})k + o(k), \quad \to 0.$$

Further, the scattering matrix $S(\lambda)$ has a finite limit as $\lambda \to 0$ and

$$S(0) = (\alpha + \alpha^{-1})^{-1} \begin{pmatrix} 2 & \alpha^{-1} - \alpha \\ \alpha - \alpha^{-1} & 2 \end{pmatrix}.$$

Thus, there is a non-zero transmission probability in the limit $\lambda \to 0$.

Concerning the high-energy asymptotics, we note that under the assumption that $V \in C^\infty(\mathbb{R})$ and for all $j \in \mathbb{N}_0$

$$|V^{(j)}(x)| \leq c_j(1 + |x|)^{-\rho-j}, \quad \rho \in (1, 2], \tag{1.43}$$

the asymptotic expansion

$$\ln m(\zeta) = \sum_{n=1}^{\infty} l_n(2i\zeta)^{-n} \tag{1.44}$$

as $|\zeta| \to \infty$, $\operatorname{Im}\zeta \geq 0$, is true with real coefficients l_n. If $\zeta = k > 0$, we can write

$$m(k) = a(k)e^{i\eta(k)} \tag{1.45}$$

with $a(k) = |m(k)| \geq 1$, because of (1.37). Here, the scattering phase is a continuous function and is normalized by the condition $\eta(\infty) = 0$. Seperating (1.44) in its real part and imaginary part, we arrive at the asymptotic expansions as $k \to \infty$,

$$\ln a(k) = \sum_{n=1}^{\infty}(-1)^n l_{2n}(2k)^{-2n} \quad \text{and} \quad \eta(k) = \sum_{n=1}^{\infty}(-1)^{n+1} l_{2n+1}(2k)^{-2n-1}. \tag{1.46}$$

Further, for $k \to \infty$, the asymptotic behaviours

$$w_0(k) = O(k^{-\infty}), \quad a(k) = 1 + O(k^{-\infty}), \quad \ln a(k) = O(k^{-\infty}) \tag{1.47}$$

and

$$s(k) = m(k)^{-1}\mathbb{1} + O(k^{-\infty}), \quad k \to \infty \tag{1.48}$$

hold. Relation (1.48) shows that the reflection coefficients $s_{12}(k) = s_{21}(k) = O(k^{-\infty})$ as $k \to \infty$. This leads to the interpretation that for high energies a particle penetrates through a potential barrier with a probability of almost one.

The coefficients l_n in (1.44) can be determined recursively. The first ones are given by

$$l_1 = -\int_{-\infty}^{\infty} V(x)\,dx, \quad l_3 = \int_{-\infty}^{\infty} V^2(x)\,dx,$$
$$l_5 = -\int_{-\infty}^{\infty} \left(V'(x)^2 + 2V^3(x)\right)\,dx.$$

The fact that $l_n = 0$ for all even n follows from the asymptotic expansion (1.46) and the asymptotic behaviour of $\ln a(k)$ in (1.47).

Assume now that (1.31) is satisfied. In order to derive the perturbation determinant for the pair $H_0 = -d^2/dx^2,\ H = -d^2/dx^2 + V(x)$ in the space $L_2(\mathbb{R})$, one may first derive

$$\operatorname{Tr}\left(R_0(z) - R(z)\right) = \frac{\dot{m}(\zeta)}{2\zeta m(\zeta)}, \quad \zeta = z^{1/2},\ \operatorname{Im}\zeta > 0, \tag{1.49}$$

where the derivative with respect to ζ is denoted by a dot "$\cdot$". The condition (1.31) implies that $|V|^{1/2}(H_0 + \mathbb{1})^{-\alpha}$ is a Hilbert-Schmidt operator for $\alpha \geq 1/4$. Therefore, the operator $R_0(z) - R(z)$ is trace class and the modified perturbation determinant $D(z) = \det(\mathbb{1} + \operatorname{sgn} V|V|^{1/2}R_0(z)|V|^{1/2})$ is correctly defined. From the well-known relation

$$\operatorname{Tr}\left(R_0(z) - R(z)\right) = D^{-1}(z)D'(z), \quad z \in \rho(H), \tag{1.50}$$

see e.g. [97], it follows together with (1.49) that

$$D(z) = Cm(z^{1/2}).$$

As the perturbation determinant satisfies $D(z) \to 1$ as $|z| \to \infty$ (see e.g. [97]), and $m(\zeta) = 1 + o(1)$ as $|\zeta| \to \infty,\ \operatorname{Im}\zeta \geq 0$, it follows that $C = 1$. The identity between the trace of the resolvent difference and the logarithmic derivative of the Jost function $m(z^{1/2})$ establishes a connection between operator and spectral theory on one side and ODE on the other side. Finally, let us state some results from [97] about the spectral shift function ξ. Assume that (1.31) is satisfied. Then the spectral shift function satisfies the condition

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

and the trace formula

$$\operatorname{Tr}\left(f(H) - f(H_0)\right) = \int_{-\infty}^{\infty} \xi(\lambda) f'(\lambda)\,d\lambda$$

is true for all functions f with two locally bounded derivatives satisfying

$$f'(\lambda) = O(\lambda^{-1/2-\varepsilon}), \quad f''(\lambda) = O(\lambda^{-1-\varepsilon}), \quad \lambda \to \infty,$$

for some $\varepsilon > 0$. In particular, one can take $f(\lambda) = (\lambda - z)^{-1}$ such that the following representation is valid,

$$\operatorname{Tr}\left(R(z) - R_0(z)\right) = -\int_{-\infty}^{\infty} \xi(\lambda)(\lambda - z)^{-2}\,d\lambda. \tag{1.51}$$

This formula remains true if an arbitrary constant is added to the spectral shift function ξ. Furthermore, formula (1.51) leads together with (1.50) to the relation

$$\ln D(z) = \int_{-\infty}^{\infty} \xi(\lambda)(\lambda - z)^{-1}\,d\lambda,$$

which implies that

$$\xi(\lambda) = \pi^{-1} \lim_{\varepsilon \to 0+} \arg D(\lambda + i\varepsilon).$$

In abstract scattering theory, the last identity is known as Kreĭn's formula. In the context of Schrödinger operators, however, D is a *modified* perturbation determinant and therefore the verification of Kreĭn's formula requires additional arguments. Another important result is the Birman-Kreĭn formula, which relates the spectral shift function to the scattering matrix,

$$\det S(\lambda) = e^{-2i\pi\xi(\lambda)}.$$

For $\lambda > 0$ the spectral shift function ξ is related to the scattering phase η, defined in (1.45), by

$$\xi(\lambda) = \pi^{-1}\eta(\lambda^{1/2}).$$

For the one-dimensional Schrödinger operator the Birman-Kreĭn formula can be verified simply by a direct computation. Using (1.37),(1.45) and the definition of $m(\zeta)$, we derive

$$\det S(k) = s_{11}(k)s_{22}(k) - s_{12}(k)s_{21}(k) = -w(k)^{-2}(4k^2 + |w_0(k)|^2) = e^{-2i\eta(k)}.$$

As an application of the scattering theory, we present two types of trace identities, the Levinson formula and Buslaev-Faddeev formulas. Both of them relate the scattering data $\eta(k)$ and $a(k)$ to the discrete spectrum of the Schrödinger operator in $L_2(\mathbb{R})$. Assume that condition (1.41) is satisfied and that the Schrödinger operator in $L_2(\mathbb{R})$ has N negative eigenvalues. Then the Levinson formula states that

$$\eta(\infty) - \eta(0) = \pi(N - 1/2), \quad \text{if } w(0) \neq 0,$$

and

$$\eta(\infty) - \eta(0) = \pi N, \quad \text{if } w(0) = 0,$$

where $\eta(\infty) = 0$ in view of (1.45), (1.47) and $m(\zeta) = 1 + o(1)$ as $|\zeta| \to \infty$, $\operatorname{Im}\zeta \geq 1$. Finally, we formulate a series of higher order trace identities known as Buslaev-Faddeev formulas. Suppose that (1.41) and (1.43) are satisfied. Then for all $n \in \mathbb{N}$,

$$\sum_{j=1}^{N} |\lambda_j|^n + (-1)^n \pi^{-1} 2n \int_0^\infty \left(\eta(k) - \sum_{j=0}^{n-1} (-1)^{j+1} l_{2j+1} (2k)^{-2j-1} \right) k^{2n-1}\, dk = 0$$

and for all $n \in \mathbb{N}_0$,

$$\sum_{j=1}^{N} |\lambda_j|^{n+1/2} + (-1)^{n+1}\pi^{-1}(2n+1) \int_0^\infty \ln a(k) k^{2n}\, dk = (2n+1)2^{-2n-2} l_{2n+1}. \qquad (1.52)$$

The proof of the Levinson formula uses the argument principle applied to the function $m(\zeta)$ and an appropriate contour of integration. Buslaev-Faddeev trace identities are obtained by applying Cauchy's residue theorem to the function $m(\zeta)$. In both cases, the low- and high-energy asymptotics are important ingredients. Also the fact, that $m(\zeta) = 0$ if and only if ζ^2 is an eigenvalue of H, is essential.

Since $\ln a(k) \geq 0$ by (1.47), identities (1.52) imply spectral inequalities. For $n = 0$, we get a lower bound for $\sum_{j=1}^{N} |\lambda_j|^{1/2}$ which is also known as Schmincke's inequality,

$$-\frac{1}{4}\int_{-\infty}^{\infty} V(x)\,dx \le \sum_{j=1}^{N} |\lambda_j|^{1/2} \le \frac{1}{2}\int_{-\infty}^{\infty} V_-(x)\,dx. \tag{1.53}$$

Remarkably, there is a two-sided estimate for the eigenvalues with moments 1/2. The upper bound in (1.53) was proved in [53, 94]. We note, that the lower bound in (1.53) also implies that the Schrödinger operator H has at least one negative eigenvalue if $\int_{-\infty}^{\infty} V(x)\,dx < 0$. If $n = 1$, we obtain the following Lieb-Thirring inequality,

$$\sum_{j=1}^{N} |\lambda_j|^{3/2} \le \frac{3}{16}\int_{-\infty}^{\infty} V^2(x)\,dx.$$

The constant 3/16 is the same constant as appears in the semi-classical limit, which means that it is sharp. By the Aizenman-Lieb argument [1] this optimal Lieb-Thirring inequality at $\gamma = 3/2$ implies optimal Lieb-Thirring inequalities for Riesz means of orders $\gamma > 3/2$.

1.6. **Scattering on metric graphs.** The scattering problem for quantum graphs was studied in [25, 34, 35, 46]. Here, we give a brief overview of results obtained in [34].

Let Γ be a star shaped graph, which is a metric graph with a single vertex in which a finite number of $n \ge 2$ edges e_j are joined. We assume that every edge has infinite length and consider the scattering problem

$$-u'' + V(x)u = zu, \quad z = \zeta^2, \tag{1.54}$$

where $\zeta \in \mathbb{C}$ and $x \in \Gamma$. We call $\psi_i(x) = \{\psi_{i1}(x_1,\zeta), \ldots, \psi_{in}(x_n,\zeta)\}$, $1 \le i \le n$, a *scattering solution* of the problem (1.54) if $\psi_i(x)$ solves equation (1.54) with the Kirchhoff vertex condition (1.4), and has the following asymptotic behaviour,

$$\begin{aligned}
\psi_{ij}(x_j,\zeta) &= T_{ij}(\zeta)e^{i\zeta x_j} + o(1), \quad x_j \to \infty,\ i \ne j,\\
\psi_{ii}(x_i,\zeta) &= e^{-i\zeta x_i} + R_{ii}(\zeta)e^{i\zeta x_i} + o(1), \quad x_i \to \infty,\ 1 \le i \le n.
\end{aligned}$$

The coefficients $T_{ij}(\zeta)$ and $R_{ii}(\zeta)$ are called *transmission coefficients* and *reflection coefficients*, respectively. The *scattering matrix* $S(\zeta)$ is a matrix with the reflection coefficients as diagonal entries and the transmission coefficients as off-diagonal entries. To construct the scattering solutions of (1.54), the *Jost solutions* of (1.54) are introduced as solutions satisfying the integral equations

$$\theta_{1i}(x_i,\zeta) = e^{i\zeta x_i} - \int_{x_i}^{\infty} \zeta^{-1}\sin(\zeta(x_i - y_i))V_i(y_i)\theta_{1i}(y_i,\zeta)\,dy_i, \tag{1.55}$$

$$\theta_{2i}(x_i,\zeta) = e^{-i\zeta x_i} + \int_{0}^{x_i} \zeta^{-1}\sin(\zeta(x_i - y_i))V_i(y_i)\theta_{2i}(y_i,\zeta)\,dy_i. \tag{1.56}$$

These solutions are characterized by their asymptotics as $x_i \to \infty$,

$$\theta_{1i}(x_i,\zeta) = e^{i\zeta x_i} + o(1), \quad \theta_{2i}(x_i,\zeta) = a_{1i}(\zeta)e^{-i\zeta x_i} + b_{1i}(\zeta)e^{i\zeta x_i} + o(1), \tag{1.57}$$

where

$$a_{1i}(\zeta) = 1 - \frac{1}{2i\zeta}\int_0^{\infty} e^{i\zeta y_i}V_i(y_i)\theta_{2i}(y_i,\zeta)\,dy_i, \quad b_{1i}(\zeta) = \frac{1}{2i\zeta}\int_0^{\infty} e^{-i\zeta y_i}V_i(y_i)\theta_{2i}(y_i,\zeta)\,dy_i.$$

Note that the solutions $\theta_{1i}(x_i,\zeta), \theta_{2i}(x_i,\zeta),\ x_i \geq 0$, are identical with the Jost solutions which arise in the study of the scattering problem for the whole-line Schrödinger operator with potential V equal to zero for $x \leq 0$ and $V_i(x_i)$ for $x \geq 0$. Hence, they have the same properties as the whole-line Jost solutions for $x \geq 0$.

For $n = 3$, the scattering solution ψ_1 is determined as follows,

$$\begin{aligned}
\psi_{11}(x_1,\zeta) &= \overline{\theta_{11}(x_1,\zeta)} + R_{11}(\zeta)\theta_{11}(x_1,\zeta),\\
\psi_{12}(x_2,\zeta) &= T_{12}(\zeta)\theta_{12}(x_2,\zeta),\\
\psi_{13}(x_3,\zeta) &= T_{13}(\zeta)\theta_{13}(x_3,\zeta).
\end{aligned}$$

$\psi_1(x,\zeta)$ can be interpreted as a continuum eigenfunction of the operator H and is analytic in the upper half-plane $\operatorname{Im}\zeta > 0$, see [34] for details. Similarly, the scattering solutions for $2 \leq i \leq n$ can be constructed via Jost solutions. The resulting scattering coefficients are given by

$$\begin{aligned}
R_{ii}(\zeta) &= \frac{2i\zeta}{\theta_{1i}(0,\zeta)\theta_{1i}(0,\zeta)K(\zeta)} - \frac{1}{a_{1i}(\zeta)\theta_{1i}(0,\zeta)} + \frac{b_{1i}(\zeta)}{a_{1i}(\zeta)},\\
T_{ij}(\zeta) &= \frac{2i\zeta}{\theta_{1i}(0,\zeta)\theta_{1j}(0,\zeta)K(\zeta)}, \quad i \neq j,
\end{aligned} \tag{1.58}$$

where $1 \leq i,j \leq n$, and $K(\zeta) = \sum_{i=1}^{n} \theta'_{1i}(0,\zeta)/\theta_{1i}(0,\zeta)$. In this context we mention that the topic of inverse scattering on quantum graphs has attracted a lot of attention recently, see e.g. [34, 42, 45]. Thereby, the question is to reconstruct the potential from the spectral data or to reconstruct the graph from given eigenvalues.

As far as we know the spectral shift function, Levinson's formula and trace identities have not been studied on star-shaped quantum graphs. This will be the topic of the third article "The spectral shift function and Levinson's theorem for quantum star graphs" in this thesis.

2. Summary

In this section, we first give an overview of the articles

I. S. Demirel and E. M. Harrell, II, *On semiclassical and universal inequalities for eigenvalues of quantum graphs*, Reviews in Mathematical Physics **22** (2010) No. 3, 305-329.

II. S. Demirel and M. Usman, *Trace formulas for Schrödinger operators on the half-line*, Bulletin of Mathematical Sciences **1**, (2011) No. 2, Page 397-427.

III. S. Demirel, *The spectral shift function and Levinson's theorem for quantum star graphs*, Journal of Mathematical Physics, to appear.

Afterwards, we summarize further results on sum rules and on Lieb-Thirring inequalities for star shaped graphs.

2.1. Overview of paper I. On semiclassical and universal inequalities for eigenvalues of quantum graphs.

Inequalities for means, moments, and ratios of eigenvalues are rather well studied for Laplacians on domains and for Schrödinger operators. For quantum graphs however only little has been known so far. We study estimates for the discrete spectrum of quantum graphs with the method of sum rules. In particular, we derive upper bounds for the negative eigenvalues of quantum graphs such as Lieb-Thirring inequalities and universal inequalities of Payne-Pólya-Weinberger, and Yang types. We show that the sharp constants of these inequalities depend on the topology of the graph and give conditions under which the sharp constants are the same as for the classical inequalities in dimension one. We also provide some counterexamples where the classical form of the inequalities is false.

The first part of the article concerns Lieb-Thirring inequalities for quantum graphs. Let Γ be a given metric graph. We consider the Schrödinger operator

$$H(\alpha)\psi(x) = -\alpha\psi''(x) + V(x)\psi(x), \quad \alpha > 0,$$

on $L_2(\Gamma)$, where the exterior potential V is a real-valued function. With Kirchhoff vertex conditions and Dirichlet boundary conditions at the ends of exterior edges, the operator H is self-adjoint. Assume that V decays at infinity in some averaged sense, then the quantum graph H has continuous spectrum on the positive semi-axis and a discrete spectrum consisting of negative eigenvalues $E_j(\alpha)$.

As already mentioned in the introduction, Lieb-Thirring inequalities for metric trees were studied in [24, 31]. The result states that under some regularity conditions on the metric tree Γ and on the potential V, the following Lieb-Thirring inequality holds for all $\gamma \geq 1/2$ with a constant depending on γ,

$$\sum_j (-E_j)^\gamma \leq C_\gamma \int_\Gamma (V_-(x))^{\gamma+1/2}\, dx. \tag{2.1}$$

The essential question here is whether these inequalities hold with the same constants as in dimension one or whether the connectedness of the graph can change the state of affairs. So far, the question about the sharp constants in (2.1) was an open problem. Our first main result gives an answer to this question for all $\gamma \geq 2$.

Theorem 2.1. *Assume that $V \in L_{\gamma+1/2}(\Gamma)$. Then for any tree graph with a finite number of vertices and edges, the mapping*

$$\alpha \mapsto \alpha^{1/2} \sum_{E_j(\alpha)<0} (-E_j(\alpha))^\gamma$$

is nonincreasing for all $\alpha > 0$ and $\gamma \geq 2$. Consequently,

$$\alpha^{1/2} \sum_{E_j(\alpha)<0} (-E_j(\alpha))^\gamma \leq L^{cl}_{\gamma,1} \int_\Gamma (V_-(x))^{\gamma+1/2}\, dx$$

for all $\alpha > 0$ and $\gamma \geq 2$. Here, the semiclassical constant $L^{cl}_{\gamma,1}$ is the best posssible one.

Remark 2.2. Theorem 2.1 is first proved for the case $\gamma = 2$. Then, by a modification of the principle of Aizenman and Lieb, [1], Theorem 2.1 is also true for eigenvalue moments of order $\gamma \geq 2$. A proof of how to extend the monotonicity of the eigenvalue moments with respect to α from $\gamma = 2$ to higher orders $\gamma > 2$ is given in Section 4.3.

The proof of Theorem 2.1 uses Stubbe's monotonicity argument, [90], which is based on general trace identities for operators [49, 50] known as sum rules. Contrary to the proofs in [24, 31] we do not use variational arguments, but combinatorial ideas instead. This allows us to obtain sharp results.

We give some further examples of metric graphs for which the analog of Theorem 2.1 is true.

We also provide a modified Lieb-Thirring inequality for a one-loop graph Γ consisting of a circle of length $2L$ to which two leaves are attached as in the following figure.

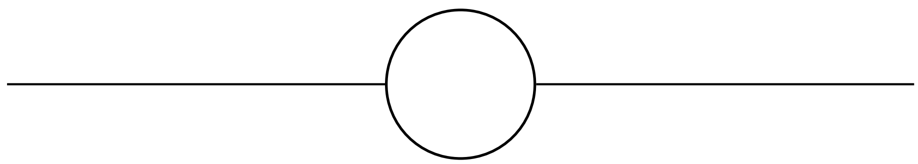

FIGURE 5. one-loop graph Γ

Theorem 2.3. *Let $q := 2\pi/L$. For all $\alpha > 0$ and $\gamma \geq 2$ the mapping*

$$\alpha \mapsto \alpha^{1/2} \sum_{E_j(\alpha)<0} \left(z - \frac{3}{16}\alpha q^2 - E_j\right)_+^{\gamma}$$

is nonincreasing. Furthermore, for all $z \in \mathbb{R}$, all $\alpha > 0$ and $\gamma \geq 2$ the following sharp Lieb-Thirring inequality holds:

$$\sum_{E_j(\alpha)<z} (z - E_j(\alpha))_+^{\gamma} \leq \alpha^{-1/2} L_{\gamma,1}^{cl} \int_\Gamma \left(V(x) - \left(z + \frac{3}{16} q^2 \alpha\right)\right)_-^{\gamma+1/2} dx.$$

We conlude the first part by identifying conditions under which the sharp constants are the same as for the classical inequalities.

The second part of the article deals with universal inqualities for quantum graphs. For bounded domains in $\mathbb{R}^d$ it is known that the means of the first n eigenvalues of the Dirirchlet Laplacian are bounded from below by the Berezin-Li-Yau inequality in terms of the volume of the domain. Furthermore, there is a large family of universal bounds on the spectrum, dating from the work of Payne, Pólya, and Weinberger [81], which give bounds on the spectrum without any reference to properties of the domain, [4].

In dimension one these questions are trivial. But the spectrum of a quantum graph responds, even in the absence of a potential, in complex ways to its connectedness. If the total length is finite and appropriate boundary conditions are imposed at exterior vertices, then the spectrum is positive and discrete $\{E_j\}_{j=1}^{\infty}$, and questions about counting functions, moments, etc. and their relation to the topology of the graph become interesting

It turns out that there are far-reaching analogies between these "universal" inequalities for Dirichlet Laplacians and Lieb-Thirring inequalities, which have led to common proofs based on sum rules. We show that the classic Payne, Pólya, and Weinberger and related inequalities can be proved for the case of trees using the method of sum rules.

First, we derive Weyl-type bounds on the averages of the eigenvalues of the Dirichlet Laplacian in $L_2(\Gamma)$. We use the following notation for the *Riesz mean of order ρ*,

$$R_\rho(z) := \sum_j (z - E_j)_+^{\rho}, \quad \rho > 0, \; z \in \mathbb{R}.$$

Theorem 2.4. *Let $|\Gamma|$ be the total length of a metric tree Γ. Then, for $z \geq 5E_1$,*

$$16E_1^{-1/2}\left(\frac{z}{5}\right)^{5/2} \leq R_2(z) \leq L^{cl}_{2,1}|\Gamma| z^{5/2}.$$

Similar estimates, related to higher eigenvalues are obtained in the following

Corollary 2.5. *Let the means of eigenvalues E_ℓ be denoted by $\overline{E}_j := \dfrac{1}{j}\sum_{\ell\leq j} E_\ell$ and suppose that $z \geq 5\overline{E_j}$. Then*

$$R_2(z) \geq \frac{16jz^{5/2}}{25(5\overline{E_j})^{1/2}}$$

and, therefore,

$$R_1(z) \geq \frac{4jz^{3/2}}{5(5\overline{E_j})^{1/2}}.$$

Using the Legendre transform one can convert bounds on $R_\rho(z)$ into bounds on the spectrum. This leads to the following result.

Corollary 2.6. *For $k \geq \frac{6}{5}j$, the means of the eigenvalues of the Dirichlet Laplacian on an arbitrary metric tree with finitely many edges and vertices satisfy a universal Weyl-type bound,*

$$\frac{\overline{E_k}}{\overline{E_j}} \leq \frac{125}{108}\left(\frac{k}{j}\right)^2.$$

2.2. **Overview of paper II. Trace formulas for Schrödinger operators on the half-line.** In paper II we study the scattering problem for the Schrödinger equation on the half-line with the Robin boundary condition at the origin.

Let H be the self-adjoint operator on $L_2[0,\infty)$ defined by

$$H = H_0 + V(x), \quad H_0 = -\frac{d^2}{dx^2}, \quad u'(0) = \gamma u(0), \tag{2.0}$$

where $\gamma \in \mathbb{R}$. The potential V is real-valued and goes to zero at infinity (in some averaged sense). Then H has a continuous spectrum on the positive semiaxis and discrete negative spectrum, consisting of eigenvalues $\{\lambda_j\}$.

The Hamiltonian H describes a one-dimensional particle restricted to the positive semi-axis. 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.

The study of trace formulas for the negative eigenvalues of H is connected with the differential equation

$$-u'' + V(x)u = zu, \qquad z = \zeta^2, \tag{2.1}$$

where $\zeta \in \mathbb{C}$ and $x > 0$. Equation (2.1) has two particular solutions. The regular solution φ is characterized by the conditions

$$\varphi(0,\zeta) = 1, \quad \varphi'_x(0,\zeta) = \gamma, \tag{2.2}$$

and the Jost solution θ by the asymptotics $\theta(x,\zeta) \sim e^{i\zeta x}$ as $x \to \infty$. By $w(\zeta)$ we denote the Wronskian of the regular solution and the Jost solution, which turns ou to be $w(\zeta) = \gamma\theta(0,\zeta) - \theta'(0,\zeta)$. Our first main result gives an expression for the trace of the difference of the perturbed and unperturbed resolvent in terms of the Wronskian $w(\zeta)$. Let us denote the resolvents of the unperturbed and perturbed operators by $R_0(z) = (H_0 - z)^{-1}$ and $R(z) = (H - z)^{-1}$, respectively.

Theorem 2.7. *Assume that*

$$\int_0^\infty |V(x)|\, dx < \infty. \tag{2.3}$$

Then

$$\operatorname{Tr}(R_0(z) - R(z)) = \frac{1}{2\zeta}\left(\frac{\frac{d}{d\zeta}w(\zeta)}{w(\zeta)} + \frac{i}{\gamma - i\zeta}\right), \quad \zeta = z^{1/2},\ \operatorname{Im}\zeta > 0. \tag{2.4}$$

This result leads to a representation for the perturbation determinant and to infinitely many trace identities of Buslaev-Faddeev type. For example, the second one in this series states that

$$\sum_{j=1}^N |\lambda_j| - M_1(\gamma) - \frac{2}{\pi}\int_0^\infty \left(\eta(k) - \frac{1}{2k}\int_0^\infty V(x)\, dx\right) k\, dk = -\frac{1}{4}V(0), \tag{2.5}$$

where $M_1(\gamma) = \gamma^2$ if $\gamma < 0$, and $M_1(\gamma) = 0$ if $\gamma \geq 0$. Here $\eta(k)$ is the so-called limit phase and has scattering theoretical nature. This formula can be interpreted as follows. We recall that if $\gamma \geq 0$, then H_0 has purely absolutely continuous spectrum $[0, \infty)$. If $\gamma < 0$, then H_0 has the simple negative eigenvalue $-\gamma^2$ and purely absolutely continuous spectrum on $[0, \infty)$. Hence the first two terms on the left-hand side of (2.5), $\sum_{j=1}^N |\lambda_j| - M_1(\gamma)$, correspond to the shift of the discrete spectrum between H and H_0. Similarly, the last term on the left-hand side corresponds to the shift of the absolutely continuous spectrum. The trace formula (2.5) and its higher order analogs proved below relate this shift of the spectrum to the potential V.

In [15] trace formulas for the half-line Schrödinger operator are derived by the application of the inverse spectral Gelfand-Levitan theory. However, these trace formulas contain norming constants and additional integrals over potentials which are obtained by the removal of eigenvalues. The appearance of additional terms distinguishes their formulas from the trace formulas of Buslaev-Faddeev type.

Further, we study the modified perturbation determinant

$$D(z) := \det(\mathbb{1} + \sqrt{V} R_0(z)\sqrt{|V|}), \quad z \in \rho(H_0),$$

which is well-defined under assumption (2.3) . Here $\rho(H_0)$ denotes the resolvent set of the operator H_0 and $\sqrt{V} := \operatorname{sgn}(V)\sqrt{|V|}$. We prove that $D(z)$ is related to the Jost function by,

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

where $\operatorname{Im} z^{1/2} > 0$.

Finally, we prove the Levinson formula which can be perceived as a trace formula of order zero. It relates the number of negative eigenvalues of H to the phase shift η.

Theorem 2.8. *Suppose that $\int_0^\infty (1 + x)|V(x)|\, dx < \infty$ and let N be the number of negative eigenvalues of the operator H. Then, the following formulas hold.*

For $w(0) \neq 0$,

$$\eta(\infty) - \eta(0) = \begin{cases} \pi N & \text{if } \gamma > 0, \\ \pi(N - \frac{1}{2}) & \text{if } \gamma = 0, \\ \pi(N-1) & \text{if } \gamma < 0. \end{cases} \tag{2.6}$$

For $w(0) = 0$,

$$\eta(\infty) - \eta(0) = \begin{cases} \pi(N + \frac{1}{2}) & \text{if } \gamma > 0, \\ \pi N & \text{if } \gamma = 0, \\ \pi(N - \frac{1}{2}) & \text{if } \gamma < 0. \end{cases} \tag{2.7}$$

We note that η satisfies for $k \in \mathbb{R}$ the identity $\eta(k) = \operatorname{Im} \ln D(k)$ and therefore it follows from the asymptotics $\lim_{\operatorname{Im} z \to \infty} D(z) = 1$ that $\eta(\infty) = 0$.

2.3. **Overview of paper III. The spectral shift function and Levinson's theorem for quantum star graphs.** The results from the previous paper, obtained for the half-line Schrödinger operator, are generalized to star shaped metric graphs Γ with n half-lines $e_j = [0, \infty)$ joined at the origin. We consider the Schrödinger operator

$$H = H_0 + V, \quad H_0 = -\frac{d^2}{dx^2}$$

on $L_2(\Gamma)$ with Kirchhoff vertex condition and denote $V_j := V|_{e_j}$. Let $R(z)$ be the resolvent of the operator H. Similarly, $R_0(z)$ denotes the resolvent of the unperturbed operator H_0 on $L_2(\Gamma)$ with Kirchhoff vertex condition. Then, the analog of Theorem 2.7 is given by

Theorem 2.9. *Let* Γ *be a star shaped graph and assume that* $\int_{e_j} |V_j(x)|\, dx < \infty$ *is satisfied for* $1 \leq j \leq n$. *Then, for the Schrödinger operator on* $L_2(\Gamma)$ *with Kirchhoff vertex condition, the following trace formula holds,*

$$\operatorname{Tr}(R_0(z) - R(z)) = \frac{1}{2\zeta} \frac{d}{d\zeta} \ln \left(\frac{K(\zeta)}{\zeta} \prod_{j=1}^{n} w_j(\zeta) \right), \quad \zeta = z^{1/2}, \quad \operatorname{Im} \zeta > 0. \tag{2.8}$$

Here, $K(\zeta) = \sum_{j=1}^{n} \theta_j'(0,\zeta)/\theta_j(0,\zeta)$ *with* $\theta_j(x,\zeta)$ *denoting the Jost solution on* e_j, *and* $w_j(\zeta) = \theta_j(0,\zeta)$.

Remark 2.10. We note that identity (2.8) is equivalent to the identity

$$\operatorname{Tr}(R_0(z) - R(z)) = \frac{1}{2\zeta} \left(\sum_{j=1}^{n} \frac{\frac{d}{d\zeta} w_j(\zeta)}{w_j(\zeta)} + \frac{\frac{d}{d\zeta} K(\zeta)}{K(\zeta)} - \frac{1}{\zeta} \right).$$

This should be compared with the analog of (2.4) for the Dirichlet case which is a classical result [16, 57], see also [87, 98]. Namely, for the half-line Schrödinger operator H_D with Dirichlet boundary condition the following identity holds,

$$\operatorname{Tr}(R_{0,D}(z) - R_D(z)) = \frac{\frac{d}{d\zeta} w(\zeta)}{2\zeta w(\zeta)}.$$

Here, $w(\zeta) = \theta(0,\zeta)$ is the corresponding Jost function on the half-line.

We note that the right-hand side of (2.8) has appeared in [46] as a Jost function in a related context.

Formula (2.8) allows us again to derive the perturbation determinant $D(\zeta)$ and the spectral shift function $\xi(\lambda; H, H_0)$. Furthermore, we derive the Levinson formula for star shaped graphs Γ. We say that the operator H on $L_2(\Gamma)$ has a *resonance* at $\zeta = 0$ if the equation $-u'' + Vu = 0$ has a non-trivial bounded solution satisfying the continuity and Kirchhoff conditions. By definition, the multiplicity of the resonance is the dimension of the corresponding solution space.

Theorem 2.11. *Assume that $\int_{e_j}(1+x)|V_j(x)|\,dx < \infty$ is satisfied for all $1 \le j \le n$ and, if $\zeta = 0$ is a resonance of multiplicity one, assume that $\int_{e_j}(1+x^2)|V_j(x)|\,dx < \infty$ for all $1 \le j \le n$. Then,*

$$\lim_{\lambda\to 0+} \xi(\lambda) = -\left(N + \frac{m-1}{2}\right), \tag{2.9}$$

where N is the number of negative eigenvalues of H and where $m \ge 1$ is the multiplicity if $\zeta = 0$ is a resonance and $m = 0$ if $\zeta = 0$ is not a resonance.

Remark 2.12. We know that $\lim_{\lambda\to 0-}\xi(\lambda) = -N$, which is an easy consequence of the definition of the spectral shift function.

In [17] a Levinson typ formula was proved for discrete graphs with only one path going to infinity. Note that in our case of the quantum star graph we have n infinite edges, which makes the situation considerably more complicated. Indeed, it was mention at the end of [17] as an interesting question to extend the result to a graph with n semi-infinite paths attached.

2.4. **Further results.** Additionally to the articles I-III, this thesis contains further results on questions arising from these articles. The first paper gives rise to the question whether it is possible to apply the sum rule method to other operators than the Schrödinger operator. In this context we consider the operator with variable coefficients. Let us define

$$H(\alpha) = -\alpha\left(\frac{d}{dx}\rho(x)\frac{d}{dx}\right) + V(x), \quad \alpha > 0, \tag{2.10}$$

in $L_2(I)$, where $I \subset \mathbb{R}$ is an open interval. At its endpoints (if any) we impose Dirichlet boundary conditions. The function ρ is assumed to be positive in the interior of I. For simplicity we assume that the real-valued function V is bounded and of compact support in I. Then, for any $\alpha > 0$, $H(\alpha)$ has at most a finite number of negative eigenvalues $E_j(\alpha)$. With the method of sum rules we prove Lieb-Thirring type inequalities for H.

Theorem 2.13. *Let ρ be a C^2-function and $\rho > 0$ in the interior of I. Assume that $\rho^{3/4}(x)$ is convex. Then the mapping*

$$\alpha \mapsto \alpha^{1/2} \sum_{E_j(\alpha)<0} (E_j(\alpha))^2$$

is nonincreasing for all $\alpha > 0$. Consequently

$$\sum_{E_j(\alpha)<0} (E_j(\alpha))^2 \le \int_{\mathbb{R}}\int_{\mathbb{R}} (\rho(x)|\xi|^2 + V(x))_-^2 \,\frac{dx\,d\xi}{2\pi\sqrt{\alpha}} = \alpha^{-1/2} L^{cl}_{2,1} \int_{\mathbb{R}} \frac{V_-^{5/2}(x)}{\sqrt{\rho(x)}}\,dx$$

for all $\alpha > 0$.

Using a different method we also show that the Lieb-Thirring inequality holds with the semi-classical constant already for $\gamma \geq 3/2$ (but we do not consider semi-classical monotonicity).

The next question arising from the first and third paper concerns Lieb-Thirring inequalities for quantum graphs. Remember that the sharp Lieb-Thirring inequalities, obtained in the first paper with the method of sum rules, do hold for $\gamma \geq 2$. In the classical case of the full space $\mathbb{R}$ however it is known that Lieb-Thirring inequalities hold for moments $\gamma \geq 1/2$. In particular, these inequalities hold with the semiclassical (and thus sharp) constants $L^{cl}_{3/2,d}$, for all $d \geq 1$ [70, 72]. We recall that it was shown in [24] that Lieb-Thirring inequalities hold for Schrödinger operators on regular metric trees for any $\gamma \geq 1/2$. The sharp constants however have not been known so far and hence the question about the sharp constants for $1/2 \leq \gamma < 2$ is still an open problem. Therefore, it is natural to ask whether Lieb-Thirring inequalities with moments $\gamma \geq 1/2$ do hold for quantum graphs with the same sharp constants $L_{\gamma,1}$ as for the whole-line case. We emphasize that the failing of the sum-rule proof for moments $\gamma < 2$ is not an artifact of the method but due to the fact that the proof provides also monotonicity of the eigenvalue moments with respect to coupling constants. However, in general the monotonicity property is no longer true for $\gamma < 2$, [90]. Hence, we have to use different methods for the case $\gamma \geq 1/2$. For a star shaped graph Γ we study the Lieb-Thirring inequalities with moments $\gamma \geq 1/2$ by applying variational arguments and the method of symmetric decomposition of the corresponding Hilbert space $L_2(\Gamma)$. In summary, we prove the following

Theorem 2.14. *Assume that Γ is a star shaped graph with n edges joined at the origin and let H be the Schrödinger operator in $L_2(\Gamma)$ with potential $V \in L_{\gamma+1/2}(\Gamma)$ and Kirchhoff vertex condition. Assume that either*

(1) *n is even*
or
(2) *V is radially symmetric.*

Then for $\gamma \geq 1/2$,

$$\operatorname{Tr}\left(-d^2/dx^2 + V\right)_-^\gamma \leq L_{\gamma,1} \int_\Gamma (V_-(x))^{\gamma+1/2}\, dx,$$

where $L_{\gamma,1}$ is the best possible Lieb-Thirring constant for the whole-line Schrödinger operator. We note that $L_{\gamma,1} \leq 2L^{cl}_{\gamma,1}$ if $\gamma \geq 1/2$ and $L_{\gamma,1} = L^{cl}_{\gamma,1}$ if $\gamma \geq 3/2$.

Remark 2.15. The proof fails to give the semi-classical constant if the graph has an odd number of edges, but it gives very good and asymptotically optimal (as $n \to \infty$) constants, nonetheless. We prove that if n is odd and $V \in L_{\gamma+1/2}(\Gamma)$ is non-symmetric, then

$$\operatorname{Tr}\left(-d^2/dx^2 + V\right)_-^\gamma \leq \left(\frac{n+1}{n}\right) L_{\gamma,1} \int_\Gamma (V_-(x))^{\gamma+1/2}\, dx$$

for all $\gamma \geq 1/2$.

We think that it is an interesting open question whether the Lieb-Thirring inequality on a star-shaped graph with an odd number of edges holds with the whole-line constant.

3. On semiclassical and universal inequalities for eigenvalues of quantum graphs

Semra Demirel and Evans M. Harrell II

Abstract. We study the spectra of quantum graphs with the method of trace identities (sum rules), which are used to derive inequalities of Lieb-Thirring, Payne-Pólya-Weinberger, and Yang types, among others. We show that the sharp constants of these inequalities and even their forms depend on the topology of the graph. Conditions are identified under which the sharp constants are the same as for the classical inequalities; in particular, this is true in the case of trees. We also provide some counterexamples where the classical form of the inequalities is false.

3.1. **Introduction.** This article is focused on inequalities for the means, moments, and ratios of eigenvalues of quantum graphs. A quantum graph is a metric graph with one-dimensional Schrödinger operators acting on the edges and appropriate boundary conditions imposed at the vertices and at the finite external ends, if any. Here we shall define the Hamiltonian H on a quantum graph as the minimal (Friedrichs) self-adjoint extension of the quadratic form

$$\phi \in C_c^\infty \mapsto E(\phi) := \int_\Gamma |\phi'|^2 ds, \tag{3.1}$$

which leads to vanishing Dirichlet boundary conditions at the ends of exterior edges and to the conditions at each vertex v_k that ϕ is continuous and moreover

$$\sum_j \frac{\partial \phi}{\partial x_{kj}}(0^+) = 0, \tag{3.2}$$

where the sum runs over all edges emanating from v_k, and x_{kj} designates the distance from v_k along the j-th edge. (Edges connecting v_k to itself are accounted twice.) In the literature these vertex conditions are usually known as Kirchhoff or Neumann conditions. Other vertex conditions are possible, and are amenable to our methods with some complications, but they will not be considered in this article. For details about the definition of H we refer to [66].

Quantum mechanics on graphs has a long history in physics and physical chemistry [43,80], but recent progress in experimental solid state physics has renewed attention on them as idealized models for thin domains. While the problem of quantum systems in high dimensions has to be solved numerically, since quantum graphs are locally one dimensional their spectra can often be determined explicitly. A large literature on the subject has arisen, for which we refer to the bibliography given in [7, 27].

The subject of inequalities for means, moments, and ratios of eigenvalues is rather well developed for Laplacians on domains and for Schrödinger operators, and it is our aim to determine the extent to which analogous theorems apply to quantum graphs. For example, when there is a potential energy $V(x)$ in appropriate function spaces, Lieb-Thirring inequalities provide an upper bound for the moments of the negative eigenvalues $E_j(\alpha)$ of the Schrödinger operator $H(\alpha) = -\alpha\nabla^2 + V(x)$ in $L^2(\mathbb{R}^d)$, $\alpha > 0$, of the form

$$\alpha^{d/2} \sum_{E_j(\alpha)<0} (-E_j(\alpha))^\gamma \le L_{\gamma,d} \int_{\mathbb{R}^d} (V_-(x))^{\gamma+d/2}\, dx \tag{3.3}$$

for some constant $L_{\gamma,d} \ge L^{cl}_{\gamma,d}$, where $L^{cl}_{\gamma,d}$, known as the *classical constant*, is given by

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

It is known that (3.3) holds true for various ranges of $\gamma \ge 0$ depending on the dimension d; see [18, 52, 71, 72, 83, 94]. In particular, in [70] Laptev and Weidl proved that $L_{\gamma,d} = L^{cl}_{\gamma,d}$ for all $\gamma \ge 3/2$ and $d \ge 1$, and Stubbe [90] has recently given a new proof of sharp Lieb-Thirring inequalities for $\gamma \ge 2$ and $d \ge 1$ by showing monotonicity with respect to coupling constants. His proof is based on general trace identities for operators [49, 50] known as sum rules, which will again be used as the foundation of the present article.

When there is no potential energy but instead the Laplacian is given Dirichlet conditions on the boundary of a bounded domain, then the means of the first n eigenvalues are bounded from below by the Berezin-Li-Yau inequality in terms of the volume of the domain, and in addition there is a large family of universal bounds on the spectrum, dating from the work of Payne, Pólya, and Weinberger [81], which constrain the spectrum without any reference to properties of the domain. (For a review of the subject, see [4].) It turns out that there are far-reaching analogies between these "universal" inequalities for Dirichlet Laplacians and Lieb-Thirring inequalities, which have led to common proofs based on sum rules [47–51, 90]. More precisely, some sharp Lieb-Thirring inequalities and some universal inequalities of the PPW family can be viewed as corollaries of a "Yang-type" inequality like (3.11) below, which in turn follows from a sum rule identity.

In one dimension a domain is merely an interval and the spectrum of the Dirichlet Laplacian is a familiar elementary calculation, for which the question of universal bounds is trivial and uninteresting. A quantum graph, however, has a spectrum that responds in complex ways to its connectedness; if the total length is finite and appropriate boundary conditions are imposed at exterior vertices, then the spectrum is discrete, and questions about counting functions, moments, etc. and their relation to the topology of the graph become interesting, even in the absence of a potential energy. Below we shall prove several inequalities for the spectra of finite quantum graphs, with the aid of the same trace identities we use to derive Lieb-Thirring inequalities.

For Lieb-Thirring inequalities on quantum graphs the essential question is whether a form of (3.3) holds with the sharp constant for $d = 1$, or whether the connectedness of the graph can change the state of affairs. In [24] T. Ekholm, R. L. Frank and H. Kovařík proved Lieb-Thirring inequalities for Schrödinger operators on regular metric trees for any $\gamma \ge 1/2$, but without sharp constants. We shall show below that trees enjoy a Lieb-Thirring inequality with the sharp constant when $\gamma \ge 2$, but that this circumstance depends on the topology of the graph.

We begin with some simple explicit examples showing that neither the expected Lieb-Thirring inequality nor the analogous universal inequalities for finite quantum graphs without potential hold in complete generality. As it will be convenient to have a uniform way of describing examples, we shall let x_{ij} denote the distance from vertex v_i along the j-th edge Γ_j emanating from v_i. We note that every edge corresponds to two distinct coordinates

$x_{ij} = L - x_{i'j'}$ where L is the length of the edge, and that a homoclinic loop from a vertex v_i to itself is accounted as two edges.

For the operator $-\frac{d^2}{dx^2}$ on an interval, with vanishing Dirichlet boundary conditions, the universal inequality of Payne-Pólya-Weinberger reduces to $E_2/E_1 \leq 5$, and the Ashbaugh-Benguria theorem becomes $E_2/E_1 \leq 4$, both of which are trivial in one dimension. But for which quantum graphs do these classic inequalities continue to be valid? We shall show below that the classic PPW and related inequalities can be proved for the case of trees, with Dirichlet boundary conditions imposed at all external ends of edges, using the method of sum rules. The sum-rule proof does not work for every graph, however, so the question naturally arises whether the topology makes a real difference, or whether a better method of proof is required. The following examples show that the failure of the sum-rule proof in the case of multiply connected graphs is not an artifact of the method but due to a true topological effect.

We refer to graphs consisting of a circle attached to a single external edge as "simple balloon graphs." The external edge may either be infinite or of finite length with a vanishing boundary condition at its exterior end. Consider first the graph $\Gamma := \Gamma_1 \cup \Gamma_2$, which consists of a loop Γ_1 to which a finite external interval Γ_2 is attached at a vertex v_1. Without loss of generality we may fix the length of the loop as 2π, while the "string" will be of length L.

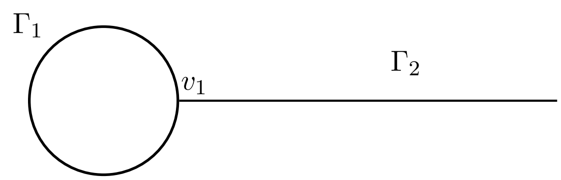

FIGURE 6. "balloon graph"

Example 3.1. (Violation of the analogue of PPW.) Let us begin with the case of a balloon graph with $L < \infty$, and assume that there is no potential. We set $\alpha = 1$. Thus H locally has the form $-\frac{d^2}{dx^2}$ with Dirichlet condition at the end of the string Γ_2 and vertex condition (3.2) at v_1 connecting it to the loop.

For convenience we slightly simplify the coordinate system, letting $x_s := x_{12}$ be the distance on $\Gamma_s := \Gamma_2$ from the node, and $x_\ell := x_{11} - \pi$ on Γ_1. Thus x_ℓ increases from $-\pi$ at v_1 to $x_2 = +\pi$ when it joins it again. It is possible to analyze the eigenvalues of the balloon graph quite explicitly: With a Dirichlet condition at $x_s = L$, any eigenfunction must be of the form $a \sin(k(L - x_s))$ on Γ_s. On Γ_1 symmetry dictates that the eigenfunction must be proportional to either $\sin kx_\ell$ or $\cos kx_\ell$. There are thus two categories of eigenfunctions and eigenvalues. Eigenfunctions of the form $\sin kx_\ell$ contribute nothing to the vertex condition (3.2) (because the outward derivatives at the node are equal in magnitude with opposite signs), and therefore the derivative of $a \sin(k(L - x_s))$ must vanish at $x_s = 0$. If k is a positive integer, then k^2 is an eigenvalue corresponding to an eigenfunction that vanishes on Γ_s. Otherwise, the conditions on Γ_s cannot be achieved without violating the condition of continuity with the eigenfunction on Γ_1. To summarize: the eigenvalues of the first category are the squares of positive integers.

The second category of eigenfunctions match $\cos kx_\ell$ on the loop to $a\sin(k(L-x_s))$ on the interval. The boundary conditions and continuity lead after a standard calculation to the transcendental equation

$$\cot kL = 2\tan k\pi. \tag{3.4}$$

There are three interesting situations to consider. In the limit $L \to 0$, an asymptotic analysis of (3.4) shows that the eigenvalues tend to $\{\left(\frac{n}{2}\right)^2\}$. In the limit $L \to \infty$, the lower eigenvalues tend to $\{\left(n+\frac{1}{2}\right)^2 \frac{\pi^2}{L^2}\}$, which are the eigenvalues of an interval of length L with Dirichlet conditions at L and Neumann conditions at 0. The ratio of the first two eigenvalues in this limit is approximately 9, which is already greater than the classically anticipated value of 5 or 4. The highest value of the ratio is, somewhat surprisingly, attained for an intermediate value of L, *viz.*, $L=\pi$, for which (3.4) can be easily solved, yielding $k = \pm\frac{1}{\pi}\arctan\frac{1}{\sqrt{2}} + j$ for a positive integer j. The corresponding fundamental ratio of the lowest two eigenvalues becomes

$$\frac{E_2}{E_1} = \left(\frac{\pi - \arctan\frac{1}{\sqrt{2}}}{\arctan\frac{1}{\sqrt{2}}}\right)^2 \doteq 16.8453.$$

(We spare the reader the direct calculation showing that the critical value of the ratio occurs precisely at $L=\pi$, establishing this value as the maximum among all simple balloons.)

Example 3.2. (Showing that E_2/E_1 can be arbitrarily large.) A modification of Example 1.1 with more complex topology shows that no upper bound on the ratio of the first two eigenvalues is possible for the graph analogue of the Dirichlet problem. We again set $\alpha = 1$ and assume $V=0$, and consider a "fancy balloon" graph consisting of an external edge, Γ_s, the "string," of length π joined at v_1 to N edges $\Gamma_m, m = 1\dots N$ of length π, all of which meet at a second vertex v_2. We observe that the eigenfunctions may be chosen either even or odd under pairwise permutation of the edges Γ_m. This is because if Pf represents the linear transformation of a function f defined on the graph by permuting two of the variables $\{x_{21}, \dots, x_{2N}\}$, and ϕ_j is an eigenfunction of the quantum graph with eigenvalue E_j, then so are $\phi_j \pm P\phi_j$. (In particular, continuity and (3.2) are preserved by these superpositions.) Moreover, the fundamental eigenfunction is even under any permutation, because it is unique and does not change sign.

By continuity and the conditions (3.2) at the vertices, as in Example 1.1, a straightforward exercise shows that $E_1 = \left(\frac{1}{\pi}\arctan(\frac{1}{\sqrt{N}})\right)^2$, and that there are other even-parity eigenvalues

$$\left(j \pm \frac{1}{\pi}\arctan\left(\frac{1}{\sqrt{N}}\right)\right)^2$$

for all positive integers j. Odd parity, when combined with continuity, forces the eigenfunctions to vanish at the nodes, and thus leads to eigenvalues of the form j^2, for positive integers j. The fundamental ratio E_2/E_1 for this example can be seen to be

$$\left(\frac{\pi - \arctan\left(\frac{1}{\sqrt{N}}\right)}{\arctan\left(\frac{1}{\sqrt{N}}\right)}\right)^2,$$

which is roughly $\pi^2 N$ for large N.

Remarks

1. With no external edges, the lowest eigenvalue of a quantum graph is $E_1 = 0$, so one might intuitively argue that for a graph with a large and complex interior part the effect of an exterior edge with a boundary condition is small. The theorems and examples given below, however, point towards a more nuanced intuition.

2. Another instructive example is the "bunch-of-balloons" graph, with many nonintersecting loops attached to the string at v_1. We leave the details to the interested reader.

Example 3.3. (Violation of classical Lieb-Thirring.) Next consider a balloon graph with $L = \infty$ and the Schrödinger operator $H(l) := -\frac{d^2}{dx^2} + V(x)$ on $L^2(\Gamma)$ with vertex conditions (3.2). Let the potential V be given by

$$V(x) := \begin{cases} V_1(x) := \dfrac{-2a^2}{\cosh^2(ax)} \ , & x_\ell \in \Gamma_1 = [-\pi, \pi] \\ \\ V_2(x) := 0 \ , & x_s \in \Gamma_2 = [0, \infty) \end{cases} .$$

Then the eigenfunction corresponding to the eigenvalue $-a^2$ is given by $C \cosh^{-1}(ax_\ell)$ on Γ_1 and by e^{-ax_s} on Γ_2. The continuity condition gives $C = \cosh(a\pi)$ and the condition (3.2) at v_1 leads to the equation

$$\tanh(a\pi) = \frac{1}{2}. \tag{3.5}$$

Denoting the ratio

$$\mathcal{Q}(\gamma, V) := \frac{|E_1|^\gamma}{\int\limits_\Gamma |V(x)|^{\gamma+1/2}\, dx},$$

we compute

$$\mathcal{Q}(3/2, V) = \frac{a^3}{2\int\limits_0^\pi \frac{4a^4}{\cosh^4(ax_\ell)}\, dx_\ell} = \left(8 \int\limits_0^{a\pi} \frac{1}{\cosh^4(y)}\, dy\right)^{-1} = \left(\frac{8}{3}\tanh(a\pi)(2 + \operatorname{sech}^2(a\pi))\right)^{-1}.$$

Because of (3.5), $\operatorname{sech}^2(a\pi) = 1 - \tanh^2(a\pi) = \frac{3}{4}$, and therefore

$$\mathcal{Q}(3/2, V) = \frac{3}{11} > \frac{3}{16} = L^{cl}_{3/2,1}. \tag{3.6}$$

Note that the ratio $\mathcal{Q}(3/2, V)$ is independent of the length of the loop, as expected because any length L can be achieved by a change of scale.
The ratio $\mathcal{Q}(\gamma, V)$ can also be calculated explicitly for the case $\gamma = 2$. In this case

$$\begin{aligned} \mathcal{Q}(2, V) &= \left[2^{7/2}\left(\frac{3}{4}\arctan(\tanh(a\pi/2)) + \frac{3}{16}\operatorname{sech}(a\pi) + \frac{1}{8}\operatorname{sech}^3(a\pi)\right)\right]^{-1} \\ &\doteq 0.2009 > L^{cl}_{2,1} = \frac{8}{15\pi} \doteq 0.1697. \end{aligned}$$

3.2. **Lieb-Thirring inequalities for quantum graphs.**

3.2.1. *Classical Lieb-Thirring inequality for metric trees.* Our point of departure is the family of sum-rule identities from [49, 50]. Let H and G be abstract self-adjoint operators satisfying certain mapping conditions. We suppose that H has nonempty discrete spectrum lying below the continuum, $\{E_j : \ H\phi_j = E_j\phi_j\}$. In the situations of interest in this article the spectrum will either be entirely discrete, in which case we focus on spectral subsets of the form $J := \{E_j, j = 1 \dots k\}$, or else, when there is a continuum, it will lie on the positive real axis and we shall take J as the negative part of the spectrum. Let P_A denote the spectral projector associated with H and a Borel set A.

Then, given a pair of self-adjoint operators H and G with domains $D(H)$ and $D(G)$, such that $G(\mathcal{J}) \subset D(H) \subset D(G)$, where $\mathcal{J}$ is the subspace spanned by the eigenfunctions ϕ_j corresponding to the eigenvalues E_j, it is shown in [49, 50] that:

$$\sum_{E_j \in J} (z - E_j)^2 \langle [G, [H, G]]\phi_j, \phi_j \rangle - 2(z - E_j) \langle [H, G]\phi_j, [H, G]\phi_j \rangle$$
$$= 2 \sum_{E_j \in J} \int_{\kappa \in J^c} (z - E_j)(z - \kappa)(\kappa - E_j)\, dG^2_{j\kappa}, \tag{3.7}$$

where $dG^2_{j\kappa} := | \langle G\phi_j, dP_\kappa G\phi_j \rangle |$ corresponds to the matrix elements of the operator G with respect to the spectral projections onto J and J^c. Because of our choice of J,

$$\sum_{E_j \in J} (z - E_j)^2 \langle [G, [H, G]]\phi_j, \phi_j \rangle - 2(z - E_j) \langle [H, G]\phi_j, [H, G]\phi_j \rangle \le 0. \tag{3.8}$$

In this section H is the Schrödinger operator on the graph Γ, namely

$$H(\alpha) = -\alpha \frac{d^2}{dx^2} + V(x) \text{ in } L^2(\Gamma),\ \alpha > 0,$$

with the usual conditions (3.2) at each vertex v_i. In particular, if any leaves (i.e. edges with one free end) are of finite length, vanishing Dirichlet boundary conditions are imposed at their ends. Without loss of generality we may assume that $V \in C_0^\infty$ for the operator $H(\alpha)$. Under this assumption, for any $\alpha > 0$, $H(\alpha)$ has at most a finite number of negative eigenvalues. We denote negative eigenvalues of $H(\alpha)$ by $E_j(\alpha)$ corresponding to the normalized eigenfunctions ϕ_j.

We shall be able to derive inequalities of the standard one-dimensional type when it is possible to choose G to be multiplication by the arclength along some distinguished subsets of the graph. This depends on the following:

Lemma 3.4. *Suppose that there exists a continuous, piecewise-linear function G on the graph Γ, such that at each vertex v_k*

$$\sum_j \frac{\partial G}{\partial x_{kj}}(0^+) = 0. \tag{3.9}$$

Suppose that $\Gamma = \cup_m \Gamma_m$ with $(G')^2 = a_m$ on Γ_m. If the spectrum has nonempty essential spectrum, assume that $z \le \inf \sigma_{\mathrm{ess}}(H)$. Then

$$\sum_{j,m} (z - E_j)_+^2 a_m \|\chi_{\Gamma_m} \phi_j\|^2 - 4\alpha(z - E_j)_+ a_m \|\chi_{\Gamma_m} \phi_j'\|^2 \le 0. \tag{3.10}$$

We observe that $\chi_{\Gamma_m} = 1 \Leftrightarrow a_m \neq 0$.

Proof. The formula (3.10) is a direct application of (3.8), when we note that locally, $[H, G] = -2G' \frac{d}{dx_{kj}} - G''$ and $[G, [H, G]] = 2(G')^2$. (A factor of 2α has been divided out.) The reason for the condition (3.9) is that $G\phi_j$ must be in the domain of definition of H, which requires that at each vertex,

$$0 = \sum_j \frac{\partial G\phi_j}{\partial x_{kj}}(0^+) = G \sum_j \frac{\partial \phi_j}{\partial x_{kj}}(0^+) + \phi_j \sum_j \frac{\partial G}{\partial x_{kj}}(0^+) = \phi_j \sum_j \frac{\partial G}{\partial x_{kj}}(0^+).$$

□

If we are so fortunate that $(G')^2$ is the same constant on every edge, then (3.10) reduces to the quadratic inequality

$$\sum_j (z - E_j)_+^2 - 4\alpha(z - E_j)_+ \|\phi_j'\|^2 \le 0, \tag{3.11}$$

familiar from [47–50, 90], where it was shown that it implies universal spectral bounds for Laplacians and Lieb-Thirring inequalities for Schrödinger operators in routine ways. Equation (3.11) can be considered as a Yang-type inequality, after [99].

Stubbe's monotonicity argument. In [90] Stubbe showed that some of the classical sharp Lieb-Thirring inequalities follow from the quadratic inequality (3.11). Here we apply the same argument to quantum graphs: For any $\alpha > 0$, the functions $E_j(\alpha)$ are non-positive, continuous and increasing. $E_j(\alpha)$ is continuously differentiable except at countably many values where $E_j(\alpha)$ fails to be isolated or enters the continuum. By the Feynman-Hellman theorem,

$$\frac{d}{d\alpha} E_j(\alpha) = \langle \phi_j, -\phi_j'' \rangle = \|\phi_j'\|^2.$$

Setting $z = 0$, (3.11) reads

$$\alpha \sum_{E_j(\alpha)<0} (-E_j(\alpha))^2 + 2\alpha^2 \frac{d}{d\alpha} \sum_{E_j(\alpha)<0} (-E_j(\alpha))^2 \le 0.$$

For any $\alpha \in]\alpha_{N+1}, \alpha_N[$ the number of eigenvalues is constant, and therefore

$$\frac{d}{d\alpha} \left(\alpha^{1/2} \sum_{E_j(\alpha)<0} (-E_j(\alpha))^2 \right) \le 0.$$

This means that $\alpha^{1/2} \sum_{E_j(\alpha)<0} (-E_j(\alpha))^2$ is monotone decreasing in α. Hence, by Weyl's asymptotics (see [10, 95]),

$$\alpha^{1/2} \sum_{E_j(\alpha)<0} (-E_j(\alpha))^2 \le \lim_{\alpha \to 0+} \alpha^{1/2} \sum_{E_j(\alpha)<0} (-E_j(\alpha))^2 = L_{2,1}^{cl} \int_\Gamma (V_-(x))^{2+1/2}\, dx.$$

Remark 3.5. Strictly speaking the Feynman-Hellman theorem only holds for nondegenerate eigenvalues. In the case of degenerate eigenvalues one has to take the right basis in the corresponding degeneracy space and to change the numbering if necessary, see e.g. [92].

The balloon counterexamples given above might lead one to think that the existence of cycles poses a barrier for a quantum graph to have an inequality of the form (3.11). Consider, however the following example.

Example 3.6. (Hash graphs.) Let Γ be a planar graph consisting of (or metrically isomorphic to) the union of a closed family of vertical lines and line segments $\mathfrak{F}_v$ and a closed family of horizontal lines and line segments $\mathfrak{F}_h$. We assume that for some $\delta > 0$ the distance between any two lines or line segments in $\mathfrak{F}_v$ is at least δ, and that the same is true of $\mathfrak{F}_h$. (The assumption on the spacing of the lines allows an unproblematic definition of the vertex conditions (3.2).) We impose Dirichlet boundary conditions at any ends of finite line segments. We also suppose a "crossing condition," that there are no vertices touching exactly three edges. (I.e., no line segment from $\mathfrak{F}_v$ has an end point in $\mathfrak{F}_h$ and *vice versa.*)
Regarding the graph as a subset of the xy-plane, we let $G(x, y) = x + y$. It is immediate from the crossing condition that G satisfies (3.9). Furthermore, the derivative of G along every edge is 1, and therefore the quadratic inequality (3.11) holds.

A quadratic inequality (3.11) can arise in a different way, if there is a family of piecewise affine functions G_ℓ each with a range of values $a_{\ell m}$, but such that $\sum_\ell a_{\ell m} = 1$ (or any other fixed positive constant). This occurs in our next example. Even when this is not possible, if we can arrange that $0 < a_{\min} \leq \sum_\ell a_{\ell m} \leq a_{\max}$, then the resulting weaker quadratic inequality

$$\sum_j (z - E_j)_+^2 - 4\alpha \frac{a_{\max}}{a_{\min}} (z - E_j)_+ \|\phi_j'\|^2 \leq 0, \tag{3.12}$$

will still lead to universal spectral bounds that may be useful. We speculate about this circumstance below.

Example 3.7. (Y-graph) As the next example we consider a simple graph, namely the Y-graph, which is a star-shaped graph with three positive halfaxes Γ_i, $i = 1, 2, 3$, joined at a single vertex v_1. If we set

$$G_1(x) := \begin{cases} g_1 := 0 \ , & x_{11} \in \Gamma_1 \\ g_2 := -x_{12} \ , & x_{12} \in \Gamma_2 \ , \\ g_3 := x_{13} \ , & x_{13} \in \Gamma_3 \end{cases}$$

then obviously $G(\mathcal{J}) \subset D(H_\Gamma(\alpha))$ holds, and with Lemma 3.4 we get

$$\sum_j (z - E_j)_+^2 \left(\|\chi_{\Gamma_2} \phi_j\|^2 + \|\chi_{\Gamma_3} \phi_j\|^2 \right) - 4\alpha (z - E_j)_+ \left(\|\chi_{\Gamma_2} \phi_j'\|^2 + \|\chi_{\Gamma_3} \phi_j'\|^2 \right) \leq 0. \tag{3.13}$$

As Γ_1 doesn't contribute to this inequality, we cyclically permute the zero part of G, i.e. we next choose $G_2(x)$, such that $g_2 = 0$, $g_1 = x_{11}$ and $g_3 = -x_{13}$, and finally $G_3(x)$, such that $g_3 = 0$, $g_1 = x_{11}$ and $g_2 = -x_{12}$. These give us two further inequalities analogous to (3.13). Summing all three inequalities, and noting that on every edge, $\sum_{\ell=1}^3 a_{\ell m} = 2$, we finally obtain

$$\sum_j 2(z - E_j)_+^2 - 8\alpha (z - E_j)_+ \|\phi_j'\|^2 \leq 0, \tag{3.14}$$

which when divided by 2 yields the quadratic inequality (3.11).

We next extend the averaging argument to prove (3.11) for arbitrary metric trees. A metric tree Γ consists of a set of vertices, a set of leaves and a set of edges, i.e., segments of the real axis, which connect the vertices, such that there is exactly one path connecting any two vertices. It is common in graph theory to distinguish between edges and leaves; a leaf is joined to a vertex at only one of its endpoints, ie. there is a free end, at which we shall set Dirichlet boundary conditions. (When the distinction is not material we shall refer to both edges and leaves as edges. It is also common to regard one free end as the distinguished "root" r of the tree, but for our purposes all free ends of the graph have the same status.) We denote the vertices by $v_i,\ i = 1, \dots, n$. The edges including leaves will be denoted by e. We shall explicitly write l_j for leaves when the distinction matters.

Theorem 3.8. *For any tree graph with a finite number of vertices and edges, the mapping*

$$\alpha \mapsto \alpha^{1/2} \sum_{E_j(\alpha)<0} (-E_j(\alpha))^2$$

is nonincreasing for all $\alpha > 0$. Consequently

$$\alpha^{1/2} \sum_{E_j(\alpha)<0} (-E_j(\alpha))^2 \le L^{cl}_{2,1} \int_\Gamma (V_-(x))^{2+1/2}\, dx$$

for all $\alpha > 0$.

Remark 3.9. By the monotonicity principle of Aizenman and Lieb (see [1]), Theorem 3.8 is also true with the sharp constant for higher moments of eigenvalues. Alternatively, the extension to higher values of γ can be obtained directly from the trace inequality of [51] for power functions with $\gamma > 2$. Furthermore, Theorem 3.8 can be extended by a density argument to potentials $V \in L^{\gamma+1/2}(\Gamma)$.

To prepare the proof of Theorem 3.8, we first formulate some auxiliary results.

Lemma 3.10. *For all $n \in \mathbb{N}$,*

$$\sum_{k=0}^{[\frac{n-1}{2}]} \binom{n-1}{2k} = \sum_{k=0}^{[\frac{n}{2}]-1} \binom{n-1}{2k+1}. \tag{3.15}$$

Proof. This is a simple computation. □

Definition 3.11. Let $\mathcal{E}$ be the set of all edges $e \subset \Gamma$. We call the mapping $\mathcal{C} : \mathcal{E} \to \{0, 1\}$ a *coloring* and say that $\mathcal{C}$ is an *admissible coloring* if at each vertex $v \in \Gamma$ the number

$$\#\{e :\ e \text{ emanates from } v :\ \mathcal{C}(e) = 1\}$$

is even. We let $\mathcal{A}(\Gamma)$ denote the set of all admissible colorings on Γ.

Theorem 3.12. *Let Γ_n be a metric tree with n vertices. For an edge $e \subset \Gamma_n$, we denote by*

$$a(e, n) := \#\{\mathcal{C}(\Gamma_n) \in \mathcal{A} :\ \mathcal{C}(e) = 1\}$$

the number of all admissible mappings $\mathcal{C} \in \mathcal{A}(\Gamma_n)$, such that $\mathcal{C}(e) = 1$ for $e \subset \Gamma_n$. Then

$$a(e, n) \text{ is independent of } e \subset \Gamma_n. \tag{3.16}$$

Proof. We shall prove (3.16) by induction over the number of vertices of Γ. The case with one vertex v_1 is trivial because of the symmetry of the graph. Given a metric tree Γ_n with n vertices, we can decompose it as follows. Γ_n consists of a metric tree Γ_{n-1} with $n-1$ vertices to which $m-1$ leaves $l_j,\ j=2,\dots,m$, are attached to the free end of a leaf $l_1 \subset \Gamma_{n-1}$. We call the vertex at which the leaves $l_j,\ j=1,\dots,m$, are joined v_n. Hence,

$$\Gamma_n := \Gamma_{n-1} \cup v_n \cup \bigcup_{j=2}^{m} l_j.$$

By the induction hypothesis,

$$a(e,n-1) := \#\{\mathcal{C} \in \mathcal{A}(\Gamma_{n-1}) :\ \mathcal{C}(e)=1\} \text{ is independent of } e \subset \Gamma_{n-1}. \tag{3.17}$$

Obviously for every edge or leaf $e \neq l_1$ in Γ_{n-1}, we have

$$a(e,n-1) = \#\{\mathcal{C} \in \mathcal{A}(\Gamma_{n-1}) :\ \mathcal{C}(e)=1 \wedge \mathcal{C}(l_1)=1\} + \#\{\mathcal{C} \in \mathcal{A}(\Gamma_{n-1}) :\ \mathcal{C}(e)=1 \wedge \mathcal{C}(l_1)=0\}. \tag{3.18}$$

Now, we have to show that $a(e,n)$ is independent of $e \subset \Gamma_n$. Note first that for each fixed leaf l_j of the subgraph $\Gamma^* = v_n \cup \bigcup_{j=1}^{m} l_j$, we have

$$\mu_1 := \#\{\mathcal{C} \in \mathcal{A}(\Gamma^*) :\ \mathcal{C}(l_j)=1,\ l_j \in \Gamma^*\} = \sum_{k=0}^{[\frac{m}{2}]-1} \binom{m-1}{2k+1} \tag{3.19}$$

and

$$\mu_0 := \#\{\mathcal{C} \in \mathcal{A}(\Gamma^*) :\ \mathcal{C}(l_j)=0,\ l_j \in \Gamma^*\} = \sum_{k=0}^{[\frac{m-1}{2}]} \binom{m-1}{2k}. \tag{3.20}$$

Hence, for arbitrary neighboring edges $e',\ e'' \subset \Gamma_{n-1}$ the following equality holds,

$$\begin{aligned} a(e',n) = \mu_1 \#\{\mathcal{C} \in \mathcal{A}(\Gamma_{n-1}) :\ \mathcal{C}(e')=1 \wedge \mathcal{C}(l_1)=1\} \\ + \mu_0 \#\{\mathcal{C} \in \mathcal{A}(\Gamma_{n-1}) :\ \mathcal{C}(e')=1 \wedge \mathcal{C}(l_1)=0\}, \end{aligned} \tag{3.21}$$

and respectively

$$\begin{aligned} a(e'',n) = \mu_1 \#\{\mathcal{C} \in \mathcal{A}(\Gamma_{n-1}) :\ \mathcal{C}(e'')=1 \wedge \mathcal{C}(l_1)=1\} \\ + \mu_0 \#\{\mathcal{C} \in \mathcal{A}(\Gamma_{n-1}) :\ \mathcal{C}(e'')=1 \wedge \mathcal{C}(l_1)=0\}. \end{aligned} \tag{3.22}$$

By Lemma 3.10, $\mu := \mu_0 = \mu_1$. Therefore, with (3.18) the equalities (3.21) and (3.22) read

$$a(e',n) = \mu a(e',n-1),$$
$$a(e'',n) = \mu a(e'',n-1).$$

Furthermore, by the induction hypothesis,

$$a(e',n-1) = a(e'',n-1),$$

from which it immediately follows that

$$a(e',n) = \mu a(e',n-1) = \mu a(e'',n-1) = a(e'',n).$$

This proves Theorem 3.12. □

Proof of Theorem 3.8. In order to apply Stubbe's monotonicity argument [90], we need to establish inequality (3.11) for metric trees. To do this, we proceed as for the example of the Y-graph. Let $\mathcal{J}$ denote the subspace spanned by the eigenfunctions ϕ_j on $L^2(\Gamma)$ corresponding to the eigenvalues E_j. Note first that there exist self-adjoint operators G, which are given by piecewise affine functions g_i on the edges (or leaves) of Γ, such that

$G(\mathcal{J}) \subset D(H(\alpha)) \subset D(G)$. Edges (or leaves) on which constant functions g_i are given, do not contribute to the sum rule. Therefore we average over a family of operators G, such that every edge e (or leaf) of the tree appears equally often in association with an affine function having $G' = \pm 1$ on e. We let $\mathcal{G}$ denote the set of continuous operators $G(x) = \{g_i(x) \text{ affine},\ x \in e_i\ (or\ l_i)\}$, which satisfy (3.2) at the vertices v of Γ. Indeed it is not necessary to average over all the operators $G \in \mathcal{G}$, because it makes no difference in Lemma 3.4, for instance, whether $g_i' = 1$ or $g_i' = -1$. Therefore we define an equivalence relation $\sim_G$ on $\mathcal{G}$ as follows: Let $\tilde{G} = \{\tilde{g}_i(x) \text{ affine},\ x \in e_i,\ (or\ l_i)\}$ be another operator in $\mathcal{G}$. We say that $G \sim \tilde{G} \Leftrightarrow \forall i \in \{1, \dots, n\} :\ |g_i'(x)| = |\tilde{g}_i'(x)|$. We define $\mathcal{G}^* := \mathcal{G}/\sim$. Then we can consider the isomorphism

$$\mathcal{I} : \mathcal{A}(\Gamma) \to \mathcal{G}^*, \tag{3.23}$$

where for each $\mathcal{C} \in \mathcal{A}(\Gamma)$ we choose an affine function $G_{\mathcal{C}} \in \mathcal{G}^*$ on Γ, such that $|G_{\mathcal{C}}'(e)| = \mathcal{C}(e)$ for every $e \subset \Gamma$. By Theorem 3.12, we know that $\#\{\mathcal{C} \in \mathcal{A}(\Gamma) :\ \mathcal{C}(e) = 1\}$ is independent of $e \subset \Gamma$. This means that summing up all inequalities corresponding to (3.10), which we get from each $G_{\mathcal{C}} \in \mathcal{G}^*$, leads to

$$\sum_j (z - E_j)_+^2 p - 4\alpha (z - E_j)_+ p \|\phi_j'\|^2 \le 0, \tag{3.24}$$

where $p := \sum_\ell a_{\ell m} = \#\{\mathcal{C} \in \mathcal{A}(\Gamma) :\ \mathcal{C}(e) = 1\}$ and we have used the normalization $\|\phi_j\| = 1$. Having the anologue of inequality (3.11) for metric trees, we can reformulate the monotonicity argument for our case. This proves Theorem 3.8. $\square$

Remark 3.13. The proof applies equally to metric trees with leaves of infinite lengths.

3.2.2. *Modified Lieb-Thirring inequalities for one-loop graphs.* In this section we consider the graph Γ consisting of a circle to which two leaves are attached. It is not hard to see that the construction leading to Lieb-Thirring inequalities with the sharp classical constant fails for one-loop graphs, because no family of auxiliary functions G_ℓ exists with the side condition that $\sum_\ell a_{\ell m} = 1$ throughout Γ. Unlike the case of the balloon graph, it is possible to replace the classical inequality with a weakened version (3.12) as mentioned above. There is, however another option, based on commutators with exponential functions, following an idea of [51]: As usual, we define the one-parameter familiy of Schrödinger operators

$$H(\alpha) = -\alpha \frac{d^2}{dx^2} + V(x),\ \alpha > 0,$$

in $L^2(\Gamma)$ with the usual conditions (3.2) at each vertex v_i of Γ. The leaves are denoted by $\Gamma_1 := [0, \infty)$ and $\Gamma_2 := [0, \infty)$, while we write Γ_3 and Γ_4 for the semicircles with lengths L. Let ϕ_j be the eigenfunctions of $H(\alpha)$ corresponding to the eigenvalues $E_j(\alpha)$.

Theorem 3.14. *Let $q := 2\pi/L$. For all $\alpha > 0$ the mapping*

$$\alpha \mapsto \alpha^{1/2} \sum_{E_j(\alpha) < 0} \left(z - \frac{3}{16}\alpha q^2 - E_j \right)_+^2 \tag{3.25}$$

is nonincreasing. Furthermore, for all $z \in \mathbb{R}$ and all $\alpha > 0$ the following sharp Lieb-Thirring inequality holds:

$$R_2(z, \alpha) \le \alpha^{-1/2} L_{2,1}^{cl} \int_\Gamma \left(V(x) - \left(z + \frac{3}{16} q^2 \alpha \right) \right)_-^{2+1/2} dx, \tag{3.26}$$

where

$$R_2(z,\alpha) := \sum_{E_j(\alpha)<z} (z - E_j(\alpha))_+^2 \,.$$

Remark 3.15. Once again, Theorem 3.14 can be extended to potentials $V \in L^{\gamma+1/2}(\Gamma)$ and is true for all $\gamma \geq 2$, either by the monotonicity principle of Aizenman and Lieb [1] or by the trace formula of [51] for $\gamma \geq 2$.

For the proof of Theorem 3.14, we make use of a theorem of Harrell and Stubbe:

Theorem 3.16 ([51, Theorem 2.1])**.** *Let H be a self-adjoint operator on $\mathcal{H}$, with a nonempty set J of finitely degenerate eigenvalues lying below the rest of the spectrum J^c and $\{\phi_j\}$ an orthonormal set of eigenfunctions of H. Let G be a linear operator with domain $\mathcal{D}_G$ and adjoint G^* defined on $\mathcal{D}_{G^*}$ such that $G(\mathcal{D}_H) \subseteq \mathcal{D}_H \subseteq \mathcal{D}_G$ and $G^*(\mathcal{D}_H) \subseteq \mathcal{D}_H \subseteq \mathcal{D}_{G^*}$, respectively. Then*

$$\begin{aligned} \frac{1}{2} \sum_{E_j \in J} (z - E_j)^2 \left(\langle [G^*, [H, G]]\phi_j, \phi_j \rangle + \langle [G, [H, G^*]]\phi_j, \phi_j \rangle \right) \\ \leq \sum_{E_j \in J} (z - E_j) \left(\|[H, G]\phi_j\|^2 + \|[H, G^*]\phi_j\|^2 \right). \end{aligned} \tag{3.27}$$

Remark 3.17. Strictly speaking, in [51] it was assumed that the spectrum was purely discrete. However, the extension to the case where continuous spectrum is allowed in J^c follows exactly as in Theorem 2.1 of [50].

Proof of Theorem 3.14. In this case it is not possible to get a quadratic inequality from Lemma 3.4 without worsening the constants. This follows from the fact that the conditions $\phi_3(0) = \phi_4(0)$ and $\phi_3(L) = \phi_4(L)$ imply that the piecewise linear function G has to be defined equally on Γ_3 and Γ_4. Consequently, the condition (3.2) can be satisfied only with different values of a_m as in (3.12), namely $a_1 = a_2 = 4a_3 = 4a_4$. Our proof of Theorem 3.14 consists of three steps. First we apply Lemma 3.4, after which we apply Theorem 3.16. Finally we combine both results and apply the line of argument given in [51].
First step: Using Lemma 3.4 with the choice,

$$G(x) := \begin{cases} g_1 := -2x_{11} \,, & x_{11} \in \Gamma_1 \\ g_2 := 2x_{22} + L \,, & x_{22} \in \Gamma_2 \\ g_3 := x_{13} \,, & x_{13} \in \Gamma_3 \\ g_4 := x_{14} \,, & x_{14} \in \Gamma_4 \end{cases},$$

we obtain

$$\begin{aligned} 4 \left(\sum_{E_j(\alpha)<0} (z - E_j(\alpha))_+^2 p_{12}(j) - 4\alpha \sum_{E_j(\alpha)<0} (z - E_j(\alpha))_+ p'_{12}(j) \right) \\ + \sum_{E_j(\alpha)<0} (z - E_j(\alpha))_+^2 p_{34}(j) - 4\alpha \sum_{E_j(\alpha)<0} (z - E_j(\alpha))_+ p'_{34}(j) \leq 0, \end{aligned} \tag{3.28}$$

where $p_{ik}(j) := \|\chi_{\Gamma_i}\phi_j\|^2 + \|\chi_{\Gamma_k}\phi_j\|^2$ and $p'_{ik}(j) := \|\chi_{\Gamma_i}\phi'_j\|^2 + \|\chi_{\Gamma_k}\phi'_j\|^2$.
Second step: Next, in Theorem 3.16 we set

$$G(x) := \begin{cases} g_1 := 1 \ , & x_{11} \in \Gamma_1 \\ g_2 := 1 \ , & x_{22} \in \Gamma_2 \\ g_3 := e^{-i2\pi x_{13}/L} \ , & x_{13} \in \Gamma_3 \\ g_4 := e^{i2\pi x_{14}/L} \ , & x_{14} \in \Gamma_4 \end{cases} .$$

It is easy to see that $G\phi_j \in D(H_\alpha)$. With $q := 2\pi/L$, the first commutators work out to be

$$[H_j, g_j] = 0, \ j = 1, 2,$$

$$[H_3, g_3] = e^{-iqx_{13}}\alpha\left(q^2 + 2iqd/dx\right), \quad [H_4, g_4] = e^{iqx_{14}}\alpha\left(q^2 - 2iqd/dx\right);$$

whereas for the second commutators,

$$\begin{aligned} &[g_j^*, [H_j, g_j]] = [g_j, [H_j, g_j^*]] = 0, \quad j = 1, 2, \\ &[g_j^*, [H_j, g_j]] = [g_j, [H_j, g_j^*]] = 2\alpha q^2, \quad j = 3, 4. \end{aligned} \tag{3.29}$$

From inequality (3.27), we get

$$\sum_{E_j(\alpha)\in J} (z - E_j(\alpha))^2 p_{34}(j) \le \alpha \sum_{E_j(\alpha)\in J} (z - E_j(\alpha)) \left(q^2 p_{34}(j) + 4p'_{34}(j)\right). \tag{3.30}$$

Third step: Adding (3.28) and (3.30) we finally obtain

$$2\left(R_2(z,\alpha) + 2\alpha\frac{d}{d\alpha}R_2(z,\alpha)\right) \le \alpha q^2 \frac{3}{2} \sum_{E_j\in J}(z - E_j)p_{34}(j), \tag{3.31}$$

or

$$2R_2(z,\alpha) + 4\alpha\frac{d}{d\alpha}R_2(z,\alpha) - \alpha q^2\frac{3}{2}R_1 \le 0, \tag{3.32}$$

which is equivalent to

$$\frac{\partial}{\partial\alpha}\left(\alpha^{1/2}R_2(z,\alpha)\right) \le \frac{3q^2}{8}\alpha^{1/2}R_1(z,\alpha). \tag{3.33}$$

Letting $U(z,\alpha) := \alpha^{1/2}R_2(z,\alpha)$, the inequality has the form

$$\frac{\partial U}{\partial\alpha} \le \frac{3}{16}q^2\frac{\partial U}{\partial z}. \tag{3.34}$$

Since the expression in (3.26) can be written as $U(z - \frac{3}{16}q^2\alpha, \alpha)$, an application of the chain rule shows that the monotonicity claimed in (3.26) follows from (3.34). (We note that (3.34) can be solved by changing to characteristic variables $\xi := \alpha - \frac{16z}{3q^2}$, $\eta := \alpha + \frac{16z}{3q^2}$, in terms of which

$$\frac{\partial U}{\partial\xi} \le 0. \tag{3.35}$$

I.e., U decreases as ξ increases while η is fixed.) By shifting the variable in (3.35), we also obtain

$$U(z,\alpha) \le U\left(z + \frac{3}{16}q^2(\alpha - \alpha_s), \alpha_s\right) \tag{3.36}$$

for $\alpha \geq \alpha_s$. By Weyl's asymptotics, for all $\gamma \geq 0$,

$$\lim_{\alpha \to 0+} \alpha^{d/2} \sum_{E_j(\alpha)<z} (z - E_j(\alpha))^\gamma = L^{cl}_{\gamma,d} \int_\Gamma (V(x) - z)_-^{\gamma+d/2}\, dx, \tag{3.37}$$

see [10, 95]. Hence, as $\alpha_s \to 0$, the right side of (3.36) tends to

$$L^{cl}_{2,1} \int_\Gamma \left(V(x) - \left(z + \frac{3}{16} q^2 \alpha \right) \right)_-^{2+1/2} dx,$$

so the conclusion of Theorem 3.14 follows. □

Remark 3.18. Theorem 3.14 can be generalized to one-loop graphs to which $2n$, $n \in \mathbb{N}$ equidistant semiaxis are attached.

To summarize, in this section we have seen that for some classes of quantum graphs a quadratic inequality (3.11) can be proved with the classical constants, and that for some other classes of graphs similar statements can be proved at the price of worse constants as in (3.12), or of a shift in the zero-point energy as in (3.26).

It is reasonable to ask whether one can look at the connectness of a graph and say whether a weak Yang-type inequality (3.12) can be proved. As we have seen, this is the case if there exists a family of continuous functions G_ℓ on the graph such that

- On each edge, all the derivatives $\{G'_\ell\}$ are constant.
- At each vertex v_k, each function G_ℓ satisfies

$$\sum_j \frac{dG_\ell}{dx_{kj}}(0^+) = 0.$$

- For each edge e there exists at least one function G_ℓ with $G'_\ell \neq 0$.

Interestingly, the question of the existence of such a family of functions can be rephrased in terms of the theory of electrical resistive circuits, a subject dating from the mid nineteenth century [60]. We first note that for a suitable family of functions to exist, there must be at least two leaves, which can be regarded as external leads of an electric circuit, bearing some resistance. (In the finite case let the resistance be equivalent to the length of the leaf, and in the infinite case let it be some fixed finite value, at least as large as the length of any finite leaf.) Each internal edge is regarded as a wire bearing a resistance equal to the length of the edge. If we regard the value of G'_ℓ as a current, then Kirchhoff's condition at the vertex of an electric circuit is exactly the condition (3.2) that $\sum_j \frac{dG_\ell}{dx_{kj}}(0^+) = 0$, and the condition that the electric potential G_ℓ must be uniquely defined at all vertices is equivalent to global continuity of G_ℓ. It has been known since Weyl [96] that the currents and potentials in an electric circuit are uniquely determined by the voltages applied at the leads. There are, however, circuits such that no matter what voltages are applied to the external leads, there will be an internal wire where no current flows; the most well-known of these is the Wheatstone bridge. (See, for instance, the Wikipedia article on the Wheatstone bridge.)

Let us call a metric graph *a generalized Wheatstone bridge* when the corresponding circuit has exactly two external leads and a configuration for which no current will flow in at least one of its wires. Then we conjecture that there are only two impediments to the existence of a suitable family of functions G_ℓ, and therefore to a weakened quadratic inequality (3.12), namely: Unless a quantum graph contains either

- a) a subgraph that can be disconnected from all leaves by the removal of one point (such as a balloon graph or a graph shaped like the letter α); or
- b) a subgraph that when disconnected from the graph by cutting two edges is a generalized Wheatstone bridge,

then an inequality of the form (3.12) holds. Otherwise the best that can be obtained may be a modified quadratic inequality with a variable shift, as in Theorem 3.14.

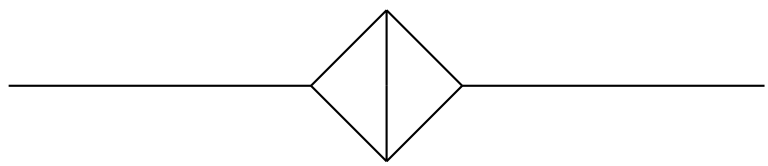

FIGURE 7. "Wheatstone bridge"

3.3. **Universal bounds for finite quantum graphs.** In this section we derive differential inequalities for Riesz means of eigenvalues of the Dirichlet Laplacian on bounded metric trees Γ with at least one leaf (free edge). From these inequalities we derive Weyl-type bounds on the averages of the eigenvalues of the Dirichlet Laplacian

$$H_D := \left(-\frac{d^2}{dx^2}\right)_D \text{ in } L^2(\Gamma),$$

with the conditions (3.2) at each vertex v_i. At the ends of the leaves, vanishing Dirichlet boundary conditions are imposed. We recall that with the methods of [47, 49] these are consequences of the same quadratic inequality (3.11) as was used above to prove Lieb-Thirring inequalities. When the total length of the graph is finite, the operator H_D on $D(H_D)$ has a positive discrete spectrum $\{E_j\}_{j=1}^{\infty}$, allowing us to define the *Riesz mean of order* ρ,

$$R_\rho(z) := \sum_j (z - E_j)_+^\rho \tag{3.38}$$

for $\rho > 0$ and real z.

Theorem 3.19. *Let Γ be a metric tree of finite length and with finitely many edges and vertices, and let H_D be the Dirichlet Laplacian in $L^2(\Gamma)$ with domain $D(H_D)$. Then for $z > 0$,*

$$R_1(z) \geq \frac{5}{4z} R_2(z); \tag{3.39}$$

$$R_2'(z) \geq \frac{5}{2z} R_2(z); \tag{3.40}$$

and consequently

$$\frac{R_2(z)}{z^{5/2}}$$

is a nondecreasing function of z.

Proof. The claims are vacuous for $z \le E_1$, so we henceforth assume $z > E_1$. The line of reasoning of the proof of Theorem 3.8 applies just as well to the operator H_D on $D(H_D)$, yielding

$$\sum_j (z - E_j)_+^2 - 4(z - E_j)_+ \|\phi_j'\|^2 \le 0. \tag{3.41}$$

Since $V \equiv 0$, $\|\phi_j'\|^2 = E_j$. Observing that

$$\sum_j (z - E_j)_+ E_j = zR_1(z) - R_2(z),$$

we get from (3.41)

$$5R_2(z) - 4zR_1(z) \le 0.$$

This proves (3.39). Inequality (3.40) follows from (3.39), as $R_2'(z) = 2R_1(z)$. ☐

Since by the Theorem 3.19, $R_2(z)z^{-5/2}$ is a nondecreasing function, we obtain a lower bound of the form $R_2(z) \ge Cz^{5/2}$ for all $z \ge z_0$ in terms of $R_2(z_0)$. Upper bounds can be obtained from the limiting behavior of $R_2(z)$ as $z \to \infty$, as given by the Weyl law. In the following, we want to follow [47] to derive Weyl-type bounds on the averages of the eigenvalues of H_D in $L^2(\Gamma)$.

Corollary 3.20. *For $z \ge 5E_1$,*

$$16E_1^{-1/2}\left(\frac{z}{5}\right)^{5/2} \le R_2(z) \le L_{2,1}^{cl}|\Gamma|z^{5/2},$$

where $L_{2,1}^{cl} := \dfrac{\Gamma(3)}{(4\pi)^{1/2}\Gamma(7/2)}$, and $|\Gamma|$ is the total length of the tree.

Proof. By Theorem 3.19, for all $z \ge z_0$,

$$\frac{R_2(z)}{z^{5/2}} \ge \frac{R_2(z_0)}{z_0^{5/2}}. \tag{3.42}$$

As $R_2(z_0) \ge (z_0 - E_1)_+^2$ for any $z_0 > E_1$, it follows from (3.42) that

$$R_2(z) \ge (z_0 - E_1)_+^2 \left(\frac{z}{z_0}\right)^{5/2}.$$

The coefficient $\dfrac{(z_0 - E_1)_+^2}{z_0^{5/2}}$ is maximized when $z_0 = 5E_1$. Thus we get

$$16E_1^{-1/2}\left(\frac{z}{5}\right)^{5/2} \le R_2(z).$$

For metric trees with total length $|\Gamma|$, the Weyl law states that

$$\lim_{n\to\infty} \frac{\sqrt{E_n}}{n} = \frac{\pi}{|\Gamma|}, \tag{3.43}$$

(see [67]). It follows that

$$\frac{R_2(z)}{z^{5/2}} \to L_{2,1}^{cl}|\Gamma|,$$

as $z \to \infty$. Since $\dfrac{R_2(z)}{z^{5/2}}$ is nondecreasing, we get

$$\frac{R_2(z)}{z^{5/2}} \leq L^{cl}_{2,1}|\Gamma|, \quad \forall z < \infty.$$

□

In summary, we get from Theorem 3.19 and Corollary 3.20 the following two-sided estimate:

$$4E_1^{-1/2}\left(\frac{z}{5}\right)^{3/2} \leq \frac{5}{4z}R_2(z) \leq R_1(z). \tag{3.44}$$

In order to obtain similar estimates, related to higher eigenvalues, we introduce the notation

$$\overline{E_j} := \frac{1}{j}\sum_{\ell \leq j} E_\ell$$

for the means of eigenvalues E_ℓ; similarly, the means of the squared eigenvalues are denoted

$$\overline{E_j^2} := \frac{1}{j}\sum_{\ell \leq j} E_\ell^2.$$

For a given z, we let $ind(z)$ be the greatest integer i such that $E_i \leq z$. Then obviously,

$$R_2(z) = ind(z)(z^2 - 2z\overline{E_{ind(z)}} + \overline{E^2_{ind(z)}}).$$

As for any integer j and all $z \geq E_j$, $ind(z) \geq j$, we get

$$R_2(z) \geq \mathcal{D}(z,j) := j(z^2 - 2z\overline{E_j} + \overline{E_j^2}).$$

Using Theorem 3.19 for $z \geq z_j \geq E_j$, it follows that

$$R_2(z) \geq \mathcal{D}(z_j, j)\left(\frac{z}{z_j}\right)^{5/2}. \tag{3.45}$$

Furthermore, $\overline{E_j}^2 \leq \overline{E_j^2}$ by the Cauchy-Schwarz inequality, and hence

$$\mathcal{D}(z,j) = j\left((z-\overline{E_j})^2 + \overline{E_j^2} - \overline{E_j}^2\right) \geq j(z-\overline{E_j})^2. \tag{3.46}$$

This establishes the following

Corollary 3.21. *Suppose that $z \geq 5\overline{E_j}$. Then*

$$R_2(z) \geq \frac{16jz^{5/2}}{25(5\overline{E_j})^{1/2}} \tag{3.47}$$

and, therefore,

$$R_1(z) \geq \frac{4jz^{3/2}}{5(5\overline{E_j})^{1/2}}. \tag{3.48}$$

Proof. Combining equations (3.45) and (3.46), we get

$$R_2(z) \geq j(z_j - \overline{E_j})^2\left(\frac{z}{z_j}\right)^{5/2}.$$

Inserting $z_j = 5\overline{E_j}$ the first statement follows. (This choice of z_j maximizes the constant appearing in (3.47).) The second statement results from substituting the first statement into (3.44). □

The Legendre transform is an effective tool for converting bounds on $R_\rho(z)$ into bounds on the spectrum, as has been realized previously, e.g., in [69]. Recall that if $f(z)$ is a convex function on $\mathbb{R}^+$ that is superlinear in z as $z \to +\infty$, its Legendre transform

$$\mathcal{L}[f](w) := \sup_z \{wz - f(z)\}$$

is likewise a superlinear convex function. Moreover, for each w, the supremum in this formula is attained at some finite value of z. We also note that if $f(z) \geq g(z)$ for all z, then $\mathcal{L}[g](w) \leq \mathcal{L}[f](w)$ for all w. The Legendre transform of the two sides of inequality (3.48) is a straightforward calculation (e.g., see [47]). The result is

$$(w - [w])E_{[w]+1} + [w]\overline{E_{[w]}} \leq \frac{w^3}{j^2}\frac{125}{108}\overline{E_j}, \tag{3.49}$$

for certain values of w and j. In Corollary 3.21 it is supposed that $z \geq 5\overline{E_j}$. Let $z_{\max}$ be the value for which $\mathcal{L}[f](w) = wz_{\max} - f(z_{\max})$, where f is the right side of (3.48). Then by an elementary calculation,

$$w = \frac{6j}{5}\left(\frac{z_{\max}}{5\overline{E_j}}\right)^{1/2}.$$

It follows that inequality (3.49) is valid for $w \geq 6j/5$. Meanwhile, for any w we can always find an integer k such that on the left side of (3.49), $k - 1 \leq w < k$. If $k > 6j/5$ and if we let approach k from below, we obtain from (3.49)

$$E_k + (k-1)\overline{E_{k-1}} \leq \frac{k^3}{j^2}\frac{125}{108}\overline{E_j}.$$

The left side of this equation is the sum of the eigenvalues E_1 through E_k, so we get the following:

Corollary 3.22. *For $k \geq \frac{6}{5}j$, the means of the eigenvalues of the Dirichlet Laplacian on an arbitrary metric tree with finitely many edges and vertices satisfy a universal Weyl-type bound,*

$$\frac{\overline{E_k}}{\overline{E_j}} \leq \frac{125}{108}\left(\frac{k}{j}\right)^2. \tag{3.50}$$

In [51] it was shown that a similar inequality with a different constant can be proved for all $k \geq j$ in the context of the Dirichlet Laplacian on Euclidian domains. The very same argument applies to quantum graphs with $V = 0$. With this assumption $\|\phi_j'\|^2 = E_j$, so with $\alpha = 1$ (3.11) can be rewritten as a quadratic inequality,

$$P_j(z) := \sum_{\ell=1}^{j}(z - E_\ell)(z - 5E_\ell) \leq 0 \tag{3.51}$$

for $z \in [E_j, E_{j+1}]$ (cf. [51], eq. (4.6)). From (3.39) and (3.42) for $z \geq z_0 \geq E_j$,

$$R_1(z) \geq \frac{5}{4z}R_2(z) \geq \frac{5}{4}z^{3/2}z_0^{-5/2}\sum_{\ell=1}^{j}(z_0 - E_j)^2. \tag{3.52}$$

The derivative of the right side of (3.52) with respect to z_0, by a calculation, is a negative quantity times $P_j(z_0)$, and therefore an optimal choice for the value of (3.52) is the root

$$z_0 = 3\overline{E_j} + \sqrt{D_j} \leq 5\overline{E_j}, \tag{3.53}$$

where D_j is the discriminant of P_j. The inequality in (3.53) results from the Cauchy-Schwarz inequality as in [49, 51]. Because $P_j(z_0) = 0$,

$$0 = \sum_{\ell=1}^{j} (z_0 - E_\ell)(z_0 - 5E_\ell) = 5 \sum_{\ell=1}^{j} (z_0 - E_\ell)^2 - 4z_0 \sum_{\ell=1}^{j} (z_0 - E_\ell),$$

so (3.52) reads

$$R_1(z) \geq \left(\frac{z}{z_0}\right)^{3/2} \sum_{\ell=1}^{j} (z_0 - E_\ell) = \left(\frac{z}{z_0}\right)^{3/2} j(z_0 - \overline{E_j}).$$

From the left side of (3.53), $z_0 - \overline{E_j} \geq \frac{2}{3} z_0$, so

$$R_1(z) \geq \left(\frac{2}{3} j z_0^{-1/2}\right) z^{3/2}. \tag{3.54}$$

The Legendre transform of (3.54) is

$$k\overline{E_k} \leq \frac{z_0}{3j^2} k^3, \tag{3.55}$$

and a calculation of the maximizing z in the Legendre transform of the right side of (3.54) shows that (3.55) is valid for all $k > j$. In particular, with the inequality on the right side of (3.53), we have established the following:

Corollary 3.23. *For $k \geq j$, the means of the eigenvalues of H_D in $L_2(\Gamma)$ satisfy*

$$\frac{\overline{E_k}}{\overline{E_j}} \leq \frac{5}{3} \left(\frac{k}{j}\right)^2. \tag{3.56}$$

Remark 3.24. Relaxing the assumption to $k \geq j$ comes at the price of making the constant on the right side larger. It would be possible to interpolate between (3.56) and (3.50) for $k \in [j, 6j/5]$ with a slightly better inequality.

Acknowledgments. The authors are grateful to several people for useful comments, including Rupert L. Frank, Lotfi Hermi, Thomas Morley, Joachim Stubbe, and Timo Weidl, and to Michael Music for calculations and insights generated by them. We also wish to express our appreciation to the Mathematisches Forschungsinstitut Oberwolfach for hosting a workshop in February, 2009, where this collaboration began, and to the Erwin Schrödinger Institut for hospitality.

4. Two remarks on sum rules

4.1. **A direct proof of the main inequality.** In the previous sections we have seen that inequality (3.8) is the starting point and key element for Stubbe's monotonicity argument. Remember that in the study of the discrete spectum of the Schrödinger operator this inequality follows from the sum rule (1.13). In this section we show that the main inequality (3.8) can also be obtained by a direct computation.

Theorem 4.1. *Let H and G be self-adjoint operators in the Hilbert space $\mathcal{H}$. We denote by D_H and D_G the domain of H and G respectively. Assume that $G(D_H) \subseteq D_H \subseteq D_G$ and that H has below a number z only finitely many negative eigenvalues $E_j < 0$, corresponding to the normalized eigenfunctions ϕ_j. Then, inequality* (3.8) *holds, that is,*

$$\sum_{E_j<0} (z-E_j)^2 \langle [G,[H,G]]\phi_j, \phi_j\rangle - 2(z-E_j)\langle [H,G]\phi_j, [H,G]\phi_j\rangle \leq 0. \tag{4.1}$$

Proof. Without loss of generality, we may assume that $z = 0$. In what follows, we use the notation $H = H_+ - H_-$, where H_- and H_+ denote respectively the negative part and the positive part of H. Thus, $H_-\phi_j = -E_j\phi_j$, where H_- has finite rank and hence is a trace class operator. We first note that $[H,G]^* = -[H,G]$ and therefore inequality (4.1) is equivalent to the following inequality

$$\operatorname{Tr}\left(H_-^2[G,[H,G]]\right) + 2\operatorname{Tr}(H_-[H,G]^2) \leq 0. \tag{4.2}$$

In what follows we compute the sum in the left-hand side of (4.2) with the help of spectral theoretic rules and show that this sum is less or equal to zero. Working out the commutators, we get

$$\begin{aligned} H_-^2[G,[H,G]] \quad &+ \quad 2H_-[H,G]^2 \\ &= \quad H_-^2GHG - H_-^2G^2H - H_-^2HG^2 + H_-^2GHG \\ &\quad\; +2\left(H_-HGHG - H_-HG^2H - H_-GH^2G + H_-GHGH\right). \end{aligned} \tag{4.3}$$

Using the relation $H_-H = HH_- = -H_-^2$ and the cyclic property of the trace, the trace of the right-hand side in equation (4.3) equals

$$\begin{aligned} &\operatorname{Tr}\left(2H_-^2GHG - H_-^2G^2H - H_-^2HG^2\right) \\ + \quad &2\operatorname{Tr}\left(-H_-^2GHG + H_-^2G^2H - H_-GH^2G - H_-^2GHG\right) \\ = \quad &\operatorname{Tr}(-2H_-^2GHG + H_-^2G^2H - H_-^2HG^2 - 2H_-GH^2G) \\ = \quad &\operatorname{Tr}\left(-2H_-^2GHG - 2H_-GH^2G\right). \end{aligned} \tag{4.4}$$

The last identity follows as both terms $\operatorname{Tr}(H_-^2G^2H)$ and $\operatorname{Tr}(H_-^2HG^2)$ are equal because of the cyclic property of the trace. Now, we replace H by $H_+ - H_-$. Then in view of $H_+H_- = H_-H_+ = 0$, (4.4) equals to

$$\begin{aligned} \operatorname{Tr}\left(-2H_-^2GH_+G + 2H_-^2GH_-G - 2H_-GH_+^2G - 2H_-GH_-^2G\right) \\ = -2\operatorname{Tr}\left(H_-^2GH_+G + H_-GH_+^2G\right). \end{aligned} \tag{4.5}$$

Recall that for operators A, B, C the identity $(ABC)^* = (BC)^*A^* = C^*B^*A^*$ is true and further $A^*A > 0$. Together with the self-adjointness of the operators $H_\pm$, $\sqrt{H_\pm}$, G, this implies that (4.5) equals

$$-2\,\mathrm{Tr}\left(H_-G\sqrt{H_+}\sqrt{H_+}GH_- + H_+G\sqrt{H_-}\sqrt{H_-}GH_+\right),$$

which is obviously non-positive.

□

4.2. **Application of the monotonicity argument to operators with variable coefficients.** Now, we apply the monotonicity argument to an operator with variable coefficients $\rho(x)$.

Consider the operator

$$H(\alpha) = -\alpha\left(\frac{d}{dx}\rho(x)\frac{d}{dx}\right) + V(x), \quad \alpha > 0, \tag{4.6}$$

in $L_2(I)$, where $I \subset \mathbb{R}$ is an open interval. We assume that $\rho > 0$ in the interior of I. For simplicity we restrict our attention to real-valued functions V which are bounded and have compact support in I. More precisely, $H(\alpha)$ is defined via the quadratic form

$$\int_I \left(\alpha\rho(x)|\phi'(x)|^2 + V(x)|\phi(x)|^2\right)\,dx \tag{4.7}$$

with form domain given by the closure of $C_0^\infty(I)$ with respect to $\int_I \rho(x)|\phi'(x)|^2\,dx$. Under the conditions below the operator $H(\alpha)$ has for any $\alpha > 0$ at most a finite number of negative eigenvalues. We denote negative eigenvalues of $H(\alpha)$ by $E_j(\alpha)$ corresponding to the normalized eigenfunctions ϕ_j.

Theorem 4.2. *Let ρ be a C^2-function and $\rho > 0$ in the interior of I. Assume that $\rho^{3/4}(x)$ is convex. Then the mapping*

$$\alpha \mapsto \alpha^{1/2}\sum_{E_j(\alpha)<0}(-E_j(\alpha))^\gamma$$

is nonincreasing for all $\alpha > 0$ and $\gamma \geq 2$. Consequently

$$\sum_{E_j(\alpha)<0}(-E_j(\alpha))^\gamma \leq \int\limits_{\mathbb{R}}\int\limits_{I}(\rho(x)|\xi|^2 + V(x))_-^\gamma\,\frac{dx\;d\xi}{2\pi\sqrt{\alpha}} = \alpha^{-1/2}L_{\gamma,1}^{cl}\int\limits_{I}\frac{V_-^{\gamma+1/2}(x)}{\sqrt{\rho(x)}}\,dx$$

for all $\alpha > 0$ and $\gamma \geq 2$.

Remark 4.3. Theorem 4.2 is first proved for the case $\gamma = 2$. Then, by a modification of the monotonicity principle of Aizenman and Lieb (see [1]), Theorem 4.2 is also true with the sharp constant for higher moments of eigenvalues, see section 4.3.

For the proof of Theorem 4.2, we will use the following

Lemma 4.4. *Let $\rho(x)$ be a C^2-function and $\rho > 0$ in the interior of I. Then the inequality*

$$\frac{1}{4}(\rho'(x))^2 - \rho(x)\rho''(x) \leq 0$$

is equivalent to the convexity of the function $\rho^{3/4}(x)$.

Proof. Let α be a positive number. Then the function $\rho^\alpha(x)$ is convex if and only if $(\rho^\alpha(x))'' \geq 0$ for all $x \in \mathbb{R}$. As $\alpha\rho^{\alpha-2}(x) \geq 0$, we see immediately from

$$(\rho^\alpha(x))'' = \alpha\rho^{\alpha-2}(x)\left((\alpha-1)(\rho'(x))^2 + \rho(x)\rho''(x)\right),$$

that the convexity of $\rho^\alpha(x)$ is equivalent to the inequality

$$(\alpha-1)(\rho'(x))^2 + \rho(x)\rho''(x) \geq 0.$$

Lemma 4.4 follows by setting $\alpha = 3/4$. □

Proof of Theorem 4.2. Let $H(\alpha)$ be the operator in (4.6) and G multiplication by a real-valued function G. Then the commutators are given by

$$[H,G]\phi = -\alpha(\rho'(x)G'\phi + \rho(x)G''\phi + 2\rho(x)G'\phi')$$

and

$$[G,[H,G]]\phi = 2\alpha\rho(x)(G')^2.$$

In inequality (3.8) we choose G to be the multiplication operator

$$G(x) = \int^x \frac{1}{\sqrt{\rho(y)}}\,dy.$$

Then,

$$G' = \frac{1}{\sqrt{\rho(x)}}, \quad G'' = -\frac{\rho'(x)}{2\rho^{3/2}(x)}.$$

Hence, the first commutator works out to be

$$[H,G] = -\alpha\left(\frac{1}{2}\frac{\rho'(x)}{\sqrt{\rho(x)}} + 2\sqrt{\rho(x)}d/dx\right);$$

whereas for the second commutator,

$$[G,[H,G]] = 2\alpha.$$

Next, we compute for any $\phi \in C_0^\infty$,

$$\langle [G,[H,G]]\phi_j, \phi_j\rangle = 2\alpha\|\phi_j\|^2$$

and

$$\langle [H,G]\phi_j, [H,G]\phi_j\rangle = \alpha^2\left(\|\frac{1}{2}\frac{\rho'(x)}{\sqrt{\rho(x)}}\phi_j\|^2 + \|2\sqrt{\rho(x)}\phi_j'\|^2 + 2\,\mathrm{Re}\int \rho'(x)\overline{\phi_j}\phi_j'\,dx\right).$$

We rewrite the last term in the right-hand side as

$$2\,\mathrm{Re}\int \rho'(x)\overline{\phi_j}\phi_j'\,dx = \int \rho'(x)(|\phi_j|^2)'\,dx = -\int \rho''(x)|\phi_j|^2\,dx$$

and note that

$$\|\frac{1}{2}\frac{\rho'(x)}{\sqrt{\rho(x)}}\phi_j\|^2 - \int \rho''(x)|\phi_j|^2\,dx = \left\langle \frac{\frac{1}{4}(\rho'(x))^2 - \rho(x)\rho''(x)}{\rho(x)}\phi_j, \phi_j\right\rangle.$$

This leads to the relation

$$\langle [H,G]\phi_j, [H,G]\phi_j\rangle \leq \alpha^2\|2\sqrt{\rho(x)}\phi_j'\|^2 \Leftrightarrow \frac{1}{4}(\rho'(x))^2 - \rho(x)\rho''(x) \leq 0,$$

which by Lemma 4.4 is equivalent to the condition that $\rho^{3/4}(x)$ is a convex function. So, for $\rho^{3/4}(x)$ convex, we have

$$\begin{aligned} \sum_{E_j(\alpha)<0} \quad & \alpha \quad |E_j(\alpha)|^2 - \alpha^2 |E_j(\alpha)| \|2\sqrt{\rho(x)}\phi_j'\|^2 \\ & \leq \quad \sum_{E_j(\alpha)<0} \alpha |E_j(\alpha)|^2 - \alpha^2 |E_j(\alpha)| \left\langle [H,G]\phi_j, [H,G]\phi_j \right\rangle \ \leq 0, \end{aligned}$$

and therefore

$$\alpha \sum_{E_j(\alpha)<0} |E_j(\alpha)|^2 - \alpha^2 \sum_{E_j(\alpha)<0} 4|E_j(\alpha)| \|\sqrt{\rho(x)}\phi_j'\|^2 \leq 0. \tag{4.8}$$

This inequality is the analog of the quadratic inequality (3.11) for Schrödinger operators and allows us again to apply the monotonicity argument. Namely, by the Feynman-Hellmann Theorem,

$$\frac{d}{d\alpha} E_j(\alpha) = \|\sqrt{\rho(x)}\phi_j'\|^2,$$

such that inequality (4.8) is equivalent to

$$\alpha \sum_{E_j(\alpha)<0} |E_j(\alpha)|^2 + 2\alpha^2 \frac{d}{d\alpha} \sum_{E_j(\alpha)<0} |E_j(\alpha)|^2 \leq 0,$$

or

$$\frac{d}{d\alpha} \left(\alpha^{1/2} \sum_{E_j(\alpha)<0} |E_j(\alpha)|^2 \right) \leq 0. \tag{4.9}$$

It follows immediately from (4.9) and Weyl's asymptotics that,

$$\begin{aligned} \alpha^{1/2} \sum_{E_j(\alpha)<0} |E_j(\alpha)|^2 \quad & \leq \quad \lim_{\alpha\to 0+} \alpha^{1/2} \sum_{E_j(\alpha)<0} |E_j(\alpha)|^2 \\ & = \quad \int_{\mathbb{R}} \int_I (\rho(x)|\xi|^2 + V(x))_-^2 \, \frac{dx\ d\xi}{2\pi} = L_{2,1}^{cl} \int_I \frac{V_-^{5/2}(x)}{\sqrt{\rho(x)}}\, dx. \end{aligned}$$

This proves Theorem 4.2. $\square$

In the following theorem we show that the Lieb-Thirring inequality in Theorem 4.2 can be extended to all moments $\gamma \geq 3/2$ by a Liouville transformation. However, the proof does not provide the monotonicity in α as in Theorem 4.2. Remarkably, we will see in what follows that the proof of the following theorem requires the same convexity condition on the function $\rho(x)$.

Theorem 4.5. *Let ρ be a C^2-function and $\rho > 0$ in the interior of I. Assume that $\rho^{3/4}(x)$ is convex. Then for all $\gamma \geq 3/2$ and for all $\alpha > 0$,*

$$\sum_{E_j(\alpha)<0} (-E_j(\alpha))^\gamma \leq \alpha^{-1/2} L_{\gamma,1}^{cl} \int_I \frac{V_-^{\gamma+1/2}(x)}{\sqrt{\rho(x)}}\, dx.$$

Proof. We consider the quadratic form (4.7) which is associated with the operator (4.6). Without loss of generality we set $\alpha = 1$. We define the transformation $\phi(x) = \varphi(x)v(\psi(x))$ and choose

$$\varphi(x) = \rho^{-1/4}(x) \quad \text{and} \quad \psi(x) = \int_c^x \rho^{-1/2}(y)\,dy, \tag{4.10}$$

where $c \in (a,b)$ is fixed and where $a := \inf I$, $b := \sup I$. Hence $|\varphi(x)|^2 = |\psi'(x)| = (|\varphi(x)|^2\rho(x))^{-1}$. Note that if ϕ satisfies Dirichlet boundary conditions at the ends of I, then v satisfies Dirichlet boundary conditions at the ends of $\tilde{I} := \left(-\int_a^c \rho^{-1/2}(y)\,dy, \int_c^b \rho^{-1/2}(y)\,dy\right)$.

First step: First, we show that if $\rho^{3/4}(x)$ is convex, then

$$h[\phi] := \int_I \left(\rho(x)|\phi'(x)|^2 + V(x)|\phi(x)|^2\right)\,dx \geq \int_{\tilde{I}} \left(|v'(t)|^2 + \tilde{V}(t)|v(t)|^2\right)\,dt =: \tilde{h}[v], \tag{4.11}$$

where $t = \psi(x)$ and $V(x) = \tilde{V}\left(\int^x \rho^{-1/2}(y)\,dy\right)$.

To show (4.11), we compute

$$\int_I \rho(x)|\phi'(x)|^2\,dx = \int_I \rho(x)\left(|\varphi(x)v'(\psi(x))\psi'(x)|^2 + |\varphi'(x)v(\psi(x))|^2\right)\,dx + \mathcal{R}, \tag{4.12}$$

where

$$\mathcal{R} = 2\,\mathrm{Re}\int_I \rho(x)\varphi(x)v'(\psi(x))\psi'(x)\overline{\varphi'(x)v(\psi(x))}\,dx = \int_I \rho(x)\varphi(x)\overline{\varphi'(x)}\frac{d}{dx}|v(\psi(x))|^2\,dx.$$

Integrating the last term by parts we get

$$\mathcal{R} = -\int_I |v(\psi(x))|^2\left(|\varphi'(x)|^2\rho(x) + \varphi(x)(\rho(x)\overline{\varphi'(x)})'\right)\,dx,$$

which in view of (4.12) implies that

$$\begin{aligned} h[\phi] : &= \int_I \rho(x)|\phi'(x)|^2 + V(x)|\phi(x)|^2\,dx \\ &= \int_I \rho(x)|\varphi(x)v'(\psi(x))\psi'(x)|^2 + V(x)|\varphi(x)|^2|v(\psi(x))|^2\,dx + \mathcal{S}, \end{aligned} \tag{4.13}$$

where $\mathcal{S} = -\int_I |v(\psi(x))|^2\varphi(x)(\rho(x)\overline{\varphi'(x)})'\,dx$. With the choice (4.10) equation (4.13) is equivalent to

$$h[\phi] = \int_I |v'(\psi(x))|^2|\psi'(x)| + V(x)|\psi'(x)||v(\psi(x))|^2\,dx + \mathcal{S}. \tag{4.14}$$

Under the assumption that the function $\rho^{3/4}$ is convex, $\mathcal{S}$ is non-negative by Lemma 4.4. Indeed, we can rewrite $\mathcal{S}$ as

$$\begin{aligned} \mathcal{S} &= \frac{1}{4}\int_I |v(\psi(x))|^2\varphi(x)(\rho(x))^{-5/4}\left(-\frac{1}{4}(\rho'(x))^2 + \rho(x)\rho''(x)\right)\,dx \\ &= \frac{1}{3}\int_I |v(\psi(x))|^2\varphi(x)\left(\rho^{3/4}(x)\right)''\,dx. \end{aligned} \tag{4.15}$$

Hence, if $\rho^{3/4}$ is convex then (4.11) follows from (4.14).

Second step: We note that, with the choice (4.10) the transformation $\phi(x) = \varphi(x)v(\psi(x))$ is unitary. Indeed

$$\int_I |\phi(x)|^2\,dx = \int_I |\varphi(x)|^2|v(\psi(x))|^2\,dx = \int_I |\psi'(x)||v(\psi(x))|^2\,dx. \tag{4.16}$$

Substituting $t=\psi(x)$ on the right-hand side of (4.16) we get

$$\int_I |\phi(x)|^2\,dx = \int_{\tilde I} |v(t)|^2\,dt.$$

Further, we substitute $t=\psi(x)$ in (4.15) and denote $\tilde{\mathcal{S}} = \int_{\tilde I} |v(t)|^2 \tilde U_\rho(t)\,dt$ with $\tilde U_\rho(\psi(x)) = (1/3)\rho^{1/4}(x)\left(\rho^{3/4}(x)\right)''$. Then, the operator H given in (4.6) is unitarily equivalent to the operator $\tilde H + \tilde U_\rho$, where $\tilde H = -\frac{d^2}{dt^2} + \tilde V$ is associated with the closed quadratic form $\tilde h[v]$. Hence, we have for the negative eigenvalues

$$E_j(H) = E_j(\tilde H + \tilde U_\rho).$$

As $\tilde U_\rho \geq 0$ under the condition that $\rho^{3/4}(x)$ is convex, it follows that $|E_j(H)| \leq |E_j(\tilde H)|$ for all j, and hence for all $\gamma > 0$,

$$\sum_j |E_j(H)|^\gamma \leq \sum_j |E_j(\tilde H)|^\gamma.$$

Now, we can use the well-known Lieb-Thirring inequality for the operator $\tilde H = -\frac{d^2}{dt^2} + \tilde V$ in $L_2(\tilde I)$ and get for all $\gamma \geq 3/2$,

$$\sum_j |E_j(H)|^\gamma \leq \sum_j |E_j(\tilde H)|^\gamma \leq L^{cl}_{\gamma,1} \int_{\tilde I} (\tilde V_-(t))^{\gamma+1/2}\,dt.$$

Noting that $\int_{\tilde I} (\tilde V_-(t))^{\gamma+1/2}\,dt = \int_I (V_-(x))^{\gamma+1/2} \rho^{-1/2}(x)\,dx$, the assertion of the theorem follows .

$\square$

4.3. **The monotonicity principle.** We recall that Theorem 2.1 and Theorem 4.2 were first proved for the case $\gamma = 2$. By a modification of the principle of Aizenman and Lieb, [1], the monotonicity property of the eigenvalue moments with respect to α can be extended from $\gamma = 2$ to higher orders $\gamma > 2$.

For $\delta > 0$ consider the integral $I := \int_0^1 \lambda^{-1+\delta}(1-\lambda)^\gamma\,d\lambda < \infty$. Then, we get for $E<0$ by scaling that

$$|E|^{\gamma+\delta} = I^{-1} \int_0^\infty \lambda^{-1+\delta} (E+\lambda)_-^\gamma\,d\lambda$$

and hence for $\gamma = 2$ and $\delta > 0$,

$$\frac{d}{d\alpha}\left(\alpha^{1/2} \sum_{E_j(\alpha)<0} |E_j(\alpha)|^{2+\delta}\right) = I^{-1} \int_0^\infty \lambda^{-1+\delta} \left(\frac{d}{d\alpha}\alpha^{1/2} \sum_{E_j(\alpha)<0} (E_j(\alpha)+\lambda)_-^2\right) d\lambda.$$

Since $\sum_{E_j(\alpha)<0}(E_j(\alpha)+\lambda)_-^2$ is the second eigenvalue moment for the Schrödinger operator $-\alpha d^2/dx^2 + V + \lambda$, the theorem, applied to this operator, yields

$$\frac{d}{d\alpha}\left(\alpha^{1/2} \sum_{E_j(\alpha)<0} (E_j(\alpha)+\lambda)_-^2\right) \leq 0.$$

Hence, $\frac{d}{d\alpha}\left(\alpha^{1/2}\sum_{E_j(\alpha)<0}|E_j(\alpha)|^{2+\delta}\right) \leq 0$, as claimed.

5. Trace formulas for Schrödinger operators on the half-line

Semra Demirel and Muhammad Usman

Abstract. We study the scattering problem for the Schrödinger equation on the half-line with the Robin boundary condition at the origin. We derive an expression for the trace of the difference of the perturbed and unperturbed resolvent in terms of a Wronskian. This leads to a representation for the perturbation determinant and to trace identities of Buslaev-Faddeev type.

5.1. **Introduction.** Let H be the self-adjoint operator on $L_2[0,\infty)$ defined by

$$H = H_0 + V(x), \quad H_0 = -\frac{d^2}{dx^2}, \quad u'(0) = \gamma u(0), \tag{5.1}$$

where $\gamma \in \mathbb{R}$. The potential V is real-valued and goes to zero at infinity (in some averaged sense). Then H has a continuous spectrum on the positive semiaxis and discrete negative spectrum, consisting of eigenvalues $\{\lambda_j\}$. If V decays fast enough, then there are only finitely many negative eigenvalues.

The Hamiltonian H describes a one-dimensional particle restricted to the positive semi-axis. 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.

In this paper we derive trace formulas for the negative eigenvalues of H. Formulas of this type first appeared in 1953 in the paper of Gel'fand and Levitan, [33], where some identities for the eigenvalues of a regular Sturm-Liouville operator were obtained. Later, also Dikiĭ studied similar formulas, see [22]. The next important contribution in this direction was made by Buslaev and Faddeev [16] in 1960. They studied the singular Sturm-Liouville operator on the half-line with Dirichlet boundary condition at the origin. Under some assumptions on the short range potential (i.e. integrable on $(0,\infty)$ with finite first moment), they proved a series of trace identities. The second one in this series states that

$$\sum_{j=1}^{N} |\lambda_j| - \frac{2}{\pi}\int_0^\infty \left(\tilde{\eta}(k) - \frac{1}{2k}\int_0^\infty V(x)\,dx\right) k\,dk = \frac{1}{4}V(0), \tag{5.2}$$

where $\tilde{\eta}(k)$ is the so-called limit phase and has a scattering theoretical nature. A more precise definition will be given later. This result was extended in 1997 by Rybkin to long-range potentials (nonintegrable on $(0,\infty)$), [6, 85]. Analog formulas for charged particles were obtained already in 1972 by Yafaev [55].

Trace formulas for the whole line Schrödinger operator as well as their generalizations to the multi-dimensional case have already been studied extensively (see, e.g., the surveys [11, 13, 39, 59]). Numerous papers are devoted to the subject of inverse spectral problems for Schrödinger operators, where trace identities turn out to be a central object, see e.g. [2,20,38] and references therein. The first application of sum rules goes back to Levinson [71] in 1949 when he studied the uniqueness of the potential in the Schrödinger equation for a given limit phase. In the context of inverse scattering, the connection between conservation laws for nonlinear evolution equations and trace formulas was studied in [13, 76, 100] and in [36] for more general settings. Other trace formulas in connection with periodic potentials and certain classes of almost periodic potentials have been important in solving the associated inverse spectral problem, see [37] and references therein. Finally, we mention that various trace identities are used also in the area of statistical mechanics and plasma physics, see [13].

An important consequence are the well-known Lieb-Thirring inequalities, which in dimension one follow from the third Faddeev-Zakharov trace formula, see [100] and [72]. This formula was extended in [70] by Laptev and Weidl to systems of Schrödinger operators, which leads to sharp Lieb-Thirring inequalities in all dimensions. These inequalities provide an upper bound for the moments of the negative eigenvalues of the corresponding Schrödinger operator and can be extended also to magnetic Schrödinger operators and Pauli operators. See also [15] for spectral estimates in the case of the half-line Schrödinger operator. Consequences for the absolutely continuous spectrum of one-dimensional Schrödinger operators were obtained by Deift and Killip in [19].

Our goal is to prove the analog of the Buslaev-Faddeev trace formulas for the half-line Schrödinger operator with Robin boundary conditions (5.1). Thereby, we follow Yafaev's book "Mathematical Scattering Theory, Analytic Theory" [98], which contains complete proofs in the case of Dirichlet boundary conditions. We aim to point out the differences arising from the Robin boundary conditions and to give an interpretation for them.

The outline of this paper is as follows. We consider the differential equation

$$-u'' + V(x)u = zu, \qquad z = \zeta^2, \tag{5.3}$$

where $\zeta \in \mathbb{C}$ and $x > 0$. We are concerned with two particular solutions of this equation, the regular solution φ and the Jost solution θ. The first one is characterized by the conditions

$$\varphi(0,\zeta) = 1, \quad \varphi'_x(0,\zeta) = \gamma, \tag{5.4}$$

and the latter one by the asymptotics $\theta(x,\zeta) \sim e^{i\zeta x}$ as $x \to \infty$.

In section 2 we prove existence and uniqueness of the regular solution. The corresponding properties of the Jost solution are well-known. Further, we introduce a quantity $w(\zeta)$, which we call the *Jost function*. We emphasize that this function depends on γ and does *not* coincide with what is called the Jost function in the Dirichlet case. More precisely , $w(\zeta)$ is defined as the Wronskian of the regular solution and the Jost solution of (5.3). It turns out that

$$w(\zeta) = \gamma\theta(0,\zeta) - \theta'(0,\zeta).$$

Section 3 contains our first main result. Denoting the resolvents of the unperturbed and perturbed operators by $R_0(z) = (H_0 - z)^{-1}$ and $R(z) = (H - z)^{-1}$, respectively, we derive an expression for $\mathrm{Tr}(R(z) - R_0(z))$ in terms of the Jost function.

Theorem 5.1. *Assume that* $\int_0^\infty |V(x)|\,dx < \infty$. *Then*

$$\mathrm{Tr}(R_0(z) - R(z)) = \frac{1}{2\zeta}\left(\frac{\dot{w}(\zeta)}{w(\zeta)} + \frac{i}{\gamma - i\zeta}\right), \quad \zeta = z^{1/2},\ \mathrm{Im}\,\zeta > 0. \tag{5.5}$$

From this relation we get a representation for the perturbation determinant in terms of $w(\zeta)$.

Section 4 deals with the asymptotic expansion of the perturbation determinant, which we shall use to derive trace identities in Section 5. For complex numbers s, we define the function

$$M_s(\gamma) := \begin{cases} (-\gamma)^{2s} & \text{if } \gamma < 0, \\ 0 & \text{if } \gamma \geq 0. \end{cases}$$

Under some regularity and decay assumptions on the potential V we prove infinitely many trace identities. The analogue to (5.2) will be given by

$$\sum_{j=1}^{N} |\lambda_j| - M_1(\gamma) - \frac{2}{\pi}\int_0^\infty \left(\eta(k) - \frac{1}{2k}\int_0^\infty V(x)\,dx\right) k\,dk = -\frac{1}{4}V(0), \tag{5.6}$$

where $\eta(k)$ is now the corresponding limit phase for the Robin boundary problem. We recall that if $\gamma \geq 0$, then H_0 has purely absolutely continuous spectrum $[0,\infty)$. If $\gamma < 0$, then H_0 has the simple negative eigenvalue $-\gamma^2$ and purely absolutely continuous spectrum on $[0,\infty)$. Hence the first two terms on the left-hand side of (5.6), $\sum_{j=1}^{N}|\lambda_j| - M_1(\gamma)$, correspond to the shift of the discrete spectrum between H and H_0. Similarly, the last term on the left-hand side corresponds to the shift of the absolutely continuous spectrum. The trace formula (5.6) and its higher order analogs proved below relate this shift of the spectrum to the potential V.

Finally, in Theorem 5.21 we prove a trace formula of order zero. Namely, the so-called *Levinson formula* for the Schrödinger operator H with Robin boundary condition.

Acknowledgments. The authors are grateful to A. Laptev, T. Weidl and D. Yafaev for helpful inputs and to F. Hantsch for providing Fig.1. Many thanks to Rupert Frank for informative discussions and references. Financial support via DAAD, grant 50022370, is gratefully acknowledged.

5.2. **The regular solution and the Jost solution.** In this section, we prove existence and uniqueness of the regular solution and recall some elementary results on the Jost solution. The γ-dependent Jost function is studied.

5.2.1. *The associated Volterra equation and auxiliary estimates.* Existence and uniqueness of the regular solution of (5.3) can be proved by using Volterra integral equations. For different boundary conditions, equation (5.3) is associated with different Volterra integral equations.

Lemma 5.2. *Let $V \in L_1^{(loc)}([0,\infty))$ and consider equation* (5.3) *on functions $\varphi \in C^1([0,\infty))$, such that φ' is absolutely continuous. Then* (5.3) *with boundary conditions* (5.4) *is equivalent to the Volterra equation*

$$\varphi(x,\zeta) = \cos(\zeta x) + \frac{\gamma}{\zeta}\sin(\zeta x) + \frac{1}{\zeta}\int_0^x \sin(\zeta(x-y))V(y)\varphi(y,\zeta)\,dy, \tag{5.7}$$

considered on locally bounded functions φ.

Proof. Suppose that equation (5.3) holds for φ. Then the equality

$$\int_0^x \zeta^{-1}\sin(\zeta(x-y))V(y)\varphi(y,\zeta)\,dy = \int_0^x \zeta^{-1}\sin(\zeta(x-y))\left(\varphi''(y,\zeta) + \zeta^2\varphi(y,\zeta)\right)\,dy$$

is true. We integrate the right-hand side twice by parts. Taking into account boundary conditions (5.4), we see that the right-hand side equals $\varphi(x,\zeta) - \cos(\zeta x) - \frac{\gamma}{\zeta}\sin(\zeta x)$. Thus equation (5.7) follows. Conversely, assume that equation (5.7) holds. Then $\varphi \in C^1_{loc}([0,\infty))$ and

$$\varphi'(x,\zeta) = -\zeta\sin(\zeta x) + \gamma\cos(\zeta x) + \int_0^x \cos(\zeta(x-y))V(y)\varphi(y,\zeta)\,dy. \tag{5.8}$$

Therefore φ' is absolutely continuous and

$$\varphi''(x,\zeta) = -\zeta^2\cos(\zeta x) - \gamma\zeta\sin(\zeta x) - \zeta\int_0^x \sin(\zeta(x-y))V(y)\varphi(y,\zeta)\,dy. \tag{5.9}$$

Comparing (5.9) with (5.7), we obtain equation (5.3). Inserting $x=0$ in (5.7) and (5.8) for $\varphi(x,\zeta)$ and $\varphi'(x,\zeta)$, we see that boundary conditions (5.4) are fullfilled. □

In the following Lemma it is proved that the regular solution $\varphi(x,\zeta)$ of (5.3) with boundary conditions (5.4) exists uniquely. For the case of Dirichlet boundary condition, this result was represented e.g. by Yafaev in [98].

Lemma 5.3. *Let $V\in L_1^{(loc)}([0,\infty))$. Then for all $\zeta\in\mathbb{C}$, equation* (5.3) *has a unique solution $\varphi(x,\zeta)$ satisfying* (5.4)*. For any fixed $x\geq 0$, $\varphi(x,\zeta)=\varphi(x,-\zeta)$ is an entire function of the variable $z=\zeta^2$. Moreover, for $\gamma\neq 0$ we have the estimate*

$$\left|\varphi(x,\zeta)-\cos(\zeta x)-\frac{\gamma}{\zeta}\sin(\zeta x)\right| \leq \tilde{c}|\gamma|xe^{|\operatorname{Im}\zeta|x}\left(\exp\left(\frac{c\int_0^x|V(y)|(1+|\gamma|y)\,dy}{|\gamma|}\right)-1\right). \tag{5.10}$$

If $\gamma=0$, then the estimate

$$|\varphi(x,\zeta)-\cos(\zeta x)| \leq \tilde{c}e^{|\operatorname{Im}\zeta|x}\left(\exp\left(cx\int_0^x|V(y)|\,dy\right)-1\right) \tag{5.11}$$

holds.

Proof. We construct a solution of integral equation (5.7), which by Lemma 5.2 is equivalent to the solution of (5.3). Set $\varphi_0(x,\zeta)=\cos(\zeta x)+\frac{\gamma}{\zeta}\sin(\zeta x)$,

$$\varphi_{n+1}(x,\zeta) = \int_0^x \zeta^{-1}\sin(\zeta(x-y))V(y)\varphi_n(y,\zeta)\,dy, \quad n\geq 0. \tag{5.12}$$

Inductively one shows that all $\varphi_n(x,\zeta)$ are entire functions of ζ^2. First, we consider the case when $\gamma\neq 0$. Using the estimates

$$\left|\frac{\sin(\zeta(x-y))}{\zeta}\right| \leq c|x-y|e^{|\operatorname{Im}\zeta|(x-y)} \quad \text{and} \quad \left|\cos(\zeta x)+\frac{\gamma}{\zeta}\sin(\zeta x)\right| \leq \tilde{c}e^{|\operatorname{Im}\zeta|x}(1+|\gamma|x), \tag{5.13}$$

we obtain

$$|\varphi_1(x,\zeta)| \leq c\tilde{c}xe^{|\operatorname{Im}\zeta|x}\int_0^x |V(y)|(1+|\gamma|\,y)\,dy.$$

Successively, we have or all $n\geq 1$,

$$|\varphi_n(x,\zeta)| \leq \frac{c^n\tilde{c}}{n!\,|\gamma|^{n-1}}xe^{|\operatorname{Im}\zeta|x}\left(\int_0^x |V(y)|(1+|\gamma|\,y)\,dy\right)^n, \tag{5.14}$$

which follows by an induction argument. Indeed, it follows from (5.12), (5.13) and (5.14) that

$$|\varphi_{n+1}(x,\zeta)| \leq \frac{c^{n+1}\tilde{c}}{n!\,|\gamma|^{n-1}}e^{|\operatorname{Im}\zeta|x}\int_0^x (x-y)y|V(y)|\left(\int_0^y |V(t)|(1+|\gamma|\,t)\,dt\right)^n dy. \tag{5.15}$$

As $|\gamma| > 0$, we have $y \le |\gamma|^{-1}(1 + |\gamma| y)$. Thus, the right-hand side in equation (5.15) is bounded by

$$\frac{c^{n+1}\tilde{c}}{n!|\gamma|^n} e^{|\operatorname{Im}\zeta| x} \int_0^x (1 + |\gamma| y)(x-y)|V(y)| \left(\int_0^y |V(t)|(1+|\gamma| t)\, dt \right)^n dy,$$

which is the same as

$$\frac{c^{n+1}\tilde{c}}{n!|\gamma|^n} e^{|\operatorname{Im}\zeta| x} \int_0^x \frac{(x-y)}{n+1} \frac{d}{dy} \left(\int_0^y |V(t)|(1+|\gamma| t)\, dt \right)^{n+1} dy.$$

Finally, the last term is bounded from above by

$$\frac{c^{n+1}\tilde{c}}{(n+1)!|\gamma|^n} e^{|\operatorname{Im}\zeta| x} x \left(\int_0^x |V(y)|(1+|\gamma| y)\, dy \right)^{n+1}.$$

Thus, the limit

$$\varphi(x,\zeta) := \lim_{N\to\infty} \sum_{n=0}^{N} \varphi_n(x,\zeta) \tag{5.16}$$

exists uniformly for bounded ζ, x and $|\gamma| > 0$. Putting together definitions (5.12) and (5.16), we see that

$$\sum_{n=0}^{N} \varphi_n(x,\zeta) = \cos(\zeta x) + \frac{\gamma}{\zeta}\sin(\zeta x) - \varphi_{N+1}(x,\zeta) + \int_0^x \zeta^{-1}\sin(\zeta(x-y))V(y) \left(\sum_{n=0}^{N} \varphi_n(y,\zeta) \right) dy.$$

From this equation, we obtain in the limit $N \to \infty$ equation (5.7). To prove estimate (5.10), we consider

$$\left| \varphi(x,\zeta) - \cos(\zeta x) - \frac{\gamma}{\zeta}\sin(\zeta x) \right| = \left| \lim_{N\to\infty} \sum_{n=1}^{N} \varphi_n(x,\zeta) \right|. \tag{5.17}$$

Because of (5.14), the right-hand side in (5.17) is bounded from above by

$$\begin{aligned} \tilde{c}|\gamma| x e^{|\operatorname{Im}\zeta| x} \sum_{n=1}^{\infty} \quad (n!)^{-1} \quad & \left(\frac{c\int_0^x |V(y)|(1+|\gamma| y)\, dy}{|\gamma|} \right)^n \\ = \quad & \tilde{c}|\gamma| x e^{|\operatorname{Im}\zeta| x} \left(\exp\left(\frac{c\int_0^x |V(y)|(1+|\gamma| y)\, dy}{|\gamma|} \right) - 1 \right). \end{aligned}$$

If $\gamma = 0$, then we use the same estimates (5.13) and get successively,

$$|\varphi_n(x,\zeta)| \le \frac{c^n \tilde{c} x^n}{n!} e^{|\operatorname{Im}\zeta| x} \left(\int_0^x |V(y)|\, dy \right)^n.$$

From this estimate it follows that

$$\begin{aligned} |\varphi(x,\zeta) - \cos(\zeta x)| \quad & \le \quad \tilde{c} e^{|\operatorname{Im}\zeta| x} \sum_{n=1}^{\infty} \frac{1}{n!} \left(cx \int_0^x |V(y)|\, dy \right)^n \\ & = \quad \tilde{c} e^{|\operatorname{Im}\zeta| x} \left(\exp\left(cx \int_0^x |V(y)|\, dy \right) - 1 \right), \end{aligned}$$

which proves estimate (5.11). The uniqueness of a bounded solution of equation (5.7) can be proved by contradiction. Suppose that φ_1 and φ_2 are two different solutions of equation (5.7). Then $\varphi_1 - \varphi_2$ satisfies the corresponding homogeneous equation and is bounded for an arbitrary n, by the right-hand side of (5.14) and hence is zero. Therefore $\varphi_1 = \varphi_2$. $\square$

5.2.2. *The Jost solution and the Jost function.* The so-called Jost solution, which was first studied by Jost, is important in scattering theory. This solution of equation (5.3) is characterized by the asymptotics $\theta(x,\zeta) \sim e^{i\zeta x}$ as $x \to \infty$. It is proved, e.g., in [98], that under the assumption

$$\int_0^\infty |V(x)|\, dx < \infty, \tag{5.18}$$

equation (5.3) has for all $\zeta \neq 0,\ \operatorname{Im}\zeta > 0$, a unique solution $\theta(x,\zeta)$ satisfying as $x \to \infty$ the conditions

$$\theta(x,\zeta) = e^{i\zeta x}(1 + o(1)), \quad \theta'(x,\zeta) = i\zeta e^{i\zeta x}(1 + o(1)). \tag{5.19}$$

For any fixed $x \geq 0$, the function $\theta(x,\zeta)$ is analytic in ζ in the upper half-plane $\operatorname{Im}\zeta > 0$ and continuous in ζ up to the real axis with a possible exception of the point $\zeta = 0$. Moreover, it satisfies the estimates

$$|\theta(x,\zeta) - e^{i\zeta x}| \leq e^{-\operatorname{Im}\zeta x}\left(\exp(|\zeta|^{-1}\int_x^\infty |V(y)|\, dy) - 1\right)$$

and consequently, for $|\zeta| \geq c > 0$,

$$|\theta(x,\zeta) - e^{i\zeta x}| \leq C|\zeta|^{-1}e^{-\operatorname{Im}\zeta x}\int_x^\infty |V(y)|\, dy, \tag{5.20}$$

where C depends on c and the value of the integral (5.18) only. We will need an analog of estimate (5.20) for the derivative of the Jost solution.

Lemma 5.4. *Assume condition* (5.18) *and* $\zeta \neq 0,\ \operatorname{Im}\zeta > 0$*. Then for the derivative of the solution* $\theta(x,\zeta)$ *with asymptotics* (5.19)*, the following estimate holds*

$$|\theta'(x,\zeta) - i\zeta e^{i\zeta x}| \leq e^{-\operatorname{Im}\zeta x}|\zeta|\left(\exp\left(|\zeta|^{-1}\int_x^\infty |V(y)|\, dy\right) - 1\right). \tag{5.21}$$

Moreover, for $|\zeta| \geq k > 0$*, we have*

$$|\theta'(x,\zeta) - i\zeta e^{i\zeta x}| \leq Ke^{-\operatorname{Im}\zeta x}\int_x^\infty |V(y)|\, dy, \tag{5.22}$$

where K *depends only on* k *and the value of the integral* (5.18)*.*

The proof of this Lemma follows closely the arguments of [98]. For the sake of completeness, we provide the necessary modifications in the appendix.

Next, we study some properties of the γ-dependent Jost function. Below we suppose that condition (5.18) is satisfied and that $\operatorname{Im}\zeta \geq 0$.

Definition 5.5. We denote by

$$w(\zeta) := \varphi'(x,\zeta)\theta(x,\zeta) - \theta'(x,\zeta)\varphi(x,\zeta) \tag{5.23}$$

the Wronskian of the regular solution and the Jost solution of the Schrödinger equation (5.3). The Wronskian $w(\zeta)$ is called *Jost function.*

Setting $x = 0$ in (5.23), we see that

$$w(\zeta) = \gamma\theta(0,\zeta) - \theta'(0,\zeta). \tag{5.24}$$

This is the definition of $w(\zeta)$ that was used in the introduction. The Jost function $w(\zeta)$ is analytic in ζ in the upper halfplane $\operatorname{Im}\zeta > 0$ and is continuous in ζ up to the real axis, with a possible exception of the point $\zeta = 0$. Moreover, it follows from (5.20) and (5.22) that

$$w(\zeta) = -i\zeta + O(1), \quad |\zeta| \to \infty, \quad \operatorname{Im}\zeta \geq 0. \tag{5.25}$$

Remark 5.6. Usually, in the literature the Wronskian w_D of the Jost solution and the regular solution satisfying a *Dirichlet* boundary condition is called Jost function. In our case of Robin boundary condition (5.4), the Wronskian differs from the usual one and depends on γ. We emphasize, that for every $\gamma \in \mathbb{R}$, the function $w(\zeta)$ grows linearly in ζ as $|\zeta| \to \infty$, whereas in the Dirichlet case we have for the corresponding Jost function $w_D(\zeta) = 1 + O(|\zeta|^{-1}),\ |\zeta| \to \infty$.

Our next goal is to give an integral representation for $w(\zeta)$.

Lemma 5.7. *For* $\operatorname{Im}\zeta \geq 0,\ \zeta \neq 0$*, the following representation for the Jost function holds*

$$w(\zeta) = \gamma - i\zeta + \int_0^\infty e^{i\zeta y} V(y)\varphi(y,\zeta)\, dy. \tag{5.26}$$

The proof of this Lemma relies on the following formula. For $\operatorname{Im}\zeta > 0$,

$$\lim_{x\to\infty} e^{i\zeta x}\left(\varphi'(x,\zeta) - i\zeta\varphi(x,\zeta)\right) = w(\zeta). \tag{5.27}$$

To show this, one can introduce, as in [98], for all ζ with $\operatorname{Im}\zeta > 0$ a solution of equation (5.3), which is linearly independent of $\theta(x,\zeta)$. Set

$$\tau(x,\zeta) = -2i\zeta\theta(x,\zeta)\int_{x_0}^x \theta(y,\zeta)^{-2}\, dy, \quad x \geq x_0,$$

where $x_0 = x_0(\zeta)$ is chosen such that $\theta(x,\zeta) \neq 0$ for all $x \geq x_0$. Then $\tau(x,\zeta)$ satisfies equation (5.3) and according to (5.19),

$$\tau(x,\zeta) = e^{-i\zeta x}(1 + o(1)), \quad \tau'(x,\zeta) = -i\zeta e^{-i\zeta x}(1 + o(1)),$$

as $x \to \infty$. Since $W\{\theta(\zeta), \tau(\zeta)\} = 2i\zeta$, we find that

$$\varphi(x,\zeta) = \frac{1}{2i\zeta}\left((\gamma\tau(0,\zeta) - \tau'(0,\zeta))\theta(x,\zeta) - (\gamma\theta(0,\zeta) - \theta'(0,\zeta))\tau(x,\zeta)\right). \tag{5.28}$$

Equation (5.27) now follows from (5.28). Given (5.27), we can prove Lemma 5.7.

Proof of Lemma 5.7. The differential equation (5.3) implies that

$$\int_0^x e^{i\zeta y} V(y)\varphi(y,\zeta)\, dy = \int_0^x e^{i\zeta y}\varphi''(y,\zeta)\, dy + \zeta^2 \int_0^x e^{i\zeta y}\varphi(y,\zeta)\, dy.$$

We integrate the first integral in the right-hand side twice by parts and get

$$\int_0^x e^{i\zeta y} V(y)\varphi(y,\zeta)\, dy = e^{i\zeta x}\left(\varphi'(x,\zeta) - i\zeta\varphi(x,\zeta)\right) - \gamma + i\zeta.$$

Passing to the limit $x \to \infty$ in the above equation and using (5.27), we arrive at (5.26) for $\operatorname{Im}\zeta > 0$. By continuity, (5.26) can be extended to the real axis. $\square$

As the Jost solution of equation (5.3) is unique, it follows that

$$\theta(x,\zeta)=\overline{\theta(x,-\bar{\zeta})},\quad \theta'(x,\zeta)=\overline{\theta'(x,-\bar{\zeta})}\quad\text{and hence}\quad w(\zeta)=\overline{w(-\bar{\zeta})}. \tag{5.29}$$

For real numbers $k>0$ both Jost solutions $\theta(x,k)$ and $\theta(x,-k)$ of the equation

$$-u''+V(x)u=k^2u,\quad k>0, \tag{5.30}$$

are correctly defined and their Wronskian $W\{\theta(\cdot,k),\theta(\cdot,-k)\}$ equals $2ik$. Thus, they are linearly independent. In particular, we get from (5.29),

$$\theta(x,-k)=\overline{\theta(x,k)}\quad\text{and hence}\quad w(-k)=\overline{w(k)}. \tag{5.31}$$

It is useful to express the regular solution in terms of the Jost solutions as follows,

$$\varphi(x,k)=\frac{1}{2ik}\left(\theta(x,k)w(-k)-\theta(x,-k)w(k)\right). \tag{5.32}$$

Indeed, it is easy to verify that the right-hand side of (5.32) satisfies equation (5.30) and conditions (5.4).

Now, we introduce the limit amplitude and phase shift for real values of k.

Definition 5.8. Set

$$w(k)=a(k)e^{i\eta(k)}(\gamma-ik),\quad a(k)=\frac{|w(k)|}{\sqrt{\gamma^2+k^2}}. \tag{5.33}$$

The functions $a(k)$ and $\eta(k)$ are called the limit amplitude and the limit phase, respectively.

These functions determine the asymptotics of the regular solution of the Schrödinger equation as $x\to\infty$. Indeed, comparing (5.19) and (5.32), we find

$$\varphi(x,k)\;=\;\frac{1}{2ik}\left(e^{ikx}w(-k)-e^{-ikx}w(k)\right)+o(1),\quad x\to\infty.$$

Furthermore,

$$w(-k)=\overline{w(k)}=a(k)e^{-i\eta(k)}(\gamma+ik).$$

Thus,

$$\varphi(x,k)=a(k)\frac{1}{2ik}\left((\gamma+ik)e^{i(kx-\eta(k))}-(\gamma-ik)e^{-i(kx-\eta(k))}\right)+o(1),\quad x\to\infty.$$

This asymptotic behavior should be compared with the exact expression for the solution $\varphi_0(x,\zeta)$ of the equation $-\varphi''=\zeta^2\varphi$ satisfying the conditions (5.4), namely,

$$\varphi_0(x,\zeta)=(2i\zeta)^{-1}((\gamma+i\zeta)e^{i\zeta x}-(\gamma-i\zeta)e^{-i\zeta x}).$$

Finally, we note that

$$w(k)\neq 0\quad\text{for all } k>0. \tag{5.34}$$

Indeed, if there was a number k such that $w(k)=0$, then it would follow from relations (5.31) and (5.32) that $\varphi(x,k)=0$ for all x.

5.3. **A Trace formula and the perturbation determinant.** We consider the Hamiltonian

$$H = -\frac{d^2}{dx^2} + V(x), \quad V = \overline{V}, \tag{5.35}$$

with boundary condition (5.4) in the space $L_2(\mathbb{R}_+)$. More precisely, H is defined through the quadratic form

$$\int_0^\infty \left(|u'(x)|^2 + V(x)|u(x)|^2\right)\, dx + \gamma |u(0)|^2$$

with form domain $H^1(\mathbb{R}_+)$. By $H_0 = -\frac{d^2}{dx^2}$ we denote the free Hamiltonian with the same boundary condition (5.4) but with $V \equiv 0$. The resolvents of H and H_0 are denoted by $R(z)$ and $R_0(z)$, respectively.

In this section, we derive an expression for $\operatorname{Tr}(R(z) - R_0(z))$ in terms of the Jost function. From this relation we get a representation for the perturbation determinant.

It is a well-known fact that $R(z)$ can be constructed in terms of solutions $\varphi(x,\zeta)$ and $\theta(x,\zeta)$ of equation (5.3) and their Wronskian (5.23). Suppose that (5.18) holds. Then for all z such that $\operatorname{Im} z \neq 0$ and $w(\zeta) \neq 0$, the resolvent is the integral operator with kernel

$$R(x,y;z) = w^{-1}(\zeta)\varphi(x,\zeta)\theta(y,\zeta), \quad x \leq y,\ \zeta = z^{1/2}, \tag{5.36}$$

and $R(x,y;z) = R(y,x;z)$. Moreover, the estimate

$$|R(x,y;z)| \leq c|w(\zeta)|^{-1}|\zeta|^{-1}\exp(-\operatorname{Im}\zeta|x-y|)$$

holds. We note that in the particular case $V \equiv 0$, the unperturbed resolvent $R_0(z)$ has the integral kernel

$$R_0(x,y;z) = R_0(y,x;z) = \frac{((\gamma + i\zeta)e^{i\zeta x} - (\gamma - i\zeta)e^{-i\zeta x})e^{i\zeta y}}{2i\zeta(\gamma - i\zeta)}, \quad x \leq y. \tag{5.37}$$

The self-adjoint operator H has discrete negative spectrum, which consists of negative eigenvalues $\lambda_j = (i\kappa_j)^2,\ \kappa_j > 0$, which possibly accumulate at zero. It is important to note that the zeros of the function $w(\zeta)$ and the eigenvalues of H are related as follows.

Lemma 5.9. *Complex zeros of the function $w(\zeta)$ are simple and lie on the imaginary axis. Moreover, $w(\zeta) = 0$ if and only if $\lambda = \zeta^2$ is a negative eigenvalue of the operator H.*

Proof. First, assume that $w(\zeta) = 0$ for $\operatorname{Im}\zeta > 0$. Then the Jost function $\theta(x,\zeta)$ fullfills boundary conditions (5.4) and is in the space $L_2(\mathbb{R}_+)$ because of (5.19) and the positive imaginary part of ζ. Thus $\theta(x,\zeta)$ is an eigenfunction of the operator H corresponding to the eigenvalue $\lambda = \zeta^2$. Since H is self-adjoint, it follows that $\lambda < 0$. Conversely, assume that λ is an eigenvalue of H. Then its resolvent $R(z)$ has a pole in λ. Therefore, it follows from (5.36) that $w(\zeta) = 0$. As the resolvent of a self-adjoint operator has only simple poles, the zeros of $w(\zeta)$ are simple. □

Remark 5.10. It follows from the proporties of the regular solution and Jost solution, that the resolvent kernel (5.36) is an analytic function in the upper half-plane $\operatorname{Im}\zeta > 0$, except for simple poles at eigenvalues of H. In view of (5.34), the resolvent kernel is a continuous function of z up to the cut along $[0,\infty)$ with the possible exception of the point $z = 0$.

Proposition 5.11. *Assume condition* (5.18), *then*

$$\operatorname{Tr}(R_0(z)-R(z)) = \frac{1}{2\zeta}\left(\frac{\dot w(\zeta)}{w(\zeta)} + \frac{i}{\gamma - i\zeta}\right), \quad \zeta = z^{1/2},\ \operatorname{Im}\zeta > 0. \tag{5.38}$$

Proof. Since $R - R_0$ is a trace class operator and kernels of the operators R and R_0 are continuous functions, we have

$$\operatorname{Tr}(R(z)-R_0(z)) = \lim_{x\to\infty}\int_0^x (R(y,y;z) - R_0(y,y;z))\,dy. \tag{5.39}$$

Using (5.37), we first compute

$$2\zeta\int_0^x R_0(y,y;z)\,dy = \frac{1}{i(\gamma - i\zeta)}\left(\frac{\gamma+i\zeta}{2i\zeta}e^{2i\zeta x} - (\gamma - i\zeta)x - \frac{\gamma+i\zeta}{2i\zeta}\right). \tag{5.40}$$

The following equation is true for any two arbitrary solutions of equation (5.3)

$$2\zeta\varphi(x,\zeta)\theta(x,\zeta) = (\varphi'(x,\zeta)\dot\theta(x,\zeta) - \varphi(x,\zeta)\dot\theta'(x,\zeta))'. \tag{5.41}$$

Applying (5.41) to the regular solution $\varphi(x,\zeta)$ and the Jost solution $\theta(x,\zeta)$, we get

$$\begin{aligned} 2\zeta w(\zeta)\int_0^x R(y,y;z)\,dy &= 2\zeta\int_0^x \varphi(y,\zeta)\theta(y,\zeta)\,dy \\ &= \Big[\varphi'(y,\zeta)\dot\theta(y,\zeta) - \varphi(y,\zeta)\dot\theta'(y,\zeta)\Big]_0^x. \end{aligned} \tag{5.42}$$

Note that the contribution of the right-hand side in (5.42) for $y = 0$ is

$$\varphi'(0,\zeta)\dot\theta(0,\zeta) - \varphi(0,\zeta)\dot\theta'(0,\zeta) = \gamma\dot\theta(0,\zeta) - \dot\theta'(0,\zeta) = \dot w(\zeta). \tag{5.43}$$

Consider now the case of potentials of compact support. Then, for all $\zeta \in \mathbb{C}$, we have $\theta(x,\zeta) = e^{i\zeta x}$ for sufficiently large x. Further, in this case we can generalize (5.32) to complex ζ, namely

$$\varphi(x,\zeta) = \frac{1}{2i\zeta}\left(\theta(x,\zeta)w(-\zeta) - \theta(x,-\zeta)w(\zeta)\right). \tag{5.44}$$

For large x we have,

$$\theta(x,\zeta) = e^{ix\zeta}, \quad \theta'(x,\zeta) = i\zeta e^{ix\zeta}, \quad \dot\theta(x,\zeta) = ixe^{ix\zeta}, \quad \dot\theta'(x,\zeta) = (i - x\zeta)e^{ix\zeta}.$$

Taking into account, that since $\operatorname{Im}\zeta > 0$, the terms containing $e^{2ix\zeta}$ tend to zero as $x\to\infty$ and using (5.44), we get for sufficiently large x

$$\varphi'(x,\zeta)\dot\theta(x,\zeta) - \varphi(x,\zeta)\dot\theta'(x,\zeta) = (ix + (2\zeta)^{-1})w(\zeta) + o(1). \tag{5.45}$$

Combining (5.43) and (5.45), we arrive at

$$2\zeta\int_0^x R(y,y;z)\,dy = ix + \frac{1}{2\zeta} - \frac{\dot w(\zeta)}{w(\zeta)} + o(1). \tag{5.46}$$

Finally, we conclude from (5.40) and (5.46) that

$$\lim_{x\to\infty}\int_0^x (R_0(y,y;z) - R(y,y;z))\,dy = \frac{1}{2\zeta}\left(\frac{\dot w(\zeta)}{w(\zeta)} + \frac{i}{\gamma - i\zeta}\right) + o(1).$$

This proves (5.38) for compactly supported potentials V. By density arguments (see [98, Prop. 4.5.3]) based on the fact, that $\sqrt{|V|}(H_0 + \mathbb{1})^{-1/2}$ is a Hilbert-Schmidt operator under condition (5.18), the result can be extended to all potentials V satisfying this condition. □

We conclude this section by relating the Jost function to the perturbation determinant. Since $\sqrt{|V|}(H_0+\mathbb{1})^{-1/2}$ is a Hilbert-Schmidt operator, the operator $\sqrt{V}R_0(z)\sqrt{|V|}$ is a trace class operator (here $\sqrt{V} := (\operatorname{sgn} V)\sqrt{|V|}$) and therefore the (modified) perturbation determinant

$$D(z) := \det(\mathbb{1} + \sqrt{V}R_0(z)\sqrt{|V|}), \quad z \in \rho(H_0)$$

is well-defined. Here $\rho(H_0)$ denotes the resolvent set of the operator H_0. Furthermore, it can easily be verified that the perturbation determinant is related to the trace of the resolvent difference by

$$\frac{D'(z)}{D(z)} = \operatorname{Tr}(R_0(z) - R(z)), \quad z \in \rho(H_0) \cap \rho(H).$$

Thus, it follows from (5.38) that

$$\frac{D'(z)}{D(z)} = \frac{1}{2\zeta}\frac{d}{d\zeta}(\ln w(\zeta) - \ln(\gamma - i\zeta)) = \frac{1}{2\zeta}\frac{d}{d\zeta}\ln\left(\frac{w(\zeta)}{\gamma - i\zeta}\right) = \frac{\left(\frac{w(\sqrt{z})}{\gamma - i\sqrt{z}}\right)'}{\left(\frac{w(\sqrt{z})}{\gamma - i\sqrt{z}}\right)}.$$

Therefore, we conclude that $D(z) = Cw(\sqrt{z})/(\gamma - i\sqrt{z})$. Because of the asymptotics (5.25), it follows that

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

This is the sought after relation.

5.4. **Low and High-energy asymptotics.** Here we derive an asymptotic expansion of the perturbation determinant $D(\zeta)$ as $|\zeta| \to \infty$.

5.4.1. *High-energy asymptotics.* In this subsection, we assume that $V \in C^\infty(\mathbb{R}_+)$ and that

$$|V^{(j)}(x)| \le C_j(1+x)^{-\rho-j}, \quad \rho \in (1,2], \quad j \in \mathbb{N}_0. \tag{5.47}$$

The asymptotic expansion of the Jost solution $\theta(x,\zeta)$ for $|\zeta| \to \infty$ can be found, e.g., in [98]. Thereby, it is more convenient to consider the function $b(x,\zeta)$ defined by

$$b(x,\zeta) := e^{-ix\zeta}\theta(x,\zeta). \tag{5.48}$$

Note that equation (5.3) for $\theta(x,\zeta)$ is equivalent to the equation

$$-b''(x,\zeta) - 2i\zeta b'(x,\zeta) + V(x)b(x,\zeta) = 0. \tag{5.49}$$

It follows from (5.48) that asymptotics (5.19) and the asymptotics

$$b(x,\zeta) = 1 + o(1), \quad b'(x,\zeta) = o(1), \quad x \to \infty, \tag{5.50}$$

are equivalent to each other. For an arbitrary N, the equality

$$b(x,\zeta) = \sum_{n=0}^{N} b_n(x)(2i\zeta)^{-n} + r_N(x,\zeta) \tag{5.51}$$

holds with the remainder satisfying the estimates

$$|\partial^j r_N(x,\zeta)/\partial x^j| \le C_{N,j}|\zeta|^{-N-1}(1+|x|)^{-(N+1)(\rho-1)-j}, \quad j \in \mathbb{N}_0,$$

for all $x \geq 0$ and $\operatorname{Im}\zeta \geq 0$, $|\zeta| \geq c > 0$. Here $b_0(x) = 1$ and $b_n(x)$ are real C^∞ functions defined by the recurrent relation

$$b_{n+1}(x) = -b_n'(x) - \int_x^\infty V(y) b_n(y)\, dy.$$

Further the following estimates hold,

$$b_n^{(j)}(x) = O(x^{-n(\rho-1)-j}), \quad j \in \mathbb{N}_0, \quad x \to \infty.$$

Now, we can prove the asymptotic expansion of the perturbation determinant for $|\zeta| \to \infty$.

Lemma 5.12. *Suppose $V \in C^\infty(\mathbb{R}_+)$ and (5.47). Then the perturbation determinant admits the expansion in the asymptotic series*

$$D(\zeta) = \sum_{n=0}^\infty d_n (2i\zeta)^{-n}, \tag{5.52}$$

as $|\zeta| \to \infty$, $\operatorname{Im}\zeta \geq 0$. The coefficients d_n are given by

$$d_0 = 1, \quad d_n := b_n(0) + 2\sum_{m=1}^{n-1} b_m'(0)(2\gamma)^{n-m-1}, \quad n \geq 1. \tag{5.53}$$

We emphasize that expansion (5.52) is understood in the sense of an asymptotic series.

Proof. It follows from (5.51) that

$$\frac{b'(x,\zeta) + (i\zeta - \gamma) b(x,\zeta)}{i\zeta - \gamma} = \frac{1}{i\zeta - \gamma} \sum_{n=0}^\infty b_n'(x)(2i\zeta)^{-n} + \sum_{n=0}^\infty b_n(x)(2i\zeta)^{-n}. \tag{5.54}$$

Applying the geometric series to the first sum in the right-hand side of (5.54) for $|\zeta| > \gamma$, we conclude

$$\frac{b'(x,\zeta) + (i\zeta - \gamma) b(x,\zeta)}{i\zeta - \gamma} = b_0(x) + \sum_{n=1}^\infty \left(b_n(x) + 2\sum_{m=0}^{n-1} b_m'(x)(2\gamma)^{n-m-1} \right)(2i\zeta)^{-n}. \tag{5.55}$$

On the other hand, it is easy to see that

$$b'(x,\zeta) + (i\zeta - \gamma) b(x,\zeta) = e^{-i\zeta x}(\theta'(x,\zeta) - \gamma\theta(x,\zeta)) \tag{5.56}$$

Thus, setting $x = 0$ and combining (5.55) with (5.56), we arrive at (5.52). $\square$

Note that because of (5.25), we have for $|\zeta| \to \infty$, $\operatorname{Im}\zeta \geq 0$,

$$D(\zeta) = \frac{w(\zeta)}{\gamma - i\zeta} = 1 + O(|\zeta|^{-1}). \tag{5.57}$$

Thus, we can fix the branch of the function $\ln D$ by the condition $\ln D(\zeta) \to 0$ as $|\zeta| \to \infty$. The following Corollary is an immediate consequence of Lemma 5.12.

Corollary 5.13. *Suppose $V \in C^\infty(\mathbb{R}_+)$ and (5.47). Then for $|\zeta| \to \infty$, $\operatorname{Im}\zeta \geq 0$, we have*

$$\ln D(\zeta) = \sum_{n=1}^\infty \ell_n (2i\zeta)^{-n},$$

where the coefficients ℓ_n are given by

$$\ell_1 := d_1, \quad \ell_n := d_n - n^{-1}\sum_{j=1}^{n-1} j d_{n-j}\ell_j, \quad n \geq 2. \tag{5.58}$$

The first coefficients ℓ_n work out to be

$$\ell_1 = -\int_0^\infty V(x)\,dx, \quad \ell_2 = V(0), \quad \ell_3 = 4\gamma V(0) - V'(0) + \int_0^\infty V^2(x)\,dx,$$

$$\ell_4 = V''(0) - 2V^2(0) - 4\gamma V'(0) + 8\gamma^2 V(0).$$

From (5.33) it follows for $k \in \mathbb{R}$ that

$$\ln D(k) = \ln\left(\frac{w(k)}{\gamma - ik}\right) = \ln a(k) + i\eta(k).$$

Seperating in Corollary 5.13 the function $\ln D(k)$ into its real and imaginary part, we finally conclude, that for $k \to \infty$,

$$\begin{aligned} \ln a(k) &= \sum_{n=1}^\infty (-1)^n \ell_{2n}(2k)^{-2n}, \\ \eta(k) &= \sum_{n=0}^\infty (-1)^{n+1}\ell_{2n+1}(2k)^{-2n-1}. \end{aligned} \tag{5.59}$$

5.4.2. *Low-energy asymptotics.* In this section we assume that

$$\int_0^\infty (1+x)|V(x)|\,dx < \infty. \tag{5.60}$$

We denote the regular solution for $\zeta = 0$ by $\varphi(x)$. This is the solution of the integral equation (5.7),

$$\varphi(x) = 1 + x\gamma + \int_0^x (x-y)V(y)\varphi(y)\,dy. \tag{5.61}$$

This solution exists under condition (5.18). As shown in [98], the stronger condition (5.60) guarantees the existence of a Jost solution $\theta(x,\zeta)$ at $\zeta = 0$. For any fixed $x \geq 0$, the Jost solution $\theta(x,\zeta)$ is continuous as $\zeta \to 0$, $\operatorname{Im}\zeta \geq 0$. Moreover,

$$|\theta(x,\zeta) - e^{i\zeta x}| \leq e^{-\operatorname{Im}\zeta x}\left(\exp\left(C\int_x^\infty y|V(y)|\,dy\right) - 1\right),$$

where C does not depend on ζ and x. The function $\theta(x) := \theta(x,0) = \overline{\theta(x,0)}$ satisfies the equation

$$-u'' + V(x)u = 0 \tag{5.62}$$

and, as $x \to \infty$,

$$\theta(x) = 1 + O\left(\int_x^\infty y|V(y)|\,dy\right) = 1 + o(1), \quad \theta'(x) = O\left(\int_x^\infty |V(y)|\,dy\right) = o(x^{-1}). \tag{5.63}$$

Indeed, asymptotics (5.63) follow from the integral equation (6.1) for $\zeta = 0$, namely,

$$\theta(x) = 1 + \int_x^\infty (y-x)V(y)\theta(y)\,dy.$$

One can also show that the Jost function $w(\zeta)$ is continuous as $\zeta \to 0$, $\operatorname{Im}\zeta \geq 0$, and from (5.26) we get for $\zeta = 0$

$$w(0) = \gamma + \int_0^\infty V(y)\varphi(y)\,dy. \tag{5.64}$$

If (5.60) holds, then the integral in (5.64) is convergent, in view of the estimate

$$|\varphi(x,0) - 1| \leq \hat{c}\gamma x,$$

following from (5.10). Moreover, we have $w(0) = \overline{w(0)}$.

After these preliminaries we claim that the operator H has no zero eigenvalue. Indeed, the function defined by

$$\tau(x) = \theta(x)\int_{x_0}^x \theta(y)^{-2}\,dy, \quad x \geq x_0,$$

is a solution of equation (5.62) and is linearly independent of $\theta(x)$. Again, x_0 is an arbitrary point such that $\theta(x) \neq 0$ for $x \geq x_0$. Further,

$$\tau(x) = x + o(x), \quad \tau'(x) = 1 + o(1) \quad \text{as } x \to \infty \text{ and } W\{\theta,\tau\} = -1.$$

Thus, the equation (5.62) does not have solutions, tending to zero at infinity, as claimed.

While the operator does not have a zero eigenvalue, it may have a so-called zero resonance.

Definition 5.14. Under assumption (5.60), one says that the operator H has a resonance at $\zeta = 0$ if $w(0) = 0$.

Since the Jost function is the Wronskian of the Jost and the regular solution, the resonance condition means that φ is a multiple of θ and therefore that equation (5.62) has a bounded solution satisfying boundary condition (5.4).

Now, we want to analyze the behavior of the Jost function $w(\zeta)$ as $\zeta \to 0$. More precisely, we want to show, that if $w(0) = 0$, then it vanishes not faster than linearly. In order to prove this, we need the following technical Lemma.

Lemma 5.15. *Assume* (5.60) *and let* $w(0) = 0$. *Then*

$$|\varphi(x,\zeta) - \varphi(x)| \leq C|\zeta| x e^{\operatorname{Im}\zeta x}, \quad \operatorname{Im}\zeta \geq 0. \tag{5.65}$$

Proof. We set $\Omega(x,\zeta) = \varphi(x,\zeta) - \varphi(x)$ and

$$\begin{aligned}\Omega_0(x,\zeta) = \cos(\zeta x) + \frac{\gamma}{\zeta}\sin(\zeta x) \quad &- \quad 1 - x\gamma - \int_0^x (x-y)V(y)\varphi(y)\,dy \\ &+ \quad \int_0^x \zeta^{-1}\sin(\zeta(x-y))V(y)\varphi(y)\,dy. \end{aligned} \tag{5.66}$$

It follows from (5.7) and (5.61) that

$$\Omega(x,\zeta) = \Omega_0(x,\zeta) + \int_0^x \zeta^{-1}\sin(\zeta(x-y))V(y)\Omega(y,\zeta)\,dy.$$

We first prove that

$$|\Omega_0(x,\zeta)| \leq C|\zeta| x e^{\operatorname{Im}\zeta x}. \tag{5.67}$$

Note that the condition $w(0) = 0$ is equivalent to the condition $\int_0^\infty V(y)\varphi(y)\,dy = -\gamma$. Therefore, we can rewrite (5.66) as

$$\Omega_0(x,\zeta) = \cos(\zeta x) - 1 - (\zeta^{-1}\sin(\zeta x) - x)\int_x^\infty V(y)\varphi(y)\,dy + \int_0^x K(x,y,\zeta)V(y)\varphi(y)\,dy, \tag{5.68}$$

where

$$K(x,y,\zeta) = -\zeta^{-1}\sin(\zeta x) + y + \zeta^{-1}\sin(\zeta(x-y)).$$

The third and fourth term in the right-hand side of (5.68) are bounded from above by $C|\zeta|xe^{\operatorname{Im}\zeta x}$. This follows in the same way as shown in [98], which only uses that $\varphi(x)$ is bounded. It remains to give an estimate for the first and second term in (5.68), which we write as

$$\cos(\zeta x) - 1 = -2\sin^2(\zeta x/2).$$

Using the estimates

$$|\sin(\zeta x/2)| \le ce^{|\operatorname{Im}\zeta|x/2} \quad \text{and} \quad |\sin(\zeta x/2)| \le c|\zeta|xe^{|\operatorname{Im}\zeta|x/2},$$

we get

$$|\cos(\zeta x) - 1| \le c|\zeta|xe^{|\operatorname{Im}\zeta|x}.$$

Thus, we conclude (5.67). This inequality implies (5.65) by Gronwall's Lemma exactly as in [98, Lemma 4.3.6]. □

Proposition 5.16. *Under the assumption* (5.60) *and* $w(0) = 0$ *we have the following asymptotics for the Jost function,*

$$w(\zeta) = -iw_0\zeta + o(\zeta), \quad \zeta \to 0, \tag{5.69}$$

where $w_0 = 1 - \int_0^\infty yV(y)\varphi(y)\,dy \neq 0$.

Proof. Since $w(0) = 0$, we have $\int_0^\infty V(y)\varphi(y)\,dy = -\gamma$ and therefore it follows from representation (5.26) that

$$\begin{aligned} w(\zeta) &= \int_0^\infty \left(e^{i\zeta x}\varphi(x,\zeta) - \varphi(x)\right)V(x)\,dx - i\zeta \\ &= -iw_0\zeta + \int_0^\infty \left(e^{i\zeta x} - 1 - i\zeta x\right)\varphi(x)V(x)\,dx \\ &+ \int_0^\infty e^{i\zeta x}\left(\varphi(x,\zeta) - \varphi(x)\right)V(x)\,dx. \end{aligned} \tag{5.70}$$

It can be shown as follows that both integrals in the right-hand side of (5.70) are $o(\zeta)$ as $\zeta \to 0$. Since the function $e^{i\zeta x} - 1 - i\zeta x$ is bounded by $C|\zeta|x$ and is $O(|\zeta|^2)$ for all fixed x, it follows that the first integral in the right-hand side is $o(\zeta)$ as $\varphi(x)$ is a bounded function. The second integral in the right-hand side of (5.70) is also $o(\zeta)$. Indeed it follows from Lemma 5.15 that the function $e^{i\zeta x}\left(\varphi(x,\zeta) - \varphi(x)\right)$ is bounded by $C|\zeta|x$ and further it is $O(|\zeta|^2)$ for all fixed x as the function φ is analytic in ζ^2. Thus the asymptotics (5.69) holds.

In order to prove that $w_0 \neq 0$, we use equation (5.61) to write

$$\begin{aligned} \varphi(x) &= x\left(\gamma + \int_0^\infty V(y)\varphi(y)\,dy\right) + w_0 - x\int_x^\infty V(y)\varphi(y)\,dy + \int_x^\infty yV(y)\varphi(y)\,dy \\ &= w_0 + o(1) \end{aligned}$$

as $x \to \infty$. On the other hand, φ is proportional to θ, which satisfies (5.63). This shows that $w_0 \neq 0$, as claimed. □

5.5. **Trace identities.** We now put the material from the previous sections together to prove our main result, namely, a family of trace formulas for the operator H. These identities provide a relation between the shift of the spectra between H and H_0 and quantities involving the potential V. The spectral shift consists of two parts, one coming from the discrete spectrum (expressed in terms of the eigenvalues of H and H_0) and the other one coming from the continuous spectrum (expressed in terms of the quantities η and a).

In this section we assume that $\int_0^\infty (1+x)|V(x)|\,dx < \infty$ which guarantees that H has only a finite number N of negative eigenvalues $\lambda_1, \dots, \lambda_N$. We recall that H_0 has a single negative eigenvalue $-\gamma^2$ if $\gamma < 0$ and no negative eigenvalues if $\gamma \geq 0$. We also recall that $M_s(\gamma)$ was defined at the end of the introduction.

While we are mainly interested in trace formulas of integer and half-integer order, we prove a version of these formulas for every complex s with $\operatorname{Re} s > 0$. We proceed by analytic continuation, where the starting point is the following proposition.

Proposition 5.17. *Suppose that* (5.60) *holds and define for* $s \in \mathbb{C}$, $0 < \operatorname{Re} s < 1/2$, *the functions*

$$F(s) := \int_0^\infty \ln a(k) k^{2s-1}\,dk, \quad G(s) := \int_0^\infty \eta(k) k^{2s-1}\,dk. \tag{5.71}$$

Then

$$\frac{\pi}{2s} \sum_{j=1}^{N} |\lambda_j|^s - \frac{\pi}{2s} M_s(\gamma) = \sin(\pi s) F(s) - \cos(\pi s) G(s). \tag{5.72}$$

Proof. Let $\Gamma_{R,\varepsilon}$ be the contour (with counterclockwise direction) which consists of the half-circles $C_R^+ = \{|\zeta| = R, \operatorname{Im}\zeta \geq 0\}$ and $C_\varepsilon^+ = \{|\zeta| = \varepsilon,\ \operatorname{Im}\zeta \geq 0\}$ and the intervals (ε, R) and $(-R, -\varepsilon)$.

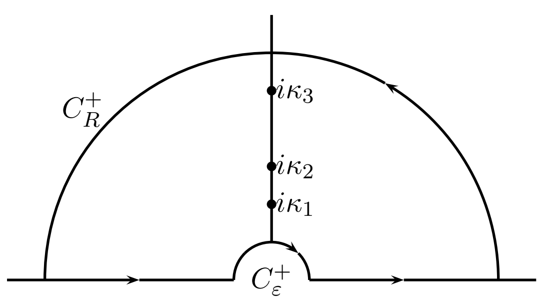

FIGURE 8. contour of integration

The argument of $\zeta \in \mathbb{C}$ is fixed by the condition $0 \leq \arg\zeta \leq \pi$. We consider the integral

$$\int_{\Gamma_{R,\varepsilon}} \frac{\frac{d}{d\zeta}\left(\frac{w(\zeta)}{\gamma - i\zeta}\right)}{\left(\frac{w(\zeta)}{\gamma - i\zeta}\right)} \zeta^{2s}\,d\zeta.$$

The set of the singularities of the integrand is the set of zeros of the function $w(\zeta)/(\gamma - i\zeta)$.

Calculating the integral by residues, we see that for $\kappa_j = |\lambda_j|^{1/2}$

$$\int_{\Gamma_{R,\varepsilon}} \frac{\frac{d}{d\zeta}\left(\frac{w(\zeta)}{\gamma - i\zeta}\right)}{\left(\frac{w(\zeta)}{\gamma - i\zeta}\right)} \zeta^{2s}\, d\zeta = 2\pi i \sum_{j=1}^{N} \mathrm{Res}_{\zeta = i\kappa_j} \frac{\frac{d}{d\zeta}\left(\frac{w(\zeta)}{\gamma - i\zeta}\right)}{\left(\frac{w(\zeta)}{\gamma - i\zeta}\right)} \zeta^{2s}$$
$$- 2\pi i \begin{cases} \mathrm{Res}_{\zeta = -i\gamma} \frac{\frac{d}{d\zeta}\left(\frac{w(\zeta)}{\gamma - i\zeta}\right)}{\left(\frac{w(\zeta)}{\gamma - i\zeta}\right)} \zeta^{2s}, & \text{if } \gamma < 0 \\ 0, & \text{if } \gamma \geq 0. \end{cases} \tag{5.73}$$

Since by Lemma 5.9, zeros $i\kappa_j$ of $w(\zeta)$ are simple, the residues work out to be $e^{i\pi s}\kappa_j^{2s}$. Hence,

$$\int_{\Gamma_{R,\varepsilon}} \frac{\frac{d}{d\zeta}\left(\frac{w(\zeta)}{\gamma - i\zeta}\right)}{\left(\frac{w(\zeta)}{\gamma - i\zeta}\right)} \zeta^{2s}\, d\zeta = 2\pi i\ e^{i\pi s} \sum_{j=1}^{N} \kappa_j^{2s} - 2\pi i\ e^{i\pi s} M_s(\gamma). \tag{5.74}$$

Next, we show that the integral over the semicircle C_r^+ tends to zero as $r \to \infty$ or $r \to 0$. Integrating by parts, we see that

$$\int_{C_r^+} \frac{\frac{d}{d\zeta}\left(\frac{w(\zeta)}{\gamma - i\zeta}\right)}{\left(\frac{w(\zeta)}{\gamma - i\zeta}\right)} \zeta^{2s}\, d\zeta = - 2s \int_{C_r^+} \ln\left(\frac{w(\zeta)}{\gamma - i\zeta}\right) \zeta^{2s-1}\, d\zeta + \ln\left(\frac{w(-r)}{\gamma + ir}\right)(-r)^{2s}$$
$$- \ln\left(\frac{w(r)}{\gamma - ir}\right) r^{2s}.$$

Note that we can choose $\ln(w(\zeta)/(\gamma - i\zeta))$ as a continuous function on C_r^+. If $r \to \infty$, then this integral tends to zero for Re $s < 1/2$ because of (5.57). If $r \to 0$, then the integral also tends to zero. Indeed, this follows from the fact that either $w(0) \neq 0$ or $w(\zeta)$ satisfies (5.69) with $w_0 \neq 0$. Therefore passing to the limits $R \to \infty$ and $\varepsilon \to 0$ in equality (5.74), we obtain that

$$\int_{-\infty}^{\infty} \frac{\frac{d}{dk}\left(\frac{w(k)}{\gamma - ik}\right)}{\left(\frac{w(k)}{\gamma - ik}\right)} k^{2s}\, dk = 2\pi i\ e^{i\pi s} \sum_{j=1}^{N} \kappa_j^{2s} - 2\pi i\ e^{i\pi s} \begin{cases} (-\gamma)^{2s}, & \text{if } \gamma < 0 \\ 0, & \text{if } \gamma \geq 0. \end{cases} \tag{5.75}$$

Integrating in the left-hand side by parts and taking into account relations (5.31) and (5.33), we obtain

$$\int_{-\infty}^{\infty} \frac{\frac{d}{dk}\left(\frac{w(k)}{\gamma - ik}\right)}{\left(\frac{w(k)}{\gamma - ik}\right)} k^{2s}\, dk = -2s \int_{-\infty}^{\infty} \ln\left(\frac{w(k)}{\gamma - ik}\right) k^{2s-1}\, dk$$
$$= -2s \int_{-\infty}^{\infty} (\ln a(k) + i\eta(k)) k^{2s-1}\, dk$$
$$= -2s \int_{0}^{\infty} (\ln a(k) + i\eta(k)) k^{2s-1}\, dk + 2s e^{2i\pi s} \int_{0}^{\infty} (\ln a(k) - i\eta(k)) k^{2s-1}\, dk$$
$$= 2s(e^{2i\pi s} - 1)F(s) - 2is(e^{2i\pi s} + 1)G(s).$$

Comparing this equation with (5.75), we arrive at (5.72). $\square$

In order to prove trace identities for arbitrary powers $s \in \mathbb{C}_+$, we need the analytic continuation of the functions $F(s)$ and $G(s)$ to the entire half-plane $\mathrm{Re}\, s > 0$.

Lemma 5.18. *Let estimates* (5.47) *and* (5.60) *be satisfied. Then the functions* F *and* G *are meromorphic in the half-plane* $\operatorname{Re} s > 0$*. The function* F *is analytic everywhere except for simple poles at integer points* $s = n$, $n \in \mathbb{N}$, *with residues*

$$\operatorname{Res}_{s=n} F(s) = (-1)^{n+1} 2^{-2n-1} \ell_{2n}, \quad n \in \mathbb{N}.$$

If $\operatorname{Re} s < 1$, *then representation* (5.71) *for* $F(s)$ *remains true. If* $n < \operatorname{Re} s < n+1$, *then*

$$F(s) = \int_0^\infty \left(\ln a(k) - \sum_{j=1}^{n} (-1)^j \ell_{2j} (2k)^{-2j} \right) k^{2s-1}\, dk.$$

The function G *is analytic everywhere except for simple poles at half-integer points* $s = n + 1/2$, $n \in \mathbb{N}_0$, *with residues*

$$\operatorname{Res}_{s=n+1/2} G(s) = (-1)^n 2^{-2n-2} \ell_{2n+1}, \quad n \in \mathbb{N}_0.$$

If $n \geq 1$ *and* $n - 1/2 < \operatorname{Re} s < n + 1/2$, *then*

$$G(s) = \int_0^\infty \left(\eta(k) - \sum_{j=0}^{n-1} (-1)^{j+1} \ell_{2j+1} (2k)^{-2j-1} \right) k^{2s-1}\, dk. \tag{5.76}$$

Proof. We can write the function F, given in Lemma 5.18 as follows

$$F(s) = \int_0^1 \ln a(k) k^{2s-1}\, dk + \int_1^\infty \left(\ln a(k) - \sum_{j=1}^{n} (-1)^j \ell_{2j} (2k)^{-2j} \right) k^{2s-1}\, dk \tag{5.77}$$
$$- \int_0^1 \sum_{j=1}^{n} (-1)^j \ell_{2j} (2k)^{-2j} k^{2s-1}\, dk.$$

The first integral in the right-hand side of equation (5.77) is an analytic function of s in the entire half-plane $\operatorname{Re} s > 0$. The second integral is in view of (5.59) an analytic function of s in the strip $0 < \operatorname{Re} s < n+1$. For $\operatorname{Re} s > n$, we have

$$\int_0^1 \sum_{j=1}^{n} (-1)^j \ell_{2j} (2k)^{-2j} k^{2s-1}\, dk = \sum_{j=1}^{n} (-1)^j 2^{-2j-1} \ell_{2j} (s-j)^{-1}.$$

Thus, the function F is an analytic function in the strip $n < \operatorname{Re} s < n+1$.
Similarly, we split the integral in the right-hand side of (5.76). Note that we now have for $n \geq 1$ and $\operatorname{Re} s > n - 1/2$,

$$\int_0^1 \sum_{j=0}^{n-1} (-1)^{j+1} \ell_{2j+1} (2k)^{-2j-1} k^{2s-1}\, dk = \sum_{j=0}^{n-1} (-1)^{j+1} \ell_{2j+1} 2^{-2j-2} (s - j - 1/2)^{-1}.$$

Therefore, it follows with analog arguments as for F that the function G, given in (5.76), is an analytic function of s in the strip $n - 1/2 < \operatorname{Re} s < n + 1/2$. $\square$

Theorem 5.19. *Let estimates* (5.47) *and* (5.60) *be satisfied. Then*

$$\sum_{j=1}^{N} |\lambda_j|^{1/2} - M_{1/2}(\gamma) - \frac{1}{\pi} \int_0^\infty \ln a(k)\, dk = \frac{1}{4} \ell_1 \tag{5.78}$$

and for $n \geq 1,\ n \in \mathbb{N}$,

$$\sum_{j=1}^{N} |\lambda_j|^n - M_n(\gamma) + (-1)^n \frac{2n}{\pi} \int_0^\infty \left(\eta(k) - \sum_{j=0}^{n-1} (-1)^{j+1} \ell_{2j+1} (2k)^{-2j-1} \right) k^{2n-1}\, dk = -\frac{n}{2^{2n}} \ell_{2n}, \tag{5.79}$$

$$\begin{aligned} \sum_{j=1}^{N} |\lambda_j|^{n+1/2} &- M_{n+1/2}(\gamma) + (-1)^{n+1} \frac{2n+1}{\pi} \int_0^\infty \left(\ln a(k) - \sum_{j=1}^{n} (-1)^j \ell_{2j} (2k)^{-2j} \right) k^{2n}\, dk \\ &= \frac{2n+1}{2^{2n+2}} \ell_{2n+1}. \end{aligned} \tag{5.80}$$

The coefficients ℓ_n *are given as in* (5.58).

Proof. Using the analytic continuation, given in Lemma 5.18, formula (5.72) can be extended to all s in the half-plane $\operatorname{Re} s > 0$. In particular, setting $s = n,\ n \in \mathbb{N}$, we obtain

$$\frac{\pi}{2n} \sum_{j=1}^{N} |\lambda_j|^n - \frac{\pi}{2n} M_n(\gamma) = (-1)^n \left(\pi \operatorname{Res}_{s=n} F(s) - G(n) \right).$$

Taking into account Lemma 5.18, we conclude formula (5.79). Similarly, we have for $s = n + 1/2$, where $n \in \mathbb{N}_0$, the following identity

$$\frac{\pi}{2n+1} \sum_{j=1}^{N} |\lambda_j|^{n+1/2} - \frac{\pi}{2n+1} M_{n+1/2}(\gamma) = (-1)^n \left(F(n+1/2) + \pi \operatorname{Res}_{s=n+1/2} G(s) \right).$$

Again, in view of Lemma 5.18, we conclude formulas (5.78) and (5.80). □

We compute the first four trace formulas.

Corollary 5.20. *Let estimates* (5.47) *and* (5.60) *be satisfied. Then*

$$\begin{aligned} \sum_{j=1}^{N} |\lambda_j|^{1/2} - M_{1/2}(\gamma) - \frac{1}{\pi} \int_0^\infty \ln a(k)\, dk &= -\frac{1}{4} \int_0^\infty V(x)\, dx, \\ \sum_{j=1}^{N} |\lambda_j| - M_1(\gamma) - \frac{2}{\pi} \int_0^\infty \left(\eta(k) - \frac{\int_0^\infty V(x)\, dx}{2k} \right) k\, dk &= -\frac{1}{4} V(0), \\ \sum_{j=1}^{N} |\lambda_j|^{3/2} - M_{3/2}(\gamma) + \frac{3}{\pi} \int_0^\infty \left(\ln a(k) + \frac{V(0)}{(2k)^2} \right) k^2\, dk &= \frac{3}{16} \ell_3, \end{aligned}$$

where

$$\ell_3 = \int_0^\infty V^2(x)\, dx - V'(0) + 4\gamma V(0),$$

$$\begin{aligned} \sum_{j=1}^{N} |\lambda_j|^2 &- M_2(\gamma) + \frac{4}{\pi} \int_0^\infty \left(\eta(k) - \frac{\int_0^\infty V(x)\, dx}{2k} - \frac{\int_0^\infty V^2(x)\, dx + 4\gamma V(0) - V'(0)}{(2k)^3} \right) k^3\, dk \\ &= -\frac{1}{8} \ell_4, \end{aligned}$$

where

$$\ell_4 = V''(0) + 8\gamma^2 V(0) - 4\gamma V'(0) - 2V^2(0).$$

Finally, we prove a trace formula of order zero for the operator H with boundary conditions (5.4). Such formulas are called in the literature the *Levinson formula* and relate the number of negative eigenvalues of H to the phase shift η.

We define $\eta(0) = \lim_{\zeta\to 0+}\eta(\zeta)$. Obviously this limit exists if $w(0) \neq 0$. In the case $w(0) = 0$ the existence follows from asymptotics (5.69).

Theorem 5.21. *Suppose* (5.60) *and let N be the number of negative eigenvalues of the operator H with boundary condition* (5.4)*. Then, the following formulas hold.*
For $w(0) \neq 0$,

$$\eta(\infty) - \eta(0) = \begin{cases} \pi N & \text{if } \gamma > 0, \\ \pi(N - \frac{1}{2}) & \text{if } \gamma = 0, \\ \pi(N-1) & \text{if } \gamma < 0. \end{cases} \tag{5.81}$$

For $w(0) = 0$,

$$\eta(\infty) - \eta(0) = \begin{cases} \pi(N + \frac{1}{2}) & \text{if } \gamma > 0, \\ \pi N & \text{if } \gamma = 0, \\ \pi(N - \frac{1}{2}) & \text{if } \gamma < 0. \end{cases} \tag{5.82}$$

Proof. We apply the argument principle to the function $D(\zeta)$ and the contour $\Gamma_{R,\varepsilon}$ given in Figure 1. We choose R and ε such that all of the N negative eigenvalues of H lie inside the contour $\Gamma_{R,\varepsilon}$. Remember that if $\gamma < 0$, then H_0 has a simple negative eigenvalue $-\gamma^2$. Thus, it follows with Lemma 5.9 that

$$\int_{\Gamma_{R,\varepsilon}} \frac{\frac{d}{d\zeta}\left(\frac{w(\zeta)}{\gamma - i\zeta}\right)}{\left(\frac{w(\zeta)}{\gamma - i\zeta}\right)}\, d\zeta = \begin{cases} 2\pi i N & \text{if } \gamma \geq 0, \\ 2\pi i (N-1) & \text{if } \gamma < 0. \end{cases} \tag{5.83}$$

Note that the branch of the function $\ln D(\zeta)$ was fixed by the condition $\ln D(\zeta) \to 0$ as $|\zeta| \to \infty$. Thus, we have $\ln D(\zeta) = \ln|D(\zeta)| + i\arg\, D(\zeta)$. As for $k \in \mathbb{R}$, $\arg\, D(k) = \eta(k)$ and $\eta(-k) = -\eta(k)$, it follows from equation (5.83) that

$$2(\eta(R) - \eta(\varepsilon)) + \mathrm{var}_{C_R^+}\arg\, D(\zeta) + \mathrm{var}_{C_\varepsilon^+}\arg\, D(\zeta) = \begin{cases} 2\pi N & \text{if } \gamma \geq 0, \\ 2\pi(N-1) & \text{if } \gamma < 0. \end{cases} \tag{5.84}$$

Note that $\lim_{R\to\infty} \mathrm{var}_{C_R^+}\arg\, D(\zeta) = 0$ because of (5.57). To compute $\lim_{\varepsilon\to 0}\mathrm{var}_{C_\varepsilon^+}\arg\, D(\zeta)$, we rewrite

$$\mathrm{var}_{C_\varepsilon^+}\arg\, D(\zeta) = \mathrm{var}_{C_\varepsilon^+}\arg\, w(\zeta) - \mathrm{var}_{C_\varepsilon^+}\arg(\gamma - i\zeta). \tag{5.85}$$

Considering (5.69), we get

$$\lim_{\varepsilon\to 0}\mathrm{var}_{C_\varepsilon^+}\arg\, w(\zeta) = \begin{cases} 0 & \text{if } w(0) \neq 0, \\ -\pi & \text{if } w(0) = 0. \end{cases} \tag{5.86}$$

The second term in the right-hand side of (5.85) depends on the sign of γ and turns out to be in the limit,

$$\lim_{\varepsilon\to 0}\mathrm{var}_{C_\varepsilon^+}\arg(\gamma - i\zeta) = \begin{cases} 0 & \text{if } \gamma > 0, \\ -\pi & \text{if } \gamma = 0, \\ 0 & \text{if } \gamma < 0. \end{cases} \tag{5.87}$$

Combining (5.86) and (5.87) with equation (5.84), formulas (5.81) and (5.82) follow immediately. □

6. Appendix A. Proof of Lemma 5.4

For the sake of completeness, we prove here Lemma 5.4. In order to do so, we have to recall the construction of the Jost solution from [98, Lemma 4.1.4] .

Instead of constructing $\theta(x,\zeta)$, it is more convenient to construct the function $b(x,\zeta)$, defined in (5.48) with asymptotics (5.50). The differential equation (5.49) is equivalent to the integral equation

$$b(x,\zeta) = 1 + (2i\zeta)^{-1}\int_x^\infty (e^{2i\zeta(y-x)} - 1)V(y)b(y,\zeta)\, dy \tag{6.1}$$

considered on the class of bounded functions $b(x,\zeta)$. Its solution $b(x,\zeta)$ can be constructed by the method of successive approximations. Set $b_0(x,\zeta) = 1$ and

$$b_{n+1}(x,\zeta) = (2i\zeta)^{-1}\int_x^\infty (e^{2i\zeta(y-x)} - 1)V(y)b_n(y,\zeta)\, dy. \tag{6.2}$$

Under assumption (5.18), it follows successively that

$$|b_n(x,\zeta)| \le |\zeta|^{-n}(n!)^{-1}\left(\int_x^\infty |V(y)|\, dy\right)^n. \tag{6.3}$$

This follows inductively as follows. Using the estimate

$$|e^{2i\zeta(y-x)} - 1| \le 2, \quad x \le y,\ \operatorname{Im}\zeta \ge 0,$$

we get from (6.2) the estimate

$$\begin{aligned} |b_{n+1}(x,\zeta)| &\le |\zeta|^{-n-1}(n!)^{-1}\int_x^\infty |V(y)|\left(\int_y^\infty |V(t)|\, dt\right)^n dy \\ &= |\zeta|^{-n-1}(n!)^{-1}(n+1)^{-1}\int_x^\infty \frac{d}{dy}\left(\int_y^\infty |V(t)|\, dt\right)^{n+1} dy. \end{aligned}$$

Thus, $|b_{n+1}(x,\zeta)|$ is bounded from above by $|\zeta|^{-n-1}((n+1)!)^{-1}\left(\int_x^\infty |V(y)|\, dy\right)^{n+1}$, which proves (6.3). For any fixed $x \ge 0$, every function $b_n(x,\zeta)$ is analytic in ζ in the upper half-plane $\operatorname{Im}\zeta > 0$ and is continuous in ζ up to the real axis, with exception of the point $\zeta = 0$. It follows from (6.3) that the limit

$$b(x,\zeta) := \lim_{N\to\infty} b^{(N)}(x,\zeta), \quad \text{where } b^{(N)}(x,\zeta) = \sum_{n=0}^N b_n(x,\zeta), \tag{6.4}$$

exists for all $x \ge 0$ uniformly with respect to ζ for $|\zeta| \ge c > 0$. Therefore the function $b(x,\zeta)$ has the same analytic properties in the variable ζ as the functions $b_n(x,\zeta)$. Moreover, estimates (6.3) show that $b(x,\zeta)$ is a bounded function of x. Putting together definitions (6.2) and (6.4), we see that

$$b^{(N)}(x,\zeta) = 1 - b_{N+1}(x,\zeta) + (2i\zeta)^{-1}\int_x^\infty (e^{2i\zeta(y-x)} - 1)V(y)b^{(N)}(y,\zeta)\, dy.$$

Passing here to the limit $N \to \infty$, we arrive at equation (6.1). The uniqueness of a bounded solution $b(x,\zeta)$ of equation (6.1) follows from estimate (6.3) for a solution of the corresponding homogeneous equation. This estimate implies that $b(x,\zeta) = 0$.

Proof of Lemma 5.4. By (6.4), we have

$$\theta(x,\zeta) = e^{i\zeta x} \lim_{N\to\infty} \sum_{n=0}^{N} b_n(x,\zeta), \tag{6.5}$$

where $b_n(x,\zeta)$ is given as in (6.2). As the limit in (6.5) exists for all $x \geq 0$ uniformly with respect to ζ for $|\zeta| \geq c > 0$, it follows that

$$\theta'(x,\zeta) = i\zeta e^{i\zeta x} \lim_{N\to\infty} \sum_{n=0}^{N} b_n(x,\zeta) + e^{i\zeta x} \lim_{N\to\infty} \sum_{n=0}^{N} b_n'(x,\zeta).$$

Obviously, we have $b_0'(x,\zeta) = 0$ and from (6.2), we derive

$$b_n'(x,\zeta) = -\int_x^\infty e^{2i\zeta(y-x)} V(y) b_{n-1}(y,\zeta)\ dy.$$

Thus,

$$\begin{aligned} \left|\theta'(x,\zeta) - i\zeta e^{i\zeta x}\right| &= e^{-\operatorname{Im}\zeta x} |\zeta| \left| \lim_{N\to\infty} \sum_{n=1}^{N} b_n(x,\zeta) + \frac{1}{i\zeta} b_n'(x,\zeta) \right| \\ &= \frac{e^{-\operatorname{Im}\zeta x}}{2} \left| \lim_{N\to\infty} \sum_{n=1}^{N} \int_x^\infty \left(e^{2i\zeta(y-x)} + 1 \right) V(y) b_{n-1}(y,\zeta)\, dy \right|. \end{aligned} \tag{6.6}$$

Using the estimate

$$|e^{2i\zeta(y-x)} + 1| \leq 2, \quad x \leq y, \quad \operatorname{Im}\zeta \geq 0,$$

we see that the term in (6.6) does not exceed

$$e^{-\operatorname{Im}\zeta x} \lim_{N\to\infty} \sum_{n=0}^{N} \int_x^\infty |V(y)|\, |b_n(y,\zeta)|\, dy. \tag{6.7}$$

Because of (6.3), expression (6.7) is less or equal

$$e^{-\operatorname{Im}\zeta x} \lim_{N\to\infty} \sum_{n=0}^{N} |\zeta|^{-n} (n!)^{-1} \int_x^\infty |V(y)| \left(\int_y^\infty |V(t)|\, dt \right)^n dy,$$

which is equivalent to

$$e^{-\operatorname{Im}\zeta x} |\zeta| \left(\exp\left(|\zeta|^{-1} \int_x^\infty |V(y)|\, dy \right) - 1 \right).$$

This proves (5.21). If $|\zeta| \geq k > 0$ and condition (5.18) is satisfied, then estimate (5.22) follows from (5.21). $\square$

7. The spectral shift function and Levinson's theorem for quantum star graphs

Semra Demirel

Abstract. We consider the Schrödinger operator on a star shaped graph with n edges joined at a single vertex. We derive an expression for the trace of the difference of the perturbed and unperturbed resolvent in terms of a Wronskian. This leads to representations for the perturbation determinant and the spectral shift function, and to an analog of Levinson's formula.

7.1. **Introduction and main results.**

7.1.1. *Introduction.* This article focuses on the study of the spectral shift function and a Levinson theorem for Schrödinger operators on star shaped graphs. Quantum mechanics on graphs has a long history in physics and physical chemistry [43, 80], but recent progress in experimental solid state physics has renewed attention on them as idealized models for thin domains. A large literature on the subject has arisen and we refer, for instance, to the bibliography given in [7, 27].

A *star graph* is a metric graph Γ with a single vertex in which a finite number $n \geq 2$ of edges e_j are joined. We assume throughout that all edges e_j are infinite and we identify $e_j = [0, \infty)$. We assume that the potential V is a real-valued function on Γ satisfying

$$\int_{e_j} |V_j(x_j)|\, dx_j < \infty \quad \text{for all } 1 \leq j \leq n, \tag{7.1}$$

where we denoted the restriction of V to the edge e_j by $V_j(x_j) = V(x)|_{e_j}$. Under this condition, we can define the Schrödinger operator

$$H\psi := -\psi'' + V\psi \tag{7.2}$$

with continuity and Kirchhoff vertex conditions

$$\psi_1(0) = \ldots = \psi_n(0) =: \psi(0), \quad \sum_{j=1}^{n} \psi_j'(0) = 0, \tag{7.3}$$

as a self-adjoint operator in the Hilbert space $L_2(\Gamma) = \oplus_{j=1}^{n} L_2(e_j)$. In (7.3) we denoted by ψ_j the restriction of ψ to the edge e_j. More precisely, we define the operator H via the closed quadratic form

$$h[\phi] := \int_\Gamma |\phi'(x)|^2\, dx + \int_\Gamma V(x)|\phi(x)|^2\, dx\,,$$

with form domain $d(h) = H^1(\Gamma)$ consisting of all continuous functions ϕ on Γ such that $\phi_j \in H^1(e_j)$ for every j. If V is sufficiently regular in a neighborhood of the vertex, then functions ϕ in the operator domain of H satisfy the Kirchhoff vertex condition in (7.3); otherwise this condition has to be interpreted in a generalized sense.

Our two main results are formulas for the spectral shift function and the perturbation determinant of H with respect to the unperturbed operator H_0 (which is defined similarly as H, but with $V \equiv 0$) and an analog of Levinson's theorem. Special attention will be paid to the existence or absence of zero energy resonances.

There are several motivations for this study. The first one is the scattering theory of quantum graphs. While star graphs are certainly very special graphs, it is generally believed that they are a correct model example for a scattering process in the presence of a vertex. The direct and indirect scattering theory on star graphs has been studied in great detail in [34] and [46]. Our results complement theirs and, in contrast to them, we advertise a more operator theoretic approach including, for instance, Fredholm determinants, trace class estimates and Kreĭn's resolvent formula.

A second motivation is a line of thought that goes back at least to Jost and Pais [57]; see also [40, 79, 87]. In these works, a perturbation determinant, which is a Fredholm determinant in an infinite dimensional space, is shown to be equal to a much simpler determinant, typically in a finite dimensional space, such as a Wronski determinant. While such formulas appear in different set-ups, there seems to be no general method of knowing in advance the form of the 'simpler determinant'. One of the achievements of this paper is to derive a new formula of this kind for a star graph.

A third motivation comes from the general interest in zero energy resonances because of their key role in several diverse problems of mathematical physics; for instance, the Efimov effect in many-body quantum mechanics [23] and the time decay of wave functions [56]. Also in the study of convergence of 'thick quantum graphs' resonances play an important role. It was shown in [41] that squeezing a fattened graph with Dirichlet boundary condition can lead in the limit to a nontrivial coupling due to threshold resonances. (While this coupling is not necessarily Kirchhoff, the squeezing of a Neumann tubular manifold leads generically to Kirchhoff vertex conditions.) We also refer to the survey [13,14]. In particular, we hope that our results will allow us to remove the non-resonance assumption in the recent dispersive estimates on star graphs [75]; see also [93] for similar bounds in the whole line case.

Finally, we note that the derivation of a Levinson theorem for a graph with a finite number of unbounded edges was mentioned as an open problem in [17] (who considered the discrete case). While the compact part of the graph still has to be better understood, our analysis explains how to deal with several unbounded edges and will be useful, we believe, in further developments in this direction.

7.1.2. *Main results.* To state our main result, namely a trace formula for the operator (7.2) with vertex condition (7.3), we need some notations. By $H_{D,j}$ we denote the half-line Schrödinger operator with potential $V_j = V|_{e_j}$ and Dirichlet boundary condition at the origin. The self-adjoint operator

$$H_{D,j} = -\frac{d^2}{dx_j^2} + V_j$$

on $L_2(e_j)$ is associated with the quadratic form

$$h_{D,j}[\phi_j] := \int_{e_j} |\phi_j'(x_j)|^2 \, dx_j + \int_{e_j} V_j(x_j)|\phi_j(x_j)|^2 \, dx_j, \quad \phi_j \in H^{0,1}(e_j),$$

where the form domain is given by $d(h_{D,j}) = H^{0,1}(e_j) = \{\phi_j \in H^1(e_j) : \phi_j(0) = 0\}$. If the condition (7.1) is satisfied, then the equation

$$-u'' + Vu = zu, \quad z = \zeta^2$$

has two particular solutions, the *regular solution* φ_j and the *Jost solution* θ_j. The first one is characterized by the conditions

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

and the latter one by the asymptotics $\theta_j(x,\zeta) = e^{ix\zeta}(1 + o(1))$ as $|\zeta| \to \infty$. Both solutions are unique, see for instance [98]. The *Jost function* $w_j(\zeta)$ is defined as the Wronskian of the regular solution and the Jost solution and turns out to be $w_j(\zeta) = \theta_j(0,\zeta)$.

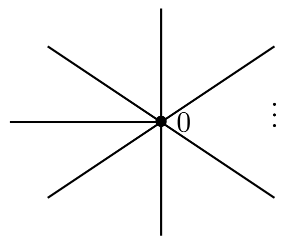

FIGURE 9. star graph Γ

Our first main result is

Theorem 7.1. *Let* Γ *be a star shaped graph and assume that* (7.1) *is satisfied for* $1 \le j \le n$. *Then, for the Schrödinger operator* (7.2) *on* $L_2(\Gamma)$ *with Kirchhoff vertex condition* (7.3), *the following trace formula holds,*

$$\operatorname{Tr}\left((H_0 - \zeta^2)^{-1} - (H - \zeta^2)^{-1}\right) = \frac{1}{2\zeta}\frac{d}{d\zeta}\ln\left(\frac{K(\zeta)}{\zeta}\prod_{j=1}^{n} w_j(\zeta)\right), \quad \operatorname{Im}\zeta > 0, \tag{7.4}$$

where $K(\zeta) = \sum_{j=1}^{n} \theta_j'(0,\zeta)/\theta_j(0,\zeta)$ *and* $w_j(\zeta) = \theta_j(0,\zeta)$.

Remark 7.2. We note that identity (7.4) is equivalent to the identity

$$\operatorname{Tr}\left((H_0 - \zeta^2)^{-1} - (H - \zeta^2)^{-1}\right) = \frac{1}{2\zeta}\left(\sum_{j=1}^{n} \frac{\frac{d}{d\zeta}w_j(\zeta)}{w_j(\zeta)} + \frac{\frac{d}{d\zeta}K(\zeta)}{K(\zeta)} - \frac{1}{\zeta}\right),$$

which should be compared with the classical result [16, 57], see also [87, 98],

$$\operatorname{Tr}\left((H_{D,j,0} - \zeta^2)^{-1} - (H_{D,j} - \zeta^2)^{-1}\right) = \frac{\frac{d}{d\zeta}w_j(\zeta)}{2\zeta w_j(\zeta)}. \tag{7.5}$$

From equation (7.4), we conclude in Section 7.3 an explicit expression for the perturbation determinant $D(z)$ and the spectral shift function $\xi(\lambda; H, H_0)$. We recall that the spectral shift function can be characterized by the formula

$$\operatorname{Tr}\left(f(H) - f(H_0)\right) = \int_{-\infty}^{\infty} \xi(\lambda; H, H_0) f'(\lambda)\, d\lambda,$$

for any $f \in C_0^\infty(\mathbb{R})$ (together with the condition $\xi(\lambda; H, H_0) = 0$ for $\lambda < \inf \sigma(H)$). An extension of this formula for a broader class of functions, as well as several equivalent definitions are discussed in Section 3.

In Section 7.4 we study the low-energy asymptotics of $D(z)$ as $|z| \to 0$. This allows us to prove an analog of Levinson's formula for the star graph. We say that the operator H on $L_2(\Gamma)$, given in (7.2), has a *resonance* at $\zeta = 0$ if the equation $-u'' + Vu = 0$ has a non-trivial bounded solution satisfying the continuity and Kirchhoff conditions. By definition, the *multiplicity of the resonance* is the dimension of the corresponding solution space.

Theorem 7.3. *Assume that*

$$\int_{e_j} (1+x)|V_j(x)|\, dx < \infty \quad \textit{for all } 1 \leq j \leq n, \tag{7.6}$$

is satisfied and, if $\zeta = 0$ is a resonance of multiplicity one, assume that

$$\int_{e_j} (1+x^2)|V_j(x)|\, dx < \infty \quad \textit{for all } 1 \leq j \leq n. \tag{7.7}$$

Then,

$$\lim_{\lambda \to 0+} \xi(\lambda) = -\left(N + \frac{m-1}{2}\right), \tag{7.8}$$

where N is the number of negative eigenvalues of H and where $m \geq 1$ is the multiplicity if $\zeta = 0$ is a resonance and $m = 0$ if $\zeta = 0$ is not a resonance.

Remark 7.4. We know from Bargmann's bound that $N < \infty$ if (7.6) is satisfied, [5]. We also know that $\lim_{\lambda \to 0-} \xi(\lambda) = -N$, which is an easy consequence of the definition of the spectral shift function.

7.2. **A Trace formula for Star Graphs.** In this section, our goal is to prove a trace formula for star graphs. More precisely, we will find an expression for $\mathrm{Tr}(R(z) - R_0(z))$ in terms of the Jost solutions θ_j on the edges e_j. Here and in the following we write $R(z) = (H - z)^{-1}$ and $R_0(z) = (H_0 - z)^{-1}$ for the perturbed and unperturbed resolvent, respectively. When deriving an expression for the resolvent $R(z)$, we will make use of Kreĭn's formula for which we refer to [3] and, in particular, to an article by Exner [26] where this formula was used in a similar context. Thereby, we need to decouple the operator H which we achieve by imposing Dirichlet vertex conditions on each edge e_j, i.e., $\psi_j(0) = 0$ for all $1 \leq j \leq n$. Then the operator (7.2) is decoupled and the half-lines are disconnected. We denote the decoupled operator by

$$H_\infty = \bigoplus_{j=1}^{n} H_{D,j}$$

and its resolvent by $R_\infty(z) = (H_\infty - z)^{-1}$. In what follows, we will skip for simplicity the indices at the coordinates and use the notation $\psi_j(x) := \psi_j(x_j),\ 1 \leq j \leq n$, for a function defined on the edge e_j of Γ.

Proof of Theorem 7.1. It is a well-known fact, see e.g. [98], that under assumption (7.1) for all $z = \zeta^2$ such that $\mathrm{Im}\, z \neq 0$ and $w_j(\zeta) \neq 0$, the resolvent $R_{D,j}(z) = (H_{D,j} - z)^{-1}$ is an integral operator with kernel

$$R_{D,j}(x,y;z) := \frac{\varphi_j(x,\zeta)\theta_j(y,\zeta)}{w_j(\zeta)}, \quad x \le y, \quad \zeta = z^{1/2},$$

and $R_{D,j}(x,y;z) = R_{D,j}(y,x;z)$. Hence, the resolvent $R_\infty(z)$ is a matrix integral operator with the kernel

$$R^\infty_{j,\ell}(x,y;z) := \delta_{j,\ell} R_{D,j}(x,y,z), \quad 1 \le j,\ell \le n.$$

Having the resolvent kernel $R^\infty_{j,\ell}$ of the decoupled operator H_∞, we can use Kreĭn's formula [3] to determine the kernel of the resolvent $R(z)$. Let $\rho(H)$ be the resolvent set of the operator H and $\rho(H_0)$ the resolvent set of H_0. The formula states that for any ζ, such that $\operatorname{Im}\zeta \ge 0$ and $z = \zeta^2 \in \rho(H_\infty) \cap \rho(H)$, the resolvent $R(z)$ is a matrix integral operator with kernel $R_{j,\ell}(x,y;z) = R^\infty_{j,\ell}(x,y;z) + \lambda_{j\ell}\theta_j(x,\zeta)\theta_\ell(y,\zeta)$. In order to determine the coefficients $\lambda_{j\ell}$ we proceed as follows. For any $f = (f_1(x),\ldots,f_n(x))^T \in L_2(\Gamma)$, the function $\psi(x) := \int R(x,y;z)f(y)\,dy$ has to satisfy the equation $H\psi = \zeta^2\psi + f$ and the Kirchhoff vertex condition. This leads to a system of n linear equations for the coefficients $\lambda_{j\ell}$. It turns out that $\lambda_{j\ell} = (-K(\zeta)\theta_j(0,\zeta)\theta_\ell(0,\zeta))^{-1}$, with $K(\zeta) = \sum_{j=1}^n \theta_j'(0,\zeta)/\theta_j(0,\zeta)$, see also [26]. Thus,

$$R_{j,\ell}(x,y;z) := R^\infty_{j,\ell}(x,y;z) - \frac{\theta_j(x,\zeta)\theta_\ell(y,\zeta)}{K(\zeta)\theta_j(0,\zeta)\theta_\ell(0,\zeta)}. \tag{7.9}$$

This representation allows us to compute $\operatorname{Tr}(R(z) - R_0(z))$. First, we note that the operator $R(z) - R_0(z)$ is a trace class operator. This can be seen as follows. As the quotient in (7.9) is a perturbation of finite rank, we only have to show that the difference $R_\infty(z) - R^{(0)}_\infty(z)$ is trace class. Here $R^{(0)}_\infty(z)$ is the resolvent of the unperturbed decoupled operator $H^{(0)}_\infty = \bigoplus_{j=1}^n \left(-d^2/dx^2\right)$ on $\bigoplus_{j=1}^n L_2(e_j)$. Similarly, we denote by $R^{(0)}_{D,j}(z)$ the resolvent of the unperturbed operator $H^{(0)}_{D,j} = -d^2/dx^2$ on $L_2(e_j)$. Under condition (7.1) the operator $\sqrt{|V_j|}\left(R^{(0)}_{D,j}(z)\right)^\alpha$ is Hilbert-Schmidt for all $\alpha > 1/4$ and all $1 \le j \le n$, as can be easily checked, see e.g. [Lemma 4.5.1, [98]]. Hence, the Birman-Schwinger operator $\sqrt{|V_j|}R^{(0)}_{D,j}(z)\sqrt{V_j}$, with $\sqrt{V_j} := \operatorname{sgn}(V_j)\sqrt{|V_j|}$, is trace class and has for $z \in \rho(H_{D,j})$ no eigenvalue -1. Thus, the following resolvent identity for the half-line Schrödinger operator holds,

$$R_{D,j}(z) - R^{(0)}_{D,j}(z) = -R^{(0)}_{D,j}(z)\sqrt{V_j}\left(\mathbb{1} + \sqrt{|V_j|}R^{(0)}_{D,j}(z)\sqrt{V_j}\right)^{-1}\sqrt{|V_j|}R^{(0)}_{D,j}(z).$$

It follows from this resolvent identity that $R_\infty(z) - R^{(0)}_\infty(z)$ is a trace class operator. In view of (7.9) it follows that also $R(z) - R_0(z)$ is a trace class operator and

$$\begin{aligned} \operatorname{Tr}(R(z) - R_0(z)) &= \sum_{j=1}^n \int_{e_j} \left(R_{D,j}(x,x,z) - R^{(0)}_{D,j}(x,x,z)\right) dx \\ &\quad + \sum_{j=1}^n \int_{e_j} \left(-\frac{\theta_j^2(x,\zeta)}{\theta_j^2(0,\zeta)K(\zeta)} + \frac{e^{2ix\zeta}}{ni\zeta}\right) dx. \end{aligned} \tag{7.10}$$

The computation of the first integral on the right-hand side is the classical Jost-Pais result [57] recalled in Remark 7.2,

$$\int_{e_j} \left(R_{D,j}(x,x,z) - R^{(0)}_{D,j}(x,x,z) \right) dx = -\frac{\dot{w}_j(\zeta)}{2\zeta w_j(\zeta)}. \tag{7.11}$$

Here the derivative with respect to ζ is denoted by a dot, "$\cdot = d/d\zeta$". To compute the second integral, we use the following equation which is true for any two arbitrary solutions of the equation $H_{D,j}\psi_j = \zeta^2\psi_j$, namely

$$2\zeta u_j(x,\zeta)v_j(x,\zeta) = (u_j'(x,\zeta)\dot{v}_j(x,\zeta) - u_j(x,\zeta)\dot{v}_j'(x,\zeta))'.$$

Applying this identity to $u_j = v_j = \theta_j$, we get

$$\int_{\mathbb{R}_+} \frac{\theta_j^2(x,\zeta)}{K(\zeta)\theta_j^2(0,\zeta)}\, dx = \frac{\left[\theta_j'(x,\zeta)\dot{\theta}_j(x,\zeta) - \theta_j(x,\zeta)\dot{\theta}_j'(x,\zeta)\right]_0^\infty}{2\zeta K(\zeta)\theta_j^2(0,\zeta)}.$$

First, we consider the case of compactly supported potential V_j. Then, for large x the Jost solution for the half-line Schrödinger operator $H_{D,j}$ is given by $\theta_j(x,\zeta) = e^{i\zeta x}$ and we have

$$\theta_j'(x,\zeta) = i\zeta e^{i\zeta x}, \quad \dot{\theta}_j(x,\zeta) = ixe^{i\zeta x}, \quad \dot{\theta}_j'(x,\zeta) = (i - x\zeta)e^{i\zeta x}.$$

Therefore, for large x,

$$\theta_j'(x,\zeta)\dot{\theta}_j(x,\zeta) - \theta_j(x,\zeta)\dot{\theta}_j'(x,\zeta) = ie^{2i\zeta x}.$$

Note that the function $e^{2i\zeta x}$ vanishes for $x \to \infty$, as $\operatorname{Im}\zeta > 0$. We therefore get

$$\sum_{j=1}^n \int_{\mathbb{R}_+} -\frac{\theta_j^2(y,\zeta)}{\theta_j^2(0,\zeta)K(\zeta)}\, dy = \sum_{j=1}^n \frac{\theta_j'(0,\zeta)\dot{\theta}_j(0,\zeta) - \theta_j(0,\zeta)\dot{\theta}_j'(0,\zeta)}{2\zeta K(\zeta)\theta_j^2(0,\zeta)} = -\frac{\frac{d}{d\zeta}K(\zeta)}{2\zeta K(\zeta)}. \tag{7.12}$$

By density arguments (see [Prop. 4.5.3, [98]]), based on the fact that $\sqrt{|V|}(H_{D,0}+\mathbb{1})^{-1/2}$ is a Hilbert-Schmidt operator under condition (7.1), the result can be extended to all potentials V_j satisfying (7.1). Similarly, we consider the case $V = 0$ and obtain

$$\sum_{j=1}^n \int_{\mathbb{R}_+} \frac{e^{2iy\zeta}}{ni\zeta}\, dy = \frac{1}{2\zeta^2}. \tag{7.13}$$

Combining (7.11), (7.12) and (7.13) with (7.10), we finally arrive at

$$\begin{aligned} \operatorname{Tr}(R(z) - R_0(z)) &= \frac{1}{2\zeta}\left(-\frac{\dot{K}(\zeta)}{K(\zeta)} + \frac{1}{\zeta} - \sum_{j=1}^n \frac{\dot{w}_j(\zeta)}{w_j(\zeta)} \right) \\ &= \frac{1}{2\zeta}\left(-\frac{d}{d\zeta}(\ln K(\zeta)) + \frac{d}{d\zeta}(\ln\zeta) - \sum_{j=1}^n \frac{d}{d\zeta}(\ln w_j(\zeta)) \right) \\ &= -\frac{1}{2\zeta}\left(\frac{d}{d\zeta}\ln\left(\zeta^{-1}K(\zeta)\prod_{j=1}^n w_j(\zeta) \right) \right). \end{aligned} \tag{7.14}$$

This is the claimed formula. □

7.3. **The perturbation determinant and the spectral shift function.** Identity (7.4) implies an explicit expression for the perturbation determinant

$$D(z) := \det(\mathbb{1} + \sqrt{V} R_0(z)\sqrt{|V|}), \quad z \in \rho(H_0),$$

where $\sqrt{V} = (\operatorname{sgn} V)\sqrt{|V|}$. Strictly speaking this is the *modified* perturbation determinant, nevertheless we shall refer to it simply as the perturbation determinant in what follows. Note that under the assumption (7.1) the perturbation determinant $D(z)$ is well-defined since the operator $\sqrt{|V|}(H_0 - z)^{-1/2}$ is Hilbert-Schmidt and therefore $\sqrt{V} R_0(z)\sqrt{|V|}$ is trace class. This follows as above from the fact that $\sqrt{|V_j|}\left(R_{D,j}^{(0)}(z)\right)^{1/2}$ is Hilbert-Schmidt for all $1 \leq j \leq n$ together with (7.9) for $V \equiv 0$ as the corresponding second term on the right-hand side of (7.9) is of finite rank.

Furthermore, a simple computation shows, see also [(0.9.36), [97]], that the perturbation determinant is related to the trace of the resolvent difference by

$$D^{-1}(z)D'(z) = \operatorname{Tr}(R_0(z) - R(z)), \quad z \in \rho(H_0) \cap \rho(H). \tag{7.15}$$

Hence, in view of Theorem 7.1 we conclude that

$$D^{-1}(z)D'(z) = \frac{\frac{d}{dz}\left(z^{-1/2}K(z^{1/2})\prod_j w_j(z^{1/2})\right)}{z^{-1/2}K(z^{1/2})\prod_j w_j(z^{1/2})},$$

here we choose the square root of z such that $\operatorname{Im} z^{1/2} > 0$. From which it follows that $D(z) = Cz^{-1/2}K(z^{1/2})\prod_{j=1}^n w_j(z^{1/2})$, for some $C \in \mathbb{C}$. The coefficient C is fixed by the asymptotics of a perturbation determinant, namely

$$\lim_{|\operatorname{Im} z| \to \infty} D(z) = 1. \tag{7.16}$$

This asymptotics is true if the operator $|V|^{1/2}(H_0 - z)^{-1/2}$ is Hilbert-Schmidt, see e.g. [(0.9.37), [97]]. As $|\zeta| \to \infty$, we have [21, 98]

$$w_j(\zeta) = \theta_j(0, \zeta) = 1 + O(|\zeta|^{-1}) \quad \text{and} \quad K(\zeta) = ni\zeta + O(1). \tag{7.17}$$

This implies that $C = 1/in$. Thus, we have proved

Corollary 7.5. *Assume that* (7.1) *is satisfied. Then, for $z \in \rho(H)$, the perturbation determinant of H with respect to H_0 is given by*

$$D(z) = \frac{K(z^{1/2})}{inz^{1/2}} \prod_{j=1}^n w_j(z^{1/2}), \tag{7.18}$$

where $\operatorname{Im} z^{1/2} > 0$.

Our next goal is to determine an explicit expression for the spectral shift function $\xi(\lambda; H, H_0)$ for the pair of operators H, H_0 in $L_2(\Gamma)$. If (7.1) is satisfied, then by the argumentation above the resolvent difference $R(z) - R_0(z)$ is trace class for all $z \in \rho(H)$. In this case it is known from general theory that for all $-c < \inf \sigma(H)$ there exists a real-valued function $\xi_c(\lambda)$ for the pair of operators $R(-c), R_0(-c)$ such that the relation

$$\operatorname{Tr}\left(f(R(-c)) - f(R_0(-c))\right) = \int_{-\infty}^{\infty} \xi_c(\lambda) f'(\lambda)\, d\lambda \tag{7.19}$$

is true for all functions $f \in C_0^\infty(\mathbb{R})$. This formula goes back to Lifshits [73].

The spectral shift function for the pair H, H_0 is defined by the relation

$$\xi(\lambda; H, H_0) := -\xi_c((\lambda + c)^{-1}, R(-c), R_0(-c)) \tag{7.20}$$

for $\lambda > -c$ and $\xi(\lambda; H, H_0) := 0$ for $\lambda \leq -c$. It can be shown that this definition is independent of the choice of c. By a change of variables the formula (7.19) for the pair R, R_0 can then be transformed into a formula for the pair H, H_0 and yields

$$\operatorname{Tr}\left(f(H) - f(H_0)\right) = \int_{-\infty}^{\infty} \xi(\lambda; H, H_0) f'(\lambda)\, d\lambda, \tag{7.21}$$

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

The next theorem among other things extends the class of admissible functions f in this trace formula.

Theorem 7.6. *Let H be the Schrödinger operator in $L_2(\Gamma)$ given in (7.2) with the Kirchhoff vertex condition and $H_0 = -d^2/dx^2$ the corresponding unperturbed operator. Assume that condition (7.1) is satisfied. Then, the spectral shift function for the pair of operators H, H_0 is given by*

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

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

Moreover,

$$\ln D(z) = \int_{-\infty}^{\infty} \xi(\lambda; H, H_0)(\lambda - z)^{-1}\, d\lambda, \quad z \in \rho(H_0) \cap \rho(H), \tag{7.22}$$

and (7.21) holds provided f has two locally bounded derivatives and for any $\varepsilon > 0$, $m > -1/2$ as $\lambda \to \infty$,

$$f'(\lambda) = O(\lambda^{-m-1-\varepsilon}), \quad f''(\lambda) = O(\lambda^{-2m-2}). \tag{7.23}$$

Finally for $m > -1/2$,

$$\int_{-\infty}^{\infty} |\xi(\lambda; H, H_0)|(1 + |\lambda|)^{-m-1}\, d\lambda < \infty.$$

In the proof of Theorem 7.6 we make use of some results from abstract scattering theory which we collect for the reader's convenience in the following proposition. These results can be found e.g. in [Chapter 0.9, [98]].

Proposition 7.7. *Let h and h_0 be lower semi-bounded operators on a Hilbert space and $v = h - h_0$. Assume that the operator $\sqrt{|v|}\,(r_0(-c))^{1/2}$ is Hilbert-Schmidt for some $c < \inf(\sigma(h) \cup \sigma(h_0))$, where $r_0(-c) = (h_0 + c)^{-1}$ and $r(-c) = (h + c)^{-1}$. Moreover, assume that*

$$\int_c^{\infty} \|r(-t) - r_0(-t)\|_1 t^{-m}\, dt < \infty \tag{7.24}$$

for some $m \in (-1, 0)$. Let the spectral shift function $\xi(\lambda; h, h_0)$ be defined as above and the (modified) perturbation determinant by

$$d(z) = \det(\mathbb{1} + \operatorname{sgn} v \sqrt{|v|} r_0(z) \sqrt{|v|}), \quad z \in \rho(h_0).$$

Then, $d(z) \to 1$ as $\operatorname{dist}(z, \sigma(h_0)) \to \infty$ and

$$\xi(\lambda; h, h_0) = \pi^{-1} \lim_{\varepsilon \to 0+} \arg d(\lambda + i\varepsilon), \tag{7.25}$$

where $\arg d(z) = \operatorname{Im}\ln d(z)$ *is defined via* $\ln d(z) \to 0$ *as* $\operatorname{dist}(z, \sigma(h_0)) \to \infty$. *Moreover,*

$$\ln d(z) = \int_{-\infty}^{\infty} \xi(\lambda; h, h_0)(\lambda - z)^{-1}\, d\lambda, \quad z \in \rho(h_0) \cap \rho(h), \tag{7.26}$$

and

$$\operatorname{Tr}(f(h) - f(h_0)) = \int_{-\infty}^{\infty} \xi(\lambda; h, h_0) f'(\lambda)\, d\lambda \tag{7.27}$$

provided f *is as in* (7.23). *Finally,*

$$\int_{-\infty}^{\infty} |\xi(\lambda; h, h_0)|(1 + |\lambda|)^{-m-1}\, d\lambda < \infty.$$

In what follows, we prove that for the case of star graphs Γ the condition (7.24) is satisfied for all $m > -1/2$. Then, by Proposition 7.7 the assertions of Theorem 7.6 will follow. We need to compute the trace norm of a rank two operator.

Lemma 7.8. *Let* $\mathcal{H}$ *be a Hilbert space and* $f, g \in \mathcal{H}$. *Further, assume that* $\mathcal{R} = (\cdot, f)f - (\cdot, g)g$ *is an operator of rank two on* $\mathcal{H}$. *Then, the trace norm of* $\mathcal{R}$ *is given by*

$$\|\mathcal{R}\|_1 = \left((\|f\|^2 + \|g\|^2)^2 - 4|(f, g)|^2\right)^{1/2}. \tag{7.28}$$

Proof. We may assume that $f \neq 0$, for otherwise formula (7.28) is obvious. We construct an orthonormal bases on $\operatorname{Ran}(\mathcal{R})$ by applying the Gram Schmidt process,

$$\mathcal{B} = \{f/\|f\|, \left(g - (f, g)f/\|f\|^2\right) / \left(\|g\|^2 - |(f, g)|^2/\|f\|^2\right)^{-1/2}\}.$$

The operator $\mathcal{R}$ is described by a 2×2 matrix $M = (m)_{k\ell}$, where

$$m_{11} = \|f\|^2 - |(f, g)|^2/\|f\|^2, \quad m_{22} = -\|g\|^2 + |(f, g)|^2/\|f\|^2,$$

$$m_{12} = \overline{m_{21}} = -\left((f, g)/\|f\|\right)\left(\|g\|^2 - |(f, g)|^2/\|f\|^2\right)^{1/2}.$$

The singular values of M turn out to be

$$s_1 = \frac{1}{2}(\|f\|^2 - \|g\|^2 + \omega), \quad s_2 = \frac{1}{2}(\omega - \|f\|^2 + \|g\|^2),$$

where $\omega := \left((\|f\|^2 + \|g\|^2)^2 - 4|(f, g)|^2\right)^{1/2}$. Hence, $\|\mathcal{R}\|_1 = s_1 + s_2 = \omega$. This proves (7.28). $\square$

Lemma 7.9. *Let* H *be the Schrödinger operator in* $L_2(\Gamma)$ *given in* (7.2) *with the Kirchhoff vertex condition and* $H_0 = -d^2/dx^2$ *the corresponding unperturbed operator. Assume that condition* (7.1) *is satisfied. Then, the resolvents* $R(z)$ *and* $R_0(z)$ *satisfy for all* $\varepsilon > 0$ *and for* t *big enough,*

$$\|R(-t) - R_0(-t)\|_1 \leq C_\varepsilon t^{-3/2+\varepsilon}.$$

Proof. By adding zero we estimate the trace norm by

$$\|R(-t) - R_0(-t)\|_1 \leq \|\mathcal{R}\|_1 + \|R_\infty(-t) - R_\infty^{(0)}(-t)\|_1, \tag{7.29}$$

where $\mathcal{R} := R(-t) - R_\infty(-t) + R_\infty^{(0)}(-t) - R_0(-t)$ is an operator of rank two. The second norm in the right-hand side of (7.29) can be estimated by $\|R_\infty(-t) - R_\infty^{(0)}(-t)\|_1 \leq ct^{-3/2+\varepsilon}$, see [Lemma 4.5.6., [98]] Thus it remains to bound the norm of the rank two operator $\mathcal{R}$. From Kreĭn's formula (7.9) we have

$$(R_0(x_k,x_\ell,-t)-R_\infty^{(0)}(x_k,x_\ell,-t))_{k\ell}=f_k(x_k)f_\ell(x_\ell),\quad f_k(x_k)=\frac{e^{-\sqrt{t}x_k}}{\sqrt{n}t^{1/4}},$$

and hence,

$$R_0(-t)-R_\infty^{(0)}(-t)=(\cdot,f)f,\quad f=(f_1,\dots,f_n)^T.$$

Further,

$$(R(x_k,x_\ell,-t)-R_\infty(x_k,x_\ell,-t))_{k\ell}=g_k(x_k)g_\ell(x_\ell),\quad g_k(x_k)=\frac{\theta_k(x_k,i\sqrt{t})}{\sqrt{-K(i\sqrt{t})}\theta_k(0,i\sqrt{t})},$$

and

$$R(-t)-R_\infty(-t)=(\cdot,g)g,\quad g=(g_1,\dots,g_n)^T.$$

In view of (7.28) we have

$$\|R(-t)-R_\infty(-t)+R_\infty^{(0)}(-t)-R_0(-t)\|_1=\left((\|f\|^2+\|g\|^2)^2-4|(f,g)|^2\right)^{1/2}. \tag{7.30}$$

In the remaining part we show that $(\|f\|^2+\|g\|^2)^2-4|(f,g)|^2=O(t^{-3})$ as $t\to\infty$. Let us set $g=f+h$ and note that h is a real-valued function. Then by applying the Cauchy-Schwarz inequality and the arithmetic inequality,

$$(\|f\|^2+\|g\|^2)^2-4|(f,g)|^2=4(\|f\|^2+(f,h))\|h\|^2+\|h\|^4\le 6\|h\|^2\|f\|^2+3\|h\|^4. \tag{7.31}$$

We compute

$$\|f\|^2=\sum_{j=1}^n\int_0^\infty\frac{e^{-2\sqrt{t}x_j}}{n\sqrt{t}}\,dx_j=(2t)^{-1}. \tag{7.32}$$

Next, we consider $h=h_1+h_2$, where $h_k=(h_{k,1},\dots,h_{k,n})^T,\ k=1,2,$

$$\begin{aligned}
h_{1,j} &= \left(\sqrt{-K(i\sqrt{t})}\theta_j(0,i\sqrt{t})\right)^{-1}\left(\theta_j(x_j,i\sqrt{t})-e^{-\sqrt{t}x_j}\right),\\
h_{2,j} &= \left(\left(\sqrt{-K(i\sqrt{t})}\theta_j(0,i\sqrt{t})\right)^{-1}-\left(\sqrt{n}t^{1/4}\right)^{-1}\right)e^{-\sqrt{t}x_j}.
\end{aligned}$$

Because of (7.17) we have as $t\to\infty$,

$$\left|\sqrt{-K(i\sqrt{t})}\theta_j(0,i\sqrt{t})\right|^{-1}=O(t^{-1/4}) \tag{7.33}$$

and further, see e.g. [Lemma 4.1.4., [98]],

$$\left|\theta_j(x_j,i\sqrt{t})-e^{-\sqrt{t}x_j}\right|\le\frac{c}{\sqrt{t}}e^{-\sqrt{t}x_j},\quad c\in\mathbb{R}. \tag{7.34}$$

Hence, in view of (7.33) and (7.34), $\|h_1\|=O(t^{-1})$. To compute the asymptotics for h_2 we rewrite

$$\begin{aligned}
h_{2,j} &= \left(\sqrt{n}t^{1/4}-\sqrt{-K(i\sqrt{t})}\theta_j(0,i\sqrt{t})\right)\left(\sqrt{-K(i\sqrt{t})}\theta_j(0,i\sqrt{t})\right)^{-1}f_j(x_j)\\
&= \frac{\left(n\sqrt{t}+K(i\sqrt{t})\theta_j^2(0,i\sqrt{t})\right)}{\sqrt{n}t^{1/4}+\sqrt{-K(i\sqrt{t})}\theta_j(0,i\sqrt{t})}\frac{f_j(x_j)}{\sqrt{-K(i\sqrt{t})}\theta_j(0,i\sqrt{t})}.
\end{aligned}$$

Together with (7.32) and (7.33), this leads to $\|h_2\| = O(t^{-1})$ and therefore, $\|h\| = O(t^{-1})$. This yields in view of (7.28) and (7.31) that $\|\mathcal{R}\|_1 = O(t^{-3/2})$. This proves the assertion of the lemma. $\square$

With Lemma 7.9 all assumptions of Proposition 7.7 are fullfilled and therefore the spectral shift function for the pair H, H_0 in $L_2(\Gamma)$ satisfies the relations (7.26) and (7.27). Especially, we have proved Theorem 7.6.

Remark 7.10. Lemma 7.9 implies that $(H+c)^\beta - (H_0+c)^\beta$ is trace class for $\beta < 1/2$, see [98].

7.4. **Low-energy asymptotics and Levinson's formula.** In this section we study the low-energy asymptotics of $D(z)$ as $|z| \to 0$. This will allow us to prove an analog of Levinson's formula for star shaped quantum graphs. *Throughout this section we assume that* (7.6) *is satisfied.*

Definition 7.11. We say that the operator H in $L_2(\Gamma)$, given in (7.2), has a *resonance* at $\zeta = 0$ if the equation

$$-u'' + Vu = 0 \tag{7.35}$$

has a non-trivial bounded solution satisfying the continuity and Kirchhoff conditions. By definition, the *multiplicity* of the resonance is the dimension of the corresponding solution space.

Remark 7.12. We shall show below that $\zeta = 0$ is never an eigenvalue.

We recall some auxiliary results on half-line Schrödinger operators. For the half-line Schrödinger operator the Jost solution of the equation $H_j u = \zeta^2 u$ was characterized by its asymptotics $\theta_j(x,\zeta) = e^{ix\zeta}(1 + o(1))$ as $|\zeta| \to \infty$. Further, the function $\theta_j(x,0)$ satisfies the equation $H_j u = 0$ and its behavior at $\zeta = 0$ is given by

$$\theta_j(x,0) = 1 + O\left(\int_x^\infty y|V_j(y)|\,dy\right) = 1 + o(1), \quad \text{as } x \to \infty, \tag{7.36}$$

(see e.g. Lemma 4.3.1., [98]). Recall also that the Jost function is $w_j(\zeta) = \theta_j(0,\zeta)$. If $w_j(0) = 0$, the low-energy asymptotics

$$w_j(\zeta) = -iw_0^{(j)}\zeta + o(\zeta), \quad \zeta \to 0 \tag{7.37}$$

is true with some constant $w_0^{(j)} \neq 0$.

Lemma 7.13. *If* $\Theta(x,0)$ *is a bounded solution of equation* (7.35), *then for some* $c_j \in \mathbb{C}$,

$$\Theta(x,0) = \bigoplus_{j=1}^n c_j\theta_j(x,0). \tag{7.38}$$

Moreover, the operator H *cannot have a zero eigenvalue.*

Proof. If $\Theta(x,0)$ solves the equation (7.35) with $\zeta = 0$, then the restriction of $\Theta(x,0)$ to the edge e_j is a solution of the corresponding zero-energy equation on the half-line for every $1 \leq j \leq n$. As stated above, the function $\theta_j(x,0)$ solves the zero-energy equation and is bounded at infinity by (7.36). We note that $\theta_j(x,0)$ is the only solution of the zero-energy equation on the half-line, which is bounded at infinity. Indeed, the solution

$$\tau_j(x,0) = \theta_j(x,0)\int_{x_0}^x \theta_j(y,0)^{-2}\,dy, \quad x \geq x_0$$

which is linearly independent of $\theta_j(x,0)$ has as $x \to \infty$, the asymptotics

$$\tau_j(x,0) = x + o(x)$$

for all $1 \le j \le n$, (Lemma 4.3.2, [98]). Here x_0 is an arbitrary point such that $\theta(x) \neq 0$ for $x \ge x_0$. Finally, equation (7.35) cannot have a nontrivial solution belonging to $L_2(\Gamma)$ at infinity as $\Theta_j(x,0) = c_j + o(1)$ for $x \to \infty$.

□

Lemma 7.14. *Let* $M := \#\{j : \ w_j(0) = 0\}$.

(1) *If* $\zeta = 0$ *is not a resonance, then either* $M = 0$ *and* $K(0) \neq 0$ *or* $M = 1$ *and* $K(\zeta)$ *has a pole at* $\zeta = 0$.

(2) *Assume that* $\zeta = 0$ *is a resonance of multiplicity* $m \ge 1$*, then either*
a) any resonance function vanishes at the vertex and $m = M - 1 \ge 1$*, or*
b) the resonance is of multiplicity one, the corresponding resonance function is non-zero at the vertex and $m = 1,\ M = 0$ *and* $K(0) = 0$.

Proof. We first note that if $M \ge 1$, i.e. $\theta_j(0,0) = 0$ for some j, then any resonance function must vanish at $\zeta = 0$ because of the continuity condition.

(1) If $M \ge 2$, then it is always possible to construct a zero-energy function by setting $c_j = 0$ if $w_j(0) \neq 0$ and determining the c_j's such that the Kirchhoff vertex condition is fullfilled if $w_j(0) = 0$. Hence, if $\zeta = 0$ is not a resonance, then necessarily $M \le 1$. If $M = 1$, then obviously $K(\zeta)$ has a pole at $\zeta = 0$. Moreover, if $M = 0$ and $\zeta = 0$ is not a resonance, then $K(0) \neq 0$, because if $K(\zeta)$ would vanish in $\zeta = 0$, then it would follow from

$$K(0) = \sum_{j=1}^{n} \frac{\theta_j'(0,0)}{\theta_j(0,0)} = \sum_{j=1}^{n} \frac{c_j\theta_j'(0,0)}{c_j\theta_j(0,0)} = 0 \tag{7.39}$$

that the function $\Theta(x,0)$ given in (7.38) is a zero-energy resonance function for suitable c_j. Hence, $K(0) \neq 0$ if $\zeta = 0$ is not a resonance.

(2) a) If $\zeta = 0$ is a resonance, then $M \neq 1$, as it is not possible to construct a resonance function satisfying the vertex conditions and having support on only one edge of Γ. If $M \ge 2$, then because of the continuity condition any resonance function has to vanish at the vertex. Further, we set $c_j = 0$ for all j with $w_j(0) \neq 0$, then there are $M - 1$ linearly independent choices for the remaining c_j's such that the Kirchhoff vertex condition is fullfilled. Hence, the multiplicity of the resonance function is $m = M - 1 \ge 1$.
b) If ζ is a resonance with $M = 0$, then $\theta_j(0,0) \neq 0$ for all j and the coefficents c_j are determined uniquely by the $n-1$ continuity conditions and the Kirchhoff vertex condition. Further, this implies because of (7.39) that $K(0) = 0$.

□

In the following proposition, we give the low-energy asymptotics for $D(z)$ as $|z| \to 0$.

Proposition 7.15. *Let* m *be the multiplicity of the resonance* $\zeta = 0$*, with the convention that* $m = 0$ *if* $\zeta = 0$ *is not a resonance. If* $m = 1$*, we assume in addition that condition* (7.7) *is satisfied for all* $1 \le j \le n$*. Then, as* $\zeta \to 0$,

$$D(z) = c\zeta^{m-1}(1 + o(1)), \quad z = \zeta^2, \tag{7.40}$$

with $c \neq 0$.

For the proof of Proposition 7.15 we shall need the following

Lemma 7.16. *Let $H_D = -d^2/dx^2 + V(x)$ in $L_2([0,\infty))$ be given with Dirichlet boundary condition at the origin and assume that $\int_0^\infty (1+x)|V(x)|\,dx < \infty$. Let $\theta(x,\zeta)$ be the Jost solution on the half-line.*

(1) *If $\theta(0,0) = 0$, then*

$$\dot{\theta}(0,0)\theta'(0,0) = -i. \tag{7.41}$$

(2) *If $\theta(0,0) \neq 0$ and $\int_0^\infty (1+x^2)|V(x)|\,dx < \infty$, then*

$$\dot{\theta}(0,0)\theta'(0,0) - \dot{\theta}'(0,0)\theta(0,0) = -i. \tag{7.42}$$

Proof. If $\theta(0,0) = 0$, then $\dot{\theta}(0,0)$ is defined for V having a first moment and $\dot{\theta}(0,0) = -ic_0,\ c_0 \neq 0$, by [Proposition 4.3.7., [98]] Further, it was shown in [(4.3.11), [98]], that

$$\varphi(x,0) = c_0\theta(x,0), \tag{7.43}$$

where φ is the regular solution of $-u'' + Vu = \zeta^2 u$. Taking the derivative with respect to x on both sides of (7.43) and setting $x = 0$ yields that $1 = c_0\theta'(0,0)$, as the regular solution of the Dirichlet problem was defined by the condition $\varphi'(0,\zeta) = 1$. Hence, equation (7.41) follows. If $\theta(0,0) \neq 0$, then $\dot{\theta}(0,0)$ is only defined for V having a second moment and

$$\varphi(x,0) = i\dot{\theta}(0,0)\theta(x,0) - i\theta(0,0)\dot{\theta}(x,0) \tag{7.44}$$

by [Corollary 4.3.11., [98]]. Again, taking on both sides of (7.44) the derivative with respect to x and setting $x = 0$ leads to (7.42).

□

Proof of Proposition 7.15. We consider the explicit expression for the perturbation determinant $D(z)$ which was given in (7.18),

$$D(z) = \frac{K(\zeta)}{in\zeta}\prod_{j=1}^{n} w_j(\zeta), \quad z = \zeta^2. \tag{7.45}$$

Let us first consider the case $M = 0$. Then by Lemma 7.14 either $\zeta = 0$ is not a resonance and $K(0) \neq 0$ or $\zeta = 0$ is a resonance and $K(0) = 0$. If $\zeta = 0$ is not a resonance, then we see from (7.45) that as $\zeta \to 0$, $D(z) = c\zeta^{-1}(1 + o(1))$, $c \neq 0$. If $\zeta = 0$ is a resonance, then we consider $\dot{K}(0) = \sum_{j=1}^n \left(\dot{\theta}_j'(0,0)\theta_j(0,0) - \theta_j'(0,0)\dot{\theta}_j(0,0)\right)\theta_j^{-2}(0,0)$ which by (7.42) is the same as $\dot{K}(0) = \sum_{j=1}^n i\theta_j^{-2}(0,0) \neq 0$. Hence, by applying l'Hospital we have as $\zeta \to 0$, $D(z) \to c \neq 0$.

Next, we consider case $M \geq 1$. Without loss of generality let $\theta_1(0,0) = \ldots = \theta_M(0,0) = 0$. We rewrite (7.45) as

$$D(z) = \frac{1}{in\zeta}\left(\sum_{j=1}^{M}\frac{\theta_j'(0,\zeta)}{\theta_j(0,\zeta)}\prod_{k=1}^{n}\theta_k(0,\zeta) + \sum_{j=M+1}^{n}\frac{\theta_j'(0,\zeta)}{\theta_j(0,\zeta)}\prod_{k=1}^{n}\theta_k(0,\zeta)\right), \quad z = \zeta^2. \tag{7.46}$$

Obviously, the second term on the right-hand side is $O(\zeta^M)$. In the first term on the right-hand side we have for each $1 \le j \le M$, as $\zeta \to 0$

$$\begin{aligned}
\frac{\theta_j'(0,\zeta)}{\theta_j(0,\zeta)} \prod_{k=1}^n \theta_k(0,\zeta) &= \theta_j'(0,\zeta) \prod_{\substack{k=1\\k\neq j}}^n \theta_k(0,\zeta) \\
&= \zeta^{M-1}\theta_j'(0,0) \prod_{\substack{k=1\\k\neq j}}^M \dot\theta_k(0,0) \prod_{k=M+1}^n \theta_k(0,0) + O(\zeta^M) \\
&= \zeta^{M-1}\frac{\theta_j'(0,0)}{\dot\theta_j(0,0)} \prod_{k=1}^M \dot\theta_k(0,0) \prod_{k=M+1}^n \theta_k(0,0) + O(\zeta^M).
\end{aligned}$$

In view of (7.41) and (7.46) we arrive at

$$\begin{aligned}
D(z) &= \frac{\zeta^{M-1}}{in\zeta}\left(\prod_{k=1}^M \dot\theta_k(0,0) \prod_{k=M+1}^n \theta_k(0,0) i \sum_{j=1}^M (\theta_j'(0,0))^2 + O(\zeta)\right) \\
&= c\zeta^{M-2} + O(\zeta^{M-1}), \quad c \neq 0,\ z = \zeta^2.
\end{aligned}$$

□

In the remaining part we prove an analog of Levinson's formula for star shaped graphs. For $k \in \mathbb{R}$, we set $D(k^2) = a(k)e^{i\eta(k)}$, where $a(k) = |D(k^2)|$. Then it follows from the representation $D(k^2) = (K(k)/(ink)) \prod_{j=1}^n w_j(k)$ that

$$-\eta(k) = \eta(-k). \tag{7.47}$$

Indeed, it follows from the uniqueness of the Jost solutions $\theta_j(x,\zeta)$ that $\overline{\theta_j(x,k)} = \theta_j(x,-k)$, and $\overline{\theta_j'(x,k)} = \theta_j'(x,-k)$, and hence also $\overline{w_j(k)} = \overline{\theta_j(0,k)} = w_j(-k)$.

Proof of Theorem 7.3. First, we note that there is a spectral theoretical result relating the zeros of the perturbation determinant to the eigenfunctions of H as follows. The function $D(\zeta^2)$ has a zero in ζ of order r if and only if ζ^2 is an eigenvalue of multiplicity r of the operator H, [97]. Obviously, the zeros of $D(\zeta^2)$ lie on the positive imaginary axis as H is a self-adjoint operator and therefore it may have only real eigenvalues.

We apply the argument principle to the function $D(\zeta^2)$ and the contour $\Gamma_{R,\varepsilon}$ which consists of the half-circles $C_R^+ = \{|\zeta| = R, \operatorname{Im}\zeta \ge 0\}$ and $C_\varepsilon^+ = \{|\zeta| = \varepsilon,\ \operatorname{Im}\zeta \ge 0\}$ and the intervals (ε, R) and $(-R,-\varepsilon)$. We choose R and ε such that all of the N negative eigenvalues of H lie inside the contour $\Gamma_{R,\varepsilon}$. The function $D(\zeta^2)$ is analytic inside and on $\Gamma_{R,\varepsilon}$ as $w_j(\zeta)$ is analytic in the the upper half-plane $\operatorname{Im}\zeta > 0$. Thus,

$$\int_{\Gamma_{R,\varepsilon}} \frac{\frac{d}{d\zeta}D(\zeta^2)}{D(\zeta^2)}\, d\zeta = 2\pi i N. \tag{7.48}$$

Remember that $\lim_{\operatorname{Im}\zeta\to\infty} D(\zeta^2) = \lim_{\operatorname{Im}\zeta\to\infty} K(\zeta)\prod_{j=1}^n w_j(\zeta)/(ni\zeta) = 1 + O(|\zeta|^{-1})$. Thus, we can fix the branch of the function $\ln D(\zeta^2)$ by the condition $\ln D(\zeta^2) \to 0$ as $\operatorname{Im}\zeta \to \infty$. Then, we have $\ln D(\zeta^2) = \ln|D(\zeta^2)| + i\arg D(\zeta^2)$. Equation (7.48) implies that

$$\operatorname{var}_{\Gamma_{R,\varepsilon}} \arg D(\zeta^2) = 2\pi N. \tag{7.49}$$

We define $\eta(0) := \lim_{k\to 0+}\eta(k)$. This limit exists because of asymptotics (7.40). It follows with (7.47) that,

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

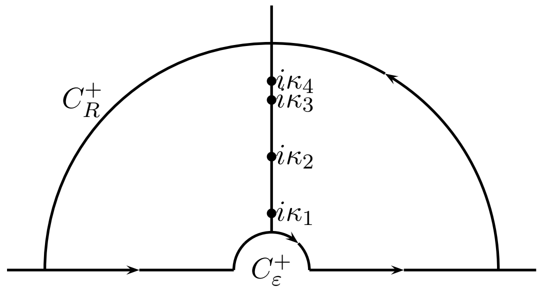

FIGURE 10. contour of integration $\Gamma_{R,\varepsilon}$

Now, we let $R\to\infty$ and $\varepsilon\to 0$. Because of (7.16), $\lim_{R\to\infty}\mathrm{var}_{C_R^+}\arg\, D(\zeta^2) = 0$. Hence, it follows from (7.49) that

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

By Proposition 7.15, $\lim_{\varepsilon\to 0}\mathrm{var}_{C_\varepsilon^+}\arg\, D(\zeta^2) = -(m-1)\pi$. Thus,

$$\eta(\infty)-\eta(0) = \pi\left(N + \frac{m-1}{2}\right). \tag{7.50}$$

Note that $\eta(\infty) = 0$ since $\ln D(\zeta^2)\to 0$ as $|\zeta|\to\infty$. It remains to note that in view of Theorem 7.6, the following identity is true for $\lambda = k^2,\ k>0$,

$$\xi(\lambda) = \pi^{-1}\lim_{\varepsilon\to 0+}\arg\, D(\lambda+i\varepsilon) = \pi^{-1}\eta(\lambda^{1/2}), \quad \lambda>0. \tag{7.51}$$

The assertion of Theorem 7.3 then follows by combining (7.50) and (7.51).

□

Acknowledgments. The author is grateful to Timo Weidl for valuable comments. Many thanks to Rupert Frank for fruitful discussions and references.

8. Remarks on Lieb-Thirring inequalities for quantum graphs

In paper I we proved that for metric trees sharp Lieb-Thirring inequalities do hold for all moments $\gamma \geq 2$ with the semiclassical constants $L^{cl}_{\gamma,1}$. In the classical case of the full space $\mathbb{R}^d$ however it is known that Lieb-Thirring inequalities hold for moments $\gamma \geq 1/2$. In particular, these inequalities hold with the semiclassical (and thus sharp) constants $L^{cl}_{3/2,d}$, for all $d \geq 1$ [70]. Hence, it is natural to ask whether Lieb-Thirring inequalities with moments $\gamma \geq 3/2$ do hold for quantum graphs with the same semiclassical constant $L^{cl}_{3/2,1}$. The method of sum rules applied in paper I fails in the case $\gamma < 2$ as it provides also monotonicity of the eigenvalue moments with respect to coupling constants, which in general is not true if $\gamma < 2$. Thus, we have to use different methods in order to obtain inequalities for the case $\gamma \geq 1/2$. For star shaped graphs Γ we derive Lieb-Thirring inequalities with moments $\gamma \geq 1/2$ by using variational arguments. If the graph has an even number of edges, this leads to sharp Lieb-Thirring inequalities for $\gamma = 1/2$ and for all $\gamma \geq 3/2$ with the same constants as in the full space case. The variational methods fail if the graph has an odd number of edges. In this case we decompose the Hilbert space $L_2(\Gamma)$ symmetrically which leads to sharp Lieb-Thirring inequalities for spherically symmetric potentials.

Let us first recall the variational principle from general theory, see [82] for more details.

The variational principle. In the study of spectral properties of self-adjoint operators the variational principle is a tool which is used very often to characterize the eigenvalues of a given self-adjoint operator. Here we shall state the variational principle in the form which we will refer to later when studying star shaped graphs. For more details, see [82].

Suppose that the operator H on a Hilbert space $\mathcal{H}$ is self-adjoint and bounded from below. Let $h[\phi]$ denote the quadratic form with which H is associated. By $d(h)$ we denote the form domain of the operator H. Define

$$\mu_k = \max_{\psi_1,\ldots,\psi_{k-1}\in\mathcal{H}} \inf_{\substack{\phi\in d(h);\|\phi\|=1\\ \phi\in[\psi_1,\ldots,\psi_{k-1}]^\perp}} h[\phi], \tag{8.1}$$

where $\phi \in [\psi_1, \ldots, \psi_{k-1}]^\perp$ is shorthand for $\{\phi : \ (\phi, \psi_i) = 0, \ i = 1, \ldots, k-1\}$. Then for each fixed $k \in \mathbb{N}$ either there are k eigenvalues (counting multiplicity) below the bottom of the essential spectrum of H and μ_k is the k-th eigenvalue counting multiplicity; or μ_k is the bottom of the essential spectrum of H and there are at most $k-1$ eigenvalues (counting multiplicity) below μ_k.

The variational principle permits to compare eigenvalues of two self-djoint operators A and B that are bounded from below. Let $d[a]$ and $d[b]$ denote the form domains of A and B respectively. We say that $A \leq B$ if and only if $d[b] \subset d[a]$ and $(\varphi, A\varphi) \leq (\varphi, B\varphi)$ for all $\varphi \in d[b]$. As a consequence, the min-max Theorem implies that

$$\mu_n(A) \leq \mu_n(B) \ \text{ for any } n \text{ if } A \leq B.$$

8.1. **Variational principle for quantum graphs.** We consider a *star graph* which is a metric graph Γ with a single vertex in which a finite number $n \geq 2$ of edges e_j are joined. We assume throughout that all edges e_j are infinite and we identify $e_j = [0, \infty)$. We assume that the potential V is a real-valued function on Γ satisfying

$$\int_{e_j} |V_j(x_j)|\, dx_j < \infty \quad \text{for all } 1 \le j \le n, \tag{8.2}$$

where we denoted the restriction of V to the edge e_j by $V_j(x_j) = V(x)|_{e_j}$. Under this condition, we can define the Schrödinger operator

$$H\psi := -\psi'' + V\psi \tag{8.3}$$

with continuity and Kirchhoff vertex conditions

$$\psi_1(0) = \ldots = \psi_n(0) =: \psi(0), \quad \sum_{j=1}^{n} \psi_j'(0) = 0, \tag{8.4}$$

as a self-adjoint operator in the Hilbert space $L_2(\Gamma) = \oplus_{j=1}^n L_2(e_j)$. In (8.4) we denoted by ψ_j the restriction of ψ to the edge e_j. More precisely, we define the operator H via the closed quadratic form

$$h[\phi] := \int_\Gamma |\phi'(x)|^2\, dx + \int_\Gamma V(x)|\phi(x)|^2\, dx\,,$$

with form domain $d(h) = H^1(\Gamma)$ consisting of all continuous functions ϕ on Γ such that $\phi_j \in H^1(e_j)$ for every j. If V is sufficiently regular in a neighborhood of the vertex, then functions ϕ in the operator domain of H satisfy the Kirchhoff vertex condition in (8.4); otherwise this condition has to be interpreted in a generalized sense. Under these conditions the spectrum of H consists of a continuous spectrum on the positive semiaxis and a discrete spectrum of negative eigenvalues E_k.

Imposing Neumann vertex condition at the origin disconnects the graph Γ into n positive half-lines. By variational arguments, the spectrum of a half-line Schrödinger operator can then be estimated from above by the spectrum of a whole-line Schrödinger operator for which Lieb-Thirring inequalities are known. In order to do this, we define the self-adjoint Schrödinger operator

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

in $L_2(\Gamma)$ which is associated with the closed quadratic form

$$h_N[\phi] := \int_\Gamma |\phi'(x)|^2\, dx + \int_\Gamma V(x)|\phi(x)|^2\, dx,$$

where ϕ is a function belonging to the form domain $d(h_N) = \bigoplus_{j=1}^n H^1(e_j)$. If V is sufficiently regular in a neighborhood of the vertex, then functions ψ in the operator domain of H satisfy the Neumann condition $\psi_j'(0) = 0$ for all $1 \le j \le n$. We note that the Neumann condition disconnects the graph Γ in n positive half-lines and the operator $H_N = \bigoplus_{j=1}^n H_N(V_j)$ is decoupled. Obviously, $d(h) \subset d(h_N)$ and it follows from the variational principle that $H_N \le H$. Denoting the negative eigenvalues of $H_N(V_j)$ in $L_2(e_j)$ by $E_k^{(N)}(V_j)$, the following inequality yields

$$\sum_k |E_k|^\gamma \le \sum_{j=1}^n \sum_k |E_k^{(N)}(V_j)|^\gamma. \tag{8.5}$$

Extending V_j to a symmetric function $\tilde{V}_j$ in $\mathbb{R}$, the right-hand side of (8.5) can be estimated from above by the corresponding moments of the whole-line operator. Indeed, the

Schrödinger operator on the whole-line with symmetric potential has alternating only Neumann and Dirichlet eigenvalues, where the ground state corresponds to a Neumann eigenvalue. Denoting the best possible Lieb-Thirring constant for the whole-line Schrödinger operator by $L_{\gamma,1}$, we arrive at

$$\sum_k |E_k^{(N)}(V_j)|^\gamma \le L_{\gamma,1} \int_{\mathbb{R}} (\tilde{V}_j(x))_-^{\gamma+1/2}\, dx = 2L_{\gamma,1} \int_{e_j} (V_j(x))_-^{\gamma+1/2}\, dx. \tag{8.6}$$

We note that $L_{\gamma,1} \le 2L_{\gamma,1}^{cl}$ if $\gamma \ge 1/2$ and $L_{\gamma,1} = L_{\gamma,1}^{cl}$ if $\gamma \ge 3/2$. Summing over j in (8.6) and combining (8.5) with (8.6) leads finally to

$$\sum_k |E_k|^\gamma \quad \le \quad 2L_{\gamma,1} \int_\Gamma (V_-(x))^{\gamma+1/2}\, dx, \quad \gamma \ge 1/2. \tag{8.7}$$

Remark 8.1. As mentioned before, the best possible Lieb-Thirring constant for the quantum graph is always greater or equal to the best possible constant for the whole-line Schrödinger operator.

The Lieb-Thirring inequalities given in (8.7) are not sharp. In fact, the constants can be improved when we distinguish the case in which Γ has an even number of edges from the case with an odd number of edges.

Theorem 8.2. *Assume that Γ has an even number of edges, i.e. $n = 2m,\ m \in \mathbb{N}$, and that $V \in L_{\gamma+1/2}(\Gamma)$. Then, the following inequalities hold,*

$$\sum_k |E_k|^\gamma \quad \le \quad L_{\gamma,1} \int_\Gamma (V_-(x))^{\gamma+1/2}\, dx, \quad \gamma \ge 1/2. \tag{8.8}$$

Proof. Given a star graph with $2m$ half-lines, we can disconnect the graph such that we obtain m whole-lines. The whole-line Schrödinger operators in $L_2(\mathbb{R})$ are denoted by

$$H_{\mathbb{R}}(V_i) = -\frac{d^2}{dx^2} + V_i(x), \tag{8.9}$$

where the potentials $V_i,\ i = 1, \dots, m$, on the disconnected lines are identified with the potential V defined on the graph. We compare the quadratic form domain of H with the quadratic form domain of $\bigoplus_{i=1}^m H_{\mathbb{R}}(V_i)$. The quadratic form domain of H is, as stated above, $d(h) = H^1(\Gamma)$. Whereas, the Schrödinger operator $H_{\mathbb{R}}(V_i)$ in $L_2(\mathbb{R})$ is associated with the closed quadratic form given by

$$h_{\mathbb{R},i}[f] := \int_{\mathbb{R}} |f'(x)|^2\, dx + \int_{\mathbb{R}} V_i(x)|f(x)|^2\, dx, \quad f \in d(h_{\mathbb{R},i}) := H^1(\mathbb{R}).$$

We denote the quadratic form domain of $\bigoplus_{i=1}^m H_{\mathbb{R}}(V_i)$ by $\bigoplus_{i=1}^m d(h_{\mathbb{R},i})$. Obviously,

$$d(h) \subset \bigoplus_{i=1}^m d(h_{\mathbb{R},i}), \tag{8.10}$$

and $\bigoplus_{i=1}^m H_{\mathbb{R}}(V_i) \le H$. Denoting the negative eigenvalues of the whole-line Schrödinger operator $H_{\mathbb{R}}(V_i)$ on the i-th line by $E_k(H_i)$, we obtain

$$\sum_k |E_k|^\gamma \le \sum_{i=1}^m \sum_k |E_k(H_i)|^\gamma. \tag{8.11}$$

It follows from the well-known Lieb-Thirring inequalities for the whole-line that the right-hand side in (8.11) is bounded from above by

$$\sum_{i=1}^{m} L_{\gamma,1} \int_{\mathbb{R}} (V_i(x))_-^{\gamma+1/2}\, dx = L_{\gamma,1} \int_{\Gamma} (V_-(x))^{\gamma+1/2}\, dx.$$

This proves Theorem 8.2. □

Inequality (8.8) is sharp for $\gamma = 1/2$ and $\gamma \geq 3/2$. As this proof does not work in the case when Γ has an odd number of edges, we shall apply other arguments to derive Lieb-Thirring inequalities in this case.

Theorem 8.3. *Assume that Γ has an odd number of edges, i.e. $n = 2m+1,\ m \in \mathbb{N}$, and that $V \in L_{\gamma+1/2}(\Gamma)$ Then, for all $\gamma \geq 1/2$ the following estimates hold,*

$$\sum_k |E_k|^\gamma \quad \leq \quad \left(\frac{n+1}{n}\right) L_{\gamma,1} \int_{\Gamma} (V_-(x))^{\gamma+1/2}\, dx. \tag{8.12}$$

Proof. Given a star graph with $2m+1$ half-lines, we can disconnect the graph such that we obtain m whole lines and one half-line. Again, the potentials on the disconnected lines are identified with the potential V defined on the graph. We choose the half-line to be the $(2m+1)$-th edge of the graph on which the potential V_{2m+1} is defined. On the half-line we define the Schrödinger operator

$$H_N(V_{2m+1}) = -\frac{d^2}{dx^2} + V_{2m+1}(x)$$

in $L_2(\mathbb{R}_+)$ with Neumann boundary condition, i.e. any function φ belonging to the operator domain of H_N satisfies the condition $\varphi'(0) = 0$. The self-adjoint operator H_N is associated with the closed quadratic form given by

$$h_N[f] := \int_{e_{2m+1}} |f'(x)|^2\, dx + \int_{e_{2m+1}} V_{2m+1}(x)|f(x)|^2\, dx, \quad f \in\ d(h_N) := H^1(e_{2m+1}).$$

For the quadratic form domains of $H,\ H_{\mathbb{R}}(V_i)$ and $H_N(V_{2m+1})$, we have the relation

$$d(h) \subset \bigoplus_{i=1}^{m} d(h_{\mathbb{R},i}) \oplus d(h_N). \tag{8.13}$$

With the argument of extending V_{2m+1} to an even function on $\mathbb{R}$, the eigenvalues of the Neumann Schrödinger operator on the half-line can be estimated from above with twice the Lieb-Thirring constant for the whole-line Schrödinger operator. Whereas for the m whole-line Schrödinger operators we have the sharp estimates from Theorem 8.2. This leads together with (8.13) to the following estimate for $\gamma \geq 1/2$,

$$\sum_k |E_k|^\gamma \leq \sum_{j=1}^{2m} L_{\gamma,1} \int_{e_j} (V_j(x))_-^{\gamma+1/2}\, dx + 2L_{\gamma,1} \int_{e_{2m+1}} (V_{2m+1}(x))_-^{\gamma+1/2}(x)\, dx. \tag{8.14}$$

We can apply the same procedure to the case where the half-line is now identified with another edge of Γ. Altogether we have $2m+1$ choices to do this, where all of them give analog inequalities of (8.14). Averaging over all of these $2m+1$ inequalities, we conclude Theorem 8.3. □

8.2. **Symmetric Decomposition for quantum graphs.** We consider the star graph given in the previous section. Let H be the self-adjoint Schrödinger operator defined in (8.3) with the Kirchhoff matching condition (8.4). The symmetry of Γ allows one to construct an orthogonal decomposition of the space $L_2(\Gamma)$ which reduces the Kirchhoff Laplacian. If, in addition V is symmetric, it also reduces the operator H. The study of the spectrum of H is then reduced to the study of the spectrum of the orthogonal components in the decomposition, where each component can be identified with a differential operator acting in the space $L_2(\mathbb{R}_+)$.

In [31, 77, 89] a decomposition of the L_2 space was given for the case of regular, rooted metric trees. In what follows, we reformulate the decomposition of $L_2(\Gamma)$ for our purposes in the special case of star graphs with finitely many edges n.

We define by $\mathcal{H}^{(0)}$ the closed subspace of $L_2(\Gamma)$ which contains all symmetric functions on Γ, i.e.,

$$\mathcal{H}^{(0)} := \{\psi \in L_2(\Gamma) : \forall r : \ \psi(r) := \psi_1(r) = \psi_2(r) = \ldots = \psi_n(r)\},$$

where $\psi_j := \psi|_{e_j}$. Any symmetric function ψ on Γ can be identified with the function $s := R\psi$ on the half-line $[0, \infty)$, such that $\psi(x) = s(|x|)$ for each $x \in \Gamma$, and

$$\int_\Gamma |\psi(x)|^2\, dx = n \int_0^\infty |s(x)|^2\, dx, \quad \psi \in \mathcal{H}^{(0)}, s = R\psi.$$

Thus, the operator $\sqrt{n}R$ defines an isometry of the subspace $\mathcal{H}^{(0)}$ onto the space $L_2(\mathbb{R}_+)$. Further,

$$\int_\Gamma |\psi'(x)|^2\, dx = n \int_0^\infty |s'(x)|^2\, dx, \quad \psi \in \mathcal{H}^{(0)} \cap H^1(\Gamma).$$

To state the orthogonal decomposition of $L_2(\Gamma)$ we define for $1 \le \ell \le n-1$, the following orthogonal subspaces $\mathcal{H}^{(\ell)}$ which are all isometric to $L_2(\mathbb{R}_+)$,

$$\mathcal{H}^{(\ell)} \ := \ \{\psi \in L_2(\Gamma) : \forall j, r : \ \psi_{j+1}(r) = e^{i2\pi(\ell/n)}\psi_j(r) \bmod n\} \sim L_2(\mathbb{R}_+).$$

Lemma 8.4. *Let Γ be a star graph. Then the subspaces $\mathcal{H}^{(\ell)}$, $\ell = 0, \ldots, n-1$, are mutually orthogonal and*

$$L_2(\Gamma) = \bigoplus_{\ell=0}^{n-1} \mathcal{H}^{(\ell)}. \tag{8.15}$$

Proof. First, we show that $L_2(\Gamma) = \operatorname{span}\{\mathcal{H}^{(\ell)} : \ell\}$, i.e., for every function $\psi \in L_2(\Gamma)$ there exists a function $\psi^{(\ell)} \in \mathcal{H}^{(\ell)}$ such that $\psi = \sum_{\ell=1}^{n-1} c_\ell \psi^{(\ell)}$.

Note that for $n = 2$ this corresponds to the fact that every function on the real line is given as a sum of even and odd functions. Namely, any function $\psi_1 = \psi|_{e_1}$ on the first edge can be written as

$$\psi_1(r) = \frac{1}{2}\left(\psi_1(r) + \psi_2(r)\right) + \frac{1}{2}\left(\psi_1(r) + e^{-i\pi}\psi_2(r)\right), \quad r \in [0, \infty),$$

where obviously $\psi_1(r) + \psi_2(r) \in \mathcal{H}^{(0)}$ is an even function and $\psi_1(r) + e^{-i\pi}\psi_2(r) \in \mathcal{H}^{(1)}$ is odd. Simlarly, $\psi_2(r)$ is given as a sum of an even and an odd function,

$$\psi_2(r) = \frac{1}{2}\left(\psi_1(r) + \psi_2(r)\right) + \frac{1}{2}\left(\psi_2(r) + e^{i\pi}\psi_1(r)\right), \quad r \in [0, \infty).$$

Returning to the general case of a star graph with n edges, any function on the k-th edge can be presented as

$$\psi_k \quad = \quad \frac{1}{n}\sum_{j=1}^{n}\psi_j + \sum_{\ell=1}^{n-1}\frac{1}{n}\left(\psi_k + \sum_{j\neq k} e^{i2\pi\ell/n}\psi_j\right), \tag{8.16}$$

where for each $1 \leq \ell \leq n-1$ the function $\psi_k + \sum_{j\neq k} e^{i2\pi\ell/n}\psi_j$ is in the subspace $\mathcal{H}^{(\ell)}$. Indeed, the right-hand side in (8.16) can be rewritten as

$$\psi_k + \frac{1}{n}\sum_{j\neq k}\psi_j + \frac{1}{n}\sum_{\ell=1}^{n-1}\sum_{j\neq k} e^{i2\pi\ell/n}\psi_j = \psi_k + \frac{1}{n}\sum_{j\neq k}\psi_j\sum_{\ell=0}^{n-1} e^{i2\pi\ell/n}.$$

As

$$\sum_{\ell=0}^{n-1} e^{i2\pi\ell/n} = \sum_{\ell=0}^{n-1}\left(e^{i2\pi/n}\right)^{\ell} = \frac{\left(e^{i2\pi/n}\right)^{n}-1}{\left(e^{i2\pi/n}\right)-1} = 0,$$

equality (8.16) follows. It remains to prove that the spaces $\mathcal{H}^{(\ell)},\ 0 \leq \ell \leq n-1$, are mutually orthogonal. For $\psi^{(\ell)} \in \mathcal{H}^{(\ell)}$ and $\psi^{(m)} \in \mathcal{H}^{(m)}$, with $\ell \neq m$, consider

$$\begin{aligned}
\int_\Gamma \psi^{(\ell)}\overline{\psi^{(m)}}\,dx \quad &= \quad \sum_{j=1}^{n}\int_{e_j}\psi_j^{(\ell)}\overline{\psi_j^{(m)}}\,dx = \sum_{j=1}^{n}\int_{e_j} e^{2i\pi\ell(j-1)/n}\psi_1^{(\ell)} e^{-2i\pi m(j-1)/n}\overline{\psi_1^{(m)}}\,dx \\
&= \quad \int_{e_1}\psi_1^{(\ell)}\overline{\psi_1^{(m)}}\,dx\sum_{j=1}^{n}\left(e^{2i\pi(\ell-m)/n}\right)^{j-1}.
\end{aligned} \tag{8.17}$$

The right-hand side in (8.17) equals zero, as

$$\sum_{j=1}^{n}\left(e^{2i\pi(\ell-m)/n}\right)^{j-1} = \sum_{j=0}^{n-1}\left(e^{2i\pi(\ell-m)/n}\right)^{j} = \frac{\left(e^{i2\pi(\ell-m)/n}\right)^{n}-1}{\left(e^{i2\pi(\ell-m)/n}\right)-1} = 0.$$

Hence, the spaces $\mathcal{H}^{(\ell)},\ 0 \leq \ell \leq n-1$, are mutually orthogonal.

□

We introduce the following notation for functions $\psi^{(\ell)} \in \mathcal{H}^{(\ell)}$ and their derivatives ,

$$\psi^{(\ell)}(x) = \left(\psi_1^{(\ell)}, \ldots, \psi_n^{(\ell)}\right)^T, \quad (\psi^{(\ell)})'(x) = \left(\left(\psi_1^{(\ell)}\right)'(x), \ldots, \left(\psi_n^{(\ell)}\right)'(x)\right)^T.$$

We recall that for all $\mathcal{H}^{(\ell)}$ there exists an isometry onto the space $L_2(\mathbb{R}_+)$ and that every function $\psi^{(\ell)} \in \mathcal{H}^{(\ell)}$ can be constructed if one of the components $\psi_j^{(\ell)}$ on the j-th edge is known. So, in order to determine $\psi \in L_2(\Gamma)$ we only need $\psi_j^{(\ell)},\ \ell = 0, \ldots, n-1$. In the following, we assume that the potential V is symmetric. Then, the operator $H|_{\mathcal{H}^{(0)}}$ is unitary equivalent to a self-adjoint half-line Schrödinger operator $H^{(0)}$ in $L_2(\mathbb{R}_+)$ associated with the quadratic form $h^{(0)}$ with form domain $d(h^{(0)}) = H^1(\mathbb{R}_+)$. Similarly the operators $H|_{\mathcal{H}^{(\ell)}},\ \ell = 1, \ldots, n-1$, are unitary equivalent to half-line Schrödinger operators $H^{(\ell)}$ on $L_2(\mathbb{R}_+)$ associated with closed quadratic forms $h^{(\ell)}$ with form domains $d(h^{(\ell)}) = H^{1,0}(\mathbb{R}_+) =$

$\{\phi \in H^1(\mathbb{R}_+) : \phi(0) = 0\}$. For $\phi \in H^1(\Gamma)$ and $\phi^{(\ell)} \in h^{(\ell)}$ the equality

$$\int_\Gamma \left(|\phi'|^2 + V|\phi|^2\right) dx = \sum_{\ell=0}^{n-1} \int_0^\infty \left(|\phi^{(\ell)\prime}|^2 + V|\phi^{(\ell)}|^2\right) dx,$$

is true, see e.g. [31]. Hence, the operator H on $L_2(\Gamma)$ is unitary equivalent to the orthogonal sum of the operators $H^{(\ell)}$ on $L_2(\mathbb{R}_+)$,

$$H \sim H_U = \bigoplus_{\ell=0}^{n-1} H^{(\ell)}, \tag{8.18}$$

where functions from the operator domain of $H^{(0)}$ satisfy Neumann boundary condition at the origin, whereas functions belonging to the operator domain of $H^{(\ell)}$ for $1 \leq \ell \leq n-1$ satisfy Dirichlet boundary condition at the origin. According to this statement, the description of the spectrum $\sigma(H)$ reduces to the description of the spectrum $\sigma(H^{(\ell)})$. Namely, it is well-known from general spectral theory that

$$\sigma(H) = \cup_{\ell=0}^{n-1} \sigma\left(H^{(\ell)}\right), \tag{8.19}$$

where the multiplicities of the eigenvalues are equal at both sides. As a consequence, we get

$$\sum_k |E_k|^\gamma = \sum_k |E_k^{(N)}|^\gamma + (n-1) \sum_k |E_k^{(D)}|^\gamma,$$

where $E_k^{(N)}$ and $E_k^{(D)}$ denote the eigenvalues of the operators $H^{(0)}$ and $H^{(\ell)}$, $\ell = 1, \ldots, n-1$, respectively.

Consider now the Schrödinger operator

$$H_\mathbb{R} = -\frac{d^2}{dx^2} + \tilde{V},$$

in $L_2(\mathbb{R})$, where the potential $\tilde{V}$ denotes the symmetric extension of the potential $V|_{e_j}$ to the whole-line. Then, it follows from (8.18) that

$$H \sim \oplus_{\ell=2}^{n-1} H^{(\ell)} \oplus H_\mathbb{R},$$

and hence,

$$\sum_k |E_k|^\gamma = \sum_k |\tilde{E}_k|^\gamma + (n-2) \sum_k |E_k^{(D)}|^\gamma,$$

where we have denoted by $\tilde{E}_k$ the negative eigenvalues of $H_\mathbb{R}$. Thus, we have proved the following

Corollary 8.5. *Let $V \in L_2(\Gamma)$ be spherically symmetric on a star graph Γ with $n \geq 2$ edges. Then, the following trace identity holds*

$$\sum_k |E_k|^\gamma = \sum_k |\tilde{E}_k|^\gamma + (n-2) \sum_k |E_k^{(D)}|^\gamma. \tag{8.20}$$

We note that the Lieb-Thirring inequalities for the whole-line Schrödinger operator hold also for the Dirichlet half-line Schrödinger operator with the same constants. Therefore, identity (8.20) implies sharp Lieb-Thirring inequalities for the Schrödinger operator H in $L_2(\Gamma)$ with symmetric potential and Kirchhoff vertex condition.

Theorem 8.6. *Let H be the Schrödinger operator defined in* (7.2) *with spherically symmetric potential $V \in L_{\gamma+1/2}(\Gamma)$ and Kirchhoff vertex condition* (7.3). *Then,*

$$\sum_k |E_k|^\gamma \quad \leq \quad L_{\gamma,1} \int_\Gamma (V_-(x))^{\gamma+1/2}\, dx, \quad \gamma \geq 1/2. \tag{8.21}$$

Remark 8.7. These inequalities are sharp for $\gamma = 1/2$ and $\gamma \geq 3/2$. Further, they hold for the star graph with an arbitrary number of edges as soon as the potential is symmetric. This gives rise to the conjecture that also the inequalities in Theorem 8.3 should hold with the sharp constants given in (8.21). We think that it is an interesting open question whether the Lieb-Thirring inequality on a star-shaped graph with an odd number of edges holds with the whole-line constant.

References

[1] Michael Aizenman and Elliott H. Lieb. On semiclassical bounds for eigenvalues of Schrödinger operators. *Phys. Lett. A*, 66(6):427–429, 1978.

[2] Tuncay Aktosun. Inverse scattering on the line with incomplete scattering data. In *Partial differential equations and inverse problems*, volume 362 of *Contemp. Math.*, pages 1–11. Amer. Math. Soc., Providence, RI, 2004.

[3] S. Albeverio, F. Gesztesy, R. Høegh-Krohn, and H. Holden. *Solvable models in quantum mechanics*. AMS Chelsea Publishing, Providence, RI, second edition, 2005. With an appendix by Pavel Exner.

[4] Mark S. Ashbaugh. The universal eigenvalue bounds of Payne-Pólya-Weinberger, Hile-Protter, and H. C. Yang. In *Spectral and inverse spectral theory (Goa, 2000)*, Proc. Indian Acad. Sci. Math. Sci, 112, pages 3–30. Indian Acad. Sci., 2002.

[5] V. Bargmann. On the number of bound states in a central field of force. *Proc. Nat. Acad. Sci. U. S. A.*, 38:961–966, 1952.

[6] S. M. Belov and A. V. Rybkin. Higher order trace formulas of the Buslaev-Faddeev-type for the half-line Schrödinger operator with long-range potentials. *J. Math. Phys.*, 44(7):2748–2761, 2003.

[7] Gregory Berkolaiko, Robert Carlson, Stephen A. Fulling, and Peter Kuchment, editors. *Quantum Graphs and Their Applications*, volume 415 of *Contemporary Mathematics*, Providence, RI, 2006. American Mathematical Society.

[8] Hans A. Bethe. *Intermediate quantum mechanics*. Notes by R. W. Jackiw. W. A. Benjamin, Inc., New York-Amsterdam, 1964.

[9] M. Š. Birman and V. V. Borzov. The asymptotic behavior of the discrete spectrum of certain singular differential operators. In *Problems of mathematical physics, No. 5: spectral theory (Russian)*, pages 24–38. Izdat. Leningrad. Univ., Leningrad, 1971.

[10] M. Sh. Birman. The spectrum of singular boundary problems. *Mat. Sb.*, 55:125–174, 1961.

[11] M. Sh. Birman and D. R. Yafaev. The spectral shift function. The papers of M. G. Kreĭn and their further development. *Algebra i Analiz*, 4(5):1–44, 1992.

[12] Jiří Blank, Pavel Exner, and Miloslav Havlíček. *Hilbert space operators in quantum physics*. Theoretical and Mathematical Physics. Springer, New York, second edition, 2008.

[13] D. Bollé. Sum rules in scattering theory and applications to statistical mechanics. In *Lectures on recent results*, volume 2 of *Mathematics+Physics*, pages 84–153. World Scientific, Singapore, 1986.

[14] D. Bollé. Schrödinger operators at tresholds. In *Ideas and Methods in Quantum Statistical Physics*, pages 173–196. Cambridge Univ. Press, Cambridge, 1992.

[15] Amin Boumenir and Vu Kim Tuan. A trace formula and Schmincke inequality on the half-line. *Proc. Amer. Math. Soc.*, 137(3):1039–1049, 2009.

[16] V. S. Buslaev and L. D. Faddeev. Formulas for traces for a singular Sturm-Liouville differential operator. *Soviet Math. Dokl.*, 1:451–454, 1960.

[17] Andrew M. Childs and DJ Strouse. Levinson's theorem for graphs. *J. Math. Phys.*, 52(8):082102, 9, 2011.

[18] Michael Cwikel. Weak type estimates for singular values and the number of bound states of Schrödinger operators. *Ann. Math. (2)*, 106(1):93–100, 1977.

[19] P. Deift and R. Killip. On the absolutely continuous spectrum of one-dimensional Schrödinger operators with square summable potentials. *Comm. Math. Phys.*, 203(2):341–347, 1999.

[20] P. Deift and E. Trubowitz. Inverse scattering on the line. *Comm. Pure Appl. Math.*, 32(2):121–251, 1979.

[21] S. Demirel and M. Usman. Trace formulas for Schrödinger operators on the half-line. *Bulletin of Mathematical Sciences*, 1(2):397–427, 2011.

[22] L. A. Dikiĭ. Trace formulas for Sturm-Liouville differential operators. *Uspehi Mat. Nauk (N.S.)*, 13(3(81)):111–143, 1958.

[23] Vitaly N. Efimov. Energy levels arising from resonant two-body forces in a three-body system. *Physics Letters B*, 33(8):563–564, 1970.

[24] Tomas Ekholm, Rupert L. Frank, and Hynek Kovařík. Eigenvalue estimates for Schrödinger operators on metric trees. *Adv. Math.*, 226(6):5165–5197, 2011.

[25] P. Exner and P. Šeba. Free quantum motion on a branching graph. *Rep. Math. Phys.*, 28(1):7–26, 1989.

[26] Pavel Exner. Weakly coupled states on branching graphs. *Lett. Math. Phys.*, 38(3):313–320, 1996.

[27] Pavel Exner, Jonathan P. Keating, Peter Kuchment, Toshikazu Sunada, and Alexander Teplyaev, editors. *Analysis on graphs and its applications*, volume 77 of *Proceedings of Symposia in Pure Mathematics*. American Mathematical Society, Providence, RI, 2008. Papers from the program held in Cambridge, January 8–June 29, 2007.

[28] Pavel Exner and Olaf Post. Convergence of spectra of graph-like thin manifolds. *J. Geom. Phys.*, 54(1):77–115, 2005.

[29] Pavel Exner and Olaf Post. Convergence of resonances on thin branched quantum waveguides. *J. Math. Phys.*, 48(9):092104, 43, 2007.

[30] Charles L. Fefferman. The uncertainty principle. *Bulletin (New Series) of the American Mathematical Society*, 9(2):129–206, 1983.

[31] Rupert L. Frank and Hynek Kovařík. Heat kernels of metric trees and applications. *arXiv:1108.6145v1*.

[32] S. A. Fulling, P. Kuchment, and J. H. Wilson. Index theorems for quantum graphs. *J. Phys. A*, 40(47):14165–14180, 2007.

[33] I. M. Gel′fand and B. M. Levitan. On a simple identity for the characteristic values of a differential operator of the second order. *Doklady Akad. Nauk SSSR (N.S.)*, 88:593–596, 1953.

[34] N. I. Gerasimenko. The inverse scattering problem on a noncompact graph. *Teoret. Mat. Fiz.*, 75(2):187–200, 1988.

[35] N. I. Gerasimenko and B. S. Pavlov. Scattering problems on noncompact graphs. *Teoret. Mat. Fiz.*, 74(3):345–359, 1988.

[36] F. Gesztesy and H. Holden. Trace formulas and conservation laws for nonlinear evolution equations. *Rev. Math. Phys.*, 6(1):51–95, 1994.

[37] F. Gesztesy and H. Holden. On new trace formulae for Schrödinger operators. *Acta Appl. Math.*, 39(1-3):315–333, 1995. KdV '95 (Amsterdam, 1995).

[38] F. Gesztesy and H. Holden. On trace formulas for Schrödinger-type operators. In *Multiparticle quantum scattering with applications to nuclear, atomic and molecular physics (Minneapolis, MN, 1995)*, volume 89 of *IMA Vol. Math. Appl.*, pages 121–145. Springer, New York, 1997.

[39] F. Gesztesy, H. Holden, B. Simon, and Z. Zhao. A trace formula for multidimensional Schrödinger operators. *J. Funct. Anal.*, 141(2):449–465, 1996.

[40] F. Gesztesy, M. Mitrea, and M. Zinchenko. Multi-dimensional versions of a determinant formula due to Jost and Pais. *Rep. Math. Phys.*, 59(3):365–377, 2007.

[41] Daniel Grieser. Spectra of graph neighborhoods and scattering. *Proc. Lond. Math. Soc. (3)*, 97(3):718–752, 2008.

[42] Boris Gutkin and Uzy Smilansky. Can one hear the shape of a graph? *J. Phys. A*, 34(31):6061–6068, 2001.

[43] Norman S. Ham and Klaus Ruedenberg. Electronic interaction in the free-electron network model for conjugated systems. I. Theory. *J. Chem. Phys.*, 25:1–13, 1956.

[44] M. Harmer. Hermitian symplectic geometry and extension theory. *J. Phys. A*, 33(50):9193–9203, 2000.

[45] M. S. Harmer. Inverse scattering for the matrix Schrödinger operator and Schrödinger operator on graphs with general self-adjoint boundary conditions. *ANZIAM J.*, 44(1):161–168, 2002. Kruskal, 2000 (Adelaide).

[46] M.S. Harmer. The matrix Schrödinger operator and Schrödinger operator on graphs. *Doctoral thesis*, 2004.

[47] Evans M. Harrell, II and Lotfi Hermi. Differential inequalities for Riesz means and Weyl-type bounds for eigenvalues. *J. Funct. Anal.*, 254(12):3173–3191, 2008.

[48] Evans M. Harrell, II and Lotfi Hermi. On Riesz means of eigenvalues. *Comm. Partial Differential Equations*, 36(9):1521–1543, 2011.

[49] Evans M. Harrell, II and Joachim Stubbe. On trace identities and universal eigenvalue estimates for some partial differential operators. *Trans. Amer. Math. Soc.*, 349(5):1797–1809, 1997.

[50] Evans M. Harrell, II and Joachim Stubbe. Universal bounds and semiclassical estimates for eigenvalues of abstract Schrödinger operators. *SIAM J. Math. Anal.*, 42(5):2261–2274, 2010.

[51] Evans M. Harrell, II and Joachim Stubbe. Trace identities for commutators, with applications to the distribution of eigenvalues. *Trans. Amer. Math. Soc.*, 363(12):6385–6405, 2011.

[52] Dirk Hundertmark. Bound state problems in Quantum Mechanics. In *Spectral theory and mathematical physics: a Festschrift in honor of Barry Simon's 60th birthday*, Proc. Sympos. Pure Math., LXXVI, part 1, pages 463–496. Amer. Math. Soc., Providence, R.I., 1980.

[53] Dirk Hundertmark, Elliott H. Lieb, and Lawrence E. Thomas. A sharp bound for an eigenvalue moment of the one-dimensional Schrödinger operator. *Adv. Theor. Math. Phys.*, 2(4):719–731, 1998.

[54] Norman E. Hurt. *Mathematical physics of quantum wires and devices*, volume 506 of *Mathematics and its Applications*. Kluwer Academic Publishers, Dordrecht, 2000. From spectral resonances to Anderson localization.

[55] D. R. Jafaev. Trace formulas for charged particles in nonrelativistic quantum mechanics. *Teoret. Mat. Fiz.*, 11(1):78–92, 1972.

[56] Arne Jensen and Tosio Kato. Spectral properties of Schrödinger operators and time-decay of the wave functions. *Duke Math. J.*, 46(3):583–611, 1979.

[57] R. Jost and A. Pais. On the scattering of a particle by a static potential. *Physical Rev. (2)*, 82:840–851, 1951.

[58] M. Kac. On the asymptotic number of bound states for certain attractive potentials. In *Topics in functional analysis (essays dedicated to M. G. Kreĭn on the occasion of his 70th birthday)*, volume 3 of *Adv. in Math. Suppl. Stud.*, pages 159–167. Academic Press, New York, 1978.

[59] Rowan Killip. Spectral theory via sum rules. In *Spectral theory and mathematical physics: a Festschrift in honor of Barry Simon's 60th birthday*, volume 76 of *Proc. Sympos. Pure Math.*, pages 907–930. Amer. Math. Soc., Providence, RI, 2007.

[60] Gustav R. Kirchhoff. Über die Auflösung der Gleichungen, auf welche man bei der Untersuchung der linearen Vertheilung galvanischer Ströme geführt wird. *Poggendorf's Ann. Phys. Chemie*, 72, 1847.

[61] V. Kostrykin and R. Schrader. Kirchhoff's rule for quantum wires. *J. Phys. A*, 32(4):595–630, 1999.

[62] V. Kostrykin and R. Schrader. Kirchhoff's rule for quantum wires. II. The inverse problem with possible applications to quantum computers. *Fortschr. Phys.*, 48(8):703–716, 2000.

[63] Peter Kuchment. Graph models for waves in thin structures. *Waves Random Media*, 12(4):R1–R24, 2002.

[64] Peter Kuchment. Differential and pseudo-differential operators on graphs as models of mesoscopic systems. In *Analysis and applications—ISAAC 2001 (Berlin)*, volume 10 of *Int. Soc. Anal. Appl. Comput.*, pages 7–30. Kluwer Acad. Publ., Dordrecht, 2003.

[65] Peter Kuchment. Quantum graphs. I. Some basic structures. *Waves Random Media*, 14(1):S107–S128, 2004. Special section on quantum graphs.

[66] Peter Kuchment. Quantum graphs: an introduction and a brief survey. In *Analysis on Graphs and its Applications*, Proc. Symp. Pure. Math., AMS 2008, pages 291–314. Amer. MAth. Soc., 2008.

[67] Pavel Kurasov. Schrödinger operators on graphs and geometry. I. Essentially bounded potentials. *J. Funct. Anal.*, 254(4):934–953, 2008.

[68] A. Laptev, S. Naboko, and O. Safronov. Absolutely continuous spectrum of Schrödinger operators with slowly decaying and oscillating potentials. *Comm. Math. Phys.*, 253(3):611–631, 2005.

[69] Ari Laptev and Timo Weidl. Recent results on Lieb-Thirring inequalities. In *Journées "Équations aux Dérivées, Partielles" (La Chapelle sur Erdre, 2000)*, pages Exp. No. XX, 14. Univ. Nantes, Nantes, 2000.

[70] Ari Laptev and Timo Weidl. Sharp Lieb-Thirring inequalities in high dimensions. *Acta Math.*, 184(1):87–111, 2000.

[71] N. Levinson. On the uniqueness of the potential in a Schrödinger equation for a given asymptotic phase. *Danske Vid. Selsk. Mat.-Fys. Medd.*, 25(9):29, 1949.

[72] Elliott H. Lieb and Walter Thirring. Inequalities for the moments of the eigenvalues of the Schrödinger Hamiltonian and their relation to Sobolev inequalities. *Studies in Mathematical Physics, Princeton University Press, Princeton, NJ*, pages 269–303, 1976.

[73] I. M. Lifshits. One problem of perturbation theory. *(Russian) Uspekhi Mat. Nauk*, 7(1):171–180, 1952.

[74] A. Martin. Bound states in the strong coupling limit. *Helv. Phys. Acta*, 45:140–148, 1972.

[75] F. Mehmeti, K. Ammari, and S. Nicaise. A dispersive estimate for the Schrödinger operator in star-shaped networks. *arXiv:1204.4998v1*, 2012.

[76] Robert M. Miura, Clifford S. Gardner, and Martin D. Kruskal. Korteweg-de Vries equation and generalizations. II. Existence of conservation laws and constants of motion. *J. Mathematical Phys.*, 9:1204–1209, 1968.

[77] K. Naimark and M. Solomyak. Eigenvalue estimates for the weighted Laplacian on metric trees. *Proc. London Math. Soc. (3)*, 80(3):690–724, 2000.

[78] K. Naimark and M. Solomyak. Geometry of Sobolev spaces on regular trees and the Hardy inequalities. *Russ. J. Math. Phys.*, 8(3):322–335, 2001.

[79] J. Östensson and D. Yafaev. A trace formula for differential operators of arbitrary order. *Operator Theory: Advances and Applications*, 218:541–570, 2012.

[80] Linus Pauling. The diamagnetic anistropy of aromatic molecules. *J. Chem. Phys.*, 4(10):673–677, 1936.

[81] L. E. Payne, G. Pólya, and H. F. Weinberger. On the ratio of consecutive eigenvalues. *J. Math. and Phys.*, 35:289–298, 1956.

[82] Michael Reed and Barry Simon. *Methods of modern mathematical physics. IV. Analysis of operators*. Academic Press [Harcourt Brace Jovanovich Publishers], New York, 1978.

[83] Grigorii V. Rozenblum. Distribution of the discrete spectrum of singular differential operators. *Izv. Vysš. Učebn. Zaved. Matematika*, (1(164)):75–86, 1976.

[84] Jacob Rubinstein and Michelle Schatzman. Variational problems on multiply connected thin strips. I. Basic estimates and convergence of the Laplacian spectrum. *Arch. Ration. Mech. Anal.*, 160(4):271–308, 2001.

[85] Alexei Rybkin. On a trace formula of the Buslaev-Faddeev type for a long-range potential. *J. Math. Phys.*, 40(3):1334–1343, 1999.

[86] Barry Simon. The bound state of weakly coupled Schrödinger operators in one and two dimensiones. *Ann. Physics*, 97(2):279–288, 1976.

[87] Barry Simon. *Trace ideals and their applications*, volume 35 of *London Mathematical Society Lecture Note Series*. Cambridge University Press, Cambridge, 1979.

[88] Uzy Smilansky and Michael Solomyak. The quantum graph as a limit of a network of physical wires. In *Quantum graphs and their applications*, volume 415 of *Contemp. Math.*, pages 283–291. Amer. Math. Soc., Providence, RI, 2006.

[89] Michael Solomyak. On the spectrum of the Laplacian on regular metric trees. *Waves Random Media*, 14(1):S155–S171, 2004. Special section on quantum graphs.

[90] Joachim Stubbe. Universal monotonicity of eigenvalue moments and sharp Lieb-Thirring inequalities. *J. Eur. Math. Soc. (JEMS)*, 12(6):1347–1353, 2010.

[91] H. Tamura. The asymptotic eigenvalue distribution for nonsmooth elliptic operators. *Proc. Jpn. Acad.*, 50:19–22, 1974.

[92] Walter Thirring. *A course in mathematical physics. Vol. 3*. Springer-Verlag, New York, 1981. Quantum mechanics of atoms and molecules, Translated from the German by Evans M. Harrell, Lecture Notes in Physics, 141.

[93] Ricardo Weder. L^p-$L^{\dot{p}}$ estimates for the Schrödinger equation on the line and inverse scattering for the nonlinear Schrödinger equation with a potential. *J. Funct. Anal.*, 170(1):37–68, 2000.

[94] Timo Weidl. On the Lieb-Thirring constants $L_{\gamma,1}$ for $\gamma \geq 1/2$. *Comm. Math. Phys.*, 178(1):135–146, 1996.

[95] Hermann Weyl. Das asymptotische Verteilungsgesetz der Eigenwerte linearer partieller Differentialgleichungen (mit einer Anwendung auf die Theorie der Hohlraumstrahlung). *Math. Ann.*, 71(4):441–479, 1912.

[96] Hermann Weyl. Repartición de corriente en una red conductora. *Rev. Mat. Hisp.-Amer*, 5(1):153–164, 1923.

[97] D. R. Yafaev. *Mathematical Scattering Theory, General Theory*, volume 105 of *Translations of Mathematical Monographs*. American Mathematical Society, Providence, RI, 1992.

[98] D. R. Yafaev. *Mathematical Scattering Theory, Analytic Theory*, volume 158 of *Mathematical Surveys and Monographs*. American Mathematical Society, Providence, RI, 2010.

[99] Hong Cang Yang. Estimates of the difference between consecutive eigenvalues. *preprint 1995 (revision of International Centre for Theoretical Physics preprint IC/91/60)*, Trieste, April 1991.

[100] V. E. Zaharov and L. D. Faddeev. The Korteweg-de Vries equation is a fully integrable Hamiltonian system. *Funkcional. Anal. i Priložen.*, 5(4):18–27, 1971.

Semra Demirel

Institute of Analysis, Dynamics and Modeling
University of Stuttgart Pfaffenwaldring 57
70569 Stuttgart, Germany

Current Position

PhD studies in Mathematics since 2008
University of Stuttgart (Germany)

Teaching Assistent in Analysis (Course head)
University of Stuttgart (Germany)

Education

Diplom der Mathematik (Masters in Mathematics) 2002 – 2007
University of Stuttgart (Germany)

Abitur (A-Levels) 1993 – 2002
Alfred-Amann-Gymnasium Bönnigheim (Germany)

Scientific Publication

S. Demirel, E. Harrell, *On semiclassical and universal inequalities for eigenvalues of Quantum Graphs*, Rev. Math. Phys. **22** (2010), 305–329.

S. Demirel, M. Usman, *Trace formulas for Schrödinger operators on the half-line*, Bull. Math. Sci. **1** (2011), 397–427.

S. Demirel, *The spectral shift function and Levinson's theorem for quantum star graphs*, arXiv:1205.1772.

Conference Contributions and Invited Seminar Talks

- *Spectral estimates for Quantum Graphs*, Tübingen, February 2012
- *Spectral estimates for Quantum Graphs*, Munich, July 2011
- *Spectral inequalities for Quantum Graphs*, Vienna, January 2011
- *Lieb-Thirring inequalities and universal bounds for eigenvalues of Quantum Graphs*, Carthage, May 2010
- *Lieb-Thirring inequalities for eigenvalues of Quantum Graphs*, London, Nov. 2009
- *Sharp Lieb-Thirring inequalities for eigenvalues of Quantum Graphs*, Mainz, Oct. 2009
- *Lieb-Thirring inequalities for eigenvalues of Quantum Graphs*, Chemnitz, Sept. 2009

Further departmental activities

Equal opportunities representative
University of Stuttgart