

The Trace Formula for Quantum Graphs with General Self Adjoint Boundary Conditions

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Abstract. We consider compact metric graphs with an arbitrary self adjoint realisation of the differential Laplacian. After discussing spectral properties of Laplacians, we prove several versions of trace formulae, relating Laplace spectra to sums over periodic orbits on the graph. This includes trace formulae with, respectively, absolutely and conditionally convergent periodic orbit sums; the convergence depending on properties of the test functions used. We also prove a trace formula for the heat kernel and provide small- t asymptotics for the trace of the heat kernel.

1. Introduction

Some ten years ago Kottos and Smilansky [19, 21] introduced quantum graphs as convenient models in the field of quantum chaos [13, 34], where a major goal is to understand the connection between dynamical properties of a quantum system and its associated classical counterpart [3]. Previously introduced models that possess classical counterparts with chaotic dynamics include quantum billiards, motions on Riemannian manifolds with negative curvatures and quantum maps. These models have been studied with considerable success, however, they have often turned out to bear unwanted complications. Quantum graphs are constructed along the lines of many of these models in that they are mainly concerned with spectral properties of Laplacians. In a sense they are maximally reduced versions of such models in that the underlying configuration space is one dimensional. The non trivial topology of the graph, however, introduces sufficient complexity such that the quantum system behaves like typical quantum systems with chaotic classical counterparts, see [19, 21]. On the other hand, many details of the classical dynamics are considerably simpler and quantum spectra are generally known to some more detail, so that quantum graph models proved to be very useful in the field of quantum chaos [11].

Trace formulae provide a direct connection between classical and quantum dynamics in that they relate quantum spectra to classical periodic orbits. In general, this connection arises in the form of an asymptotic relation, valid for large wave numbers. There are only few exceptional cases in which trace formulae are identities. Among these are, most notably, Laplacians on flat tori and on Riemannian manifolds with constant negative sectional curvatures. In both cases the configuration manifolds are Riemannian symmetric spaces, allowing for the application of powerful methods of harmonic analysis in proving the relevant trace formulae, i.e., the Poisson summation formula and the Selberg trace formula [32], respectively. Generically, however, the tools of harmonic analysis are not available, and trace formulae have to be proven using semiclassical or microlocal techniques, which naturally involve asymptotic methods. Semiclassical trace formulae were introduced by Gutzwiller [12] for the spectral density of quantum Hamiltonians. Subsequently, Balian and Bloch [1] set up analogous trace formulae for Laplacians on domains in \mathbb{R}^n in a short wavelength approximation. The first mathematical proofs, for Laplacians on Riemannian manifolds, are due to Colin de Verdière [6] as well as Duistermaat and Guillemin [7]. Later, proofs for the semiclassical case followed [27, 28].

One of the virtues of quantum graph models that led Kottos and Smilansky to introduce them to the field of quantum chaos is that their trace formulae are identities, very much in analogy to the Selberg trace formula. The first quantum graph trace formula, however, is due to Roth [29], who expressed the trace of the heat kernel for a Laplacian with Kirchhoff boundary conditions in the vertices of the graph as a sum over periodic orbits. Kottos and Smilansky [21] then introduced a trace formula for the spectral density of the Laplacian, and later Kostrykin, Potthoff and Schrader [18] extended Roth's trace formula to more general boundary conditions. In these cases the boundary conditions characterising the domain of the Laplacian were of a non-Robin type in that they do not mix boundary values of functions and their derivatives. This leads to periodic orbit sums in the trace formulae that closely resemble those occurring in the Selberg trace formula. In this paper our principal goal now is to consider general self adjoint realisations of Laplacians on compact metric graphs and to prove associated trace formulae with fairly general test functions. In particular, we do not require their Fourier transforms to be compactly supported. Allowing for Robin-type boundary conditions leads to trace formulae that are still identities, yet the amplitudes multiplying the oscillating factors in each periodic orbit contribution depend on the wave number in a non trivial way. In principle, these amplitude functions are known and possess asymptotic expansions for large wave numbers. Therefore, in a sense these trace formulae are intermediate between Selberg and Gutzwiller/Duistermaat-Guillemin trace formulae, where in the latter case only the asymptotic expansions of the amplitude functions are known, and the test functions must have compactly supported Fourier transforms.

This paper is organised as follows: In Section 2 we briefly review the construction of quantum graphs, including parametrisations of self adjoint realisations of

the Laplacian developed by Kostykin and Schrader [20] as well as Kuchment [24]. Following this we investigate various properties of quantum graph edge S-matrices as introduced in [21], focusing on their analytic properties. In Section 4 we then discuss general properties of Laplace spectra on compact graphs. The main part of this paper can be found in Section 5 where we prove several versions of quantum graph trace formulae: Theorem 5.3 contains a trace formula with a double sum over periodic orbits, of which only the sum over topological orbit lengths converges absolutely, and which allows for a large class of test functions. In Theorem 5.4, however, we restrict the class of test functions with the effect that the entire sum over periodic orbits converges absolutely. A suitable choice of a test function then allows to establish the trace of the heat kernel for arbitrary self adjoint realisations of the Laplacian, see Theorem 5.5. We finally summarise and discuss our results in Section 6. Some of the results presented here have been announced in [2].

2. Preliminaries

We begin with reviewing the relevant concepts underlying the construction of quantum graphs.

2.1. Metric graphs

In the sequel we shall consider finite, metric graphs $\Gamma = (\mathcal{V}, \mathcal{E}, \mathbf{l})$. Here \mathcal{V} is a finite set of vertices $\{v_1, \dots, v_V\}$ and \mathcal{E} is a finite set of edges $\{e_1, \dots, e_E\}$. When an edge e connects the vertices v and w , these are called edge ends. Two edges are adjacent, if they share an edge end; loops and pairs of multiply connected vertices shall be allowed. The degree d_v of a vertex v specifies the number of edges with v as one of their edge ends. A metric structure can be introduced by assigning intervals $[0, l_i]$ to edges e_i , along with coordinates $x_i \in [0, l_i]$. The E -tuple $\mathbf{l} = (l_1, \dots, l_E)$ then collects all edge lengths. Through this procedure the edge ends are mapped to the end points of the intervals in a specified manner. The edge end corresponding to $x_i = 0$ is then called initial point and, correspondingly, the other end point is the terminal point of the edge e_i . Hence not only the connectedness of the graph is specified, but also an orientation of the edges is introduced. We emphasise that the specific choice of the orientation thus made does not impact the results of this paper, in fact the choice of the initial and terminal points of the edges are arbitrary. The intervals are only used to construct the Laplace operator as a differential operator.

It is useful to arrange the $2E$ edge ends in a particular way: we list the initial points in the order as they occur in the list of edges, followed by the terminal points in the same order. For the trace formula we, moreover, require the following notions.

Definition 2.1. A *closed path* in Γ is a finite sequence of edges $(e_i)_{i=1}^n$, such that the edges e_i and e_{i+1} for $i \in \{1, \dots, n-1\}$ and the edges e_n and e_1 are adjacent. A *periodic orbit* is an equivalence class of closed paths modulo cyclic permutations of the edges.

The number n of edges in a periodic orbit p is its *topological length*, whereas the sum $l_p = l_{e_1} + \dots + l_{e_n}$ of the metric lengths of its edges is the *metric length*, or simply length, of p . A periodic orbit is primitive, if it is not a multiple repetition of another periodic orbit. Furthermore, the set of periodic orbits of the graph is called \mathcal{P} , and \mathcal{P}_n is its subset of orbits with topological length n .

2.2. Quantum graphs

Quantum mechanics on a metric graph can be studied in terms of the Schrödinger equation

$$i \frac{\partial}{\partial t} \psi_t = -\Delta \psi_t. \quad (2.1)$$

Here ψ_t is a vector in an appropriate Hilbert space and Δ is a suitable (differential) Laplace operator, acting on functions defined on the edges of the graph. Since this operator is of second order, it is independent of the choice of the coordinates x_j or $\tilde{x}_j := l_j - x_j$ on the edges e_j , and therefore also independent of the specification of edge ends as initial and terminal.

In order to be in a position to view the negative Laplacian in (2.1) as a quantum Hamiltonian, it has to be realised as a self adjoint operator on a suitable Hilbert space. We therefore introduce the space of square integrable functions on Γ as the quantum graph Hilbert space. In this context a function on the graph is a collection $F = (f_1, \dots, f_E)$ of functions $f_j : (0, l_j) \rightarrow \mathbb{C}$ on the edges. Therefore, one considers the following function spaces,

$$C^\infty(\Gamma) = \bigoplus_{j=1}^E C^\infty(0, l_j) \quad \text{and} \quad L^2(\Gamma) = \bigoplus_{j=1}^E L^2(0, l_j).$$

The latter is a closed orthogonal sum of Hilbert spaces with respect to the scalar product

$$\langle F, G \rangle := \sum_{j=1}^E \int_0^{l_j} \overline{f_j(x_j)} g_j(x_j) \, dx_j.$$

As a differential expression the (negative) Laplacian is simply given by

$$-\Delta F := (-f_1'', \dots, -f_E''),$$

where dashes denote derivatives. This expression may now serve as a way to introduce a closed, symmetric operator $(-\Delta, \mathcal{D}_0)$ with domain

$$\mathcal{D}_0 = \bigoplus_{j=1}^E H_0^2(0, l_j).$$

Here each term in the orthogonal sum consists of an L^2 -Sobolev space of functions which, together with their derivatives, vanish at the edge ends. The deficiency indices of this operator are $(2E, 2E)$, and thus it possesses self adjoint extensions that can be classified according to von Neumann's theory (see, e.g., [30]). An alternative approach has been developed in detail by Kostyrykin and Schrader [20],

which provides a convenient parametrisation that is particularly useful for later purposes. In this context one introduces the boundary values

$$\begin{aligned} F_{bv} &= (f_1(0), \dots, f_E(0), f_1(l_1), \dots, f_E(l_E))^T, \\ F'_{bv} &= (f'_1(0), \dots, f'_E(0), -f'_1(l_1), \dots, -f'_E(l_E))^T, \end{aligned} \quad (2.2)$$

of functions and their derivatives, whereby the signs ensure that inward derivatives are considered at all edge ends. Notice that the order of the terms follows the convention of arranging edge ends introduced previously. Boundary conditions on the functions in the domain of a given self adjoint operator are specified through a linear relation between boundary values; they are of the form

$$AF_{bv} + BF'_{bv} = 0, \quad (2.3)$$

see [20]. Here $A, B \in M(2E, \mathbb{C})$ are two matrices such that

- the matrix (A, B) , consisting of the columns of A and B , has maximal rank $2E$,
- AB^* is self adjoint.

These conditions then imply the self adjointness of the operator, and every self adjoint extension can be achieved in this manner. Occasionally, we shall denote a particular such self adjoint realisation of the Laplacian as $\Delta(A, B, \mathbf{l})$. This parametrisation, however, is obviously not unique because a multiplication of (2.3) with $C \in \text{GL}(2E, \mathbb{C})$ from the left does not change the boundary conditions. On the other hand, if $\Delta(A, B, \mathbf{l}) = \Delta(A', B', \mathbf{l})$, there exists $C \in \text{GL}(2E, \mathbb{C})$ with $A' = CA$ and $B' = CB$, see [20]. Thus, for any $C \in \text{GL}(2E, \mathbb{C})$ both A, B and $A' = CA, B' = CB$ provide an equivalent characterisation of the same operator.

The linear relations (2.3) can in principle relate boundary values at any set of edge ends. We wish, however, the operator to respect the connectedness of the graph and therefore we restrict ourselves to local boundary conditions. These are characterised by the condition that (2.3) only relates edge ends that form a single vertex. To this end we now group the edge ends in (2.2) according to the vertices they belong to. Local boundary conditions then lead to a block structure of the matrices A and B ,

$$A = \bigoplus_{v \in \mathcal{V}} A_v \quad \text{and} \quad B = \bigoplus_{v \in \mathcal{V}} B_v, \quad (2.4)$$

such that each block, represented by A_v and B_v , exactly relates the boundary values of functions and their derivatives at the vertex v . In this context self adjointness of the Laplacian is achieved, if for all $v \in \mathcal{V}$ the rank of (A_v, B_v) is d_v and $A_v B_v^*$ is self adjoint.

To mention a few examples, a vertex with Dirichlet boundary conditions can be characterised by $A_v = \mathbf{1}_{d_v}$, $B_v = 0$, whereas for Neumann boundary conditions one would choose $A_v = 0$, $B_v = \mathbf{1}_{d_v}$. Moreover, the generalised Kirchhoff boundary

conditions used by Kottos and Smilansky [21] can be achieved by choosing

$$A_v = \begin{pmatrix} 1 & -1 & & & \\ & \ddots & \ddots & & \\ & & 1 & -1 & \\ & & & & \mu_v \end{pmatrix} \quad \text{and} \quad B_v = \begin{pmatrix} & & & & \\ & & & & \\ & & & & \\ 1 & \dots & \dots & & 1 \end{pmatrix}, \quad (2.5)$$

where only the non vanishing matrix entries are indicated. Here μ_v must be real; when $\mu_v = 0$ the usual Kirchhoff conditions are realised.

The approach we have taken here when singling out local boundary conditions is to start from a given graph and then to realise the Laplacian as a self adjoint operator on that graph. An alternative view would be to consider the above construction as a realisation of the Laplacian as a self adjoint operator on a collection of E intervals. One can then find a graph, i.e., a way to connect the interval ends in vertices, such that a given pair of matrices A and B is local with respect to this graph; there even is a unique graph maximising the number of vertices [22]. In the following we shall, however, stick to the previous view.

The non-uniqueness in the choice of the matrices A and B can be overcome by parametrising the self adjoint realisations of the Laplacian in terms of projectors onto subspaces of the $2E$ -dimensional spaces of boundary values. To this end Kuchment [24] introduced the projector P onto the kernel of B as well as the projector $Q = \mathbf{1} - P$ onto the orthogonal complement $(\ker B)^\perp = \text{ran } B^*$ in \mathbb{C}^{2E} and proved that A maps $\text{ran } B^*$ into $\text{ran } B$. He then defined the (self adjoint) endomorphism

$$L := (B|_{\text{ran } B^*})^{-1} A Q \quad (2.6)$$

of $\text{ran } B^*$, and showed that the boundary conditions (2.3) are equivalent to

$$P F_{bv} = 0 \quad \text{and} \quad L Q F_{bv} + Q F'_{bv} = 0. \quad (2.7)$$

Moreover, there exists a $C \in \text{GL}(2E, \mathbb{C})$ such that

$$A' = C A = P + L \quad \text{and} \quad B' = C B = Q, \quad (2.8)$$

implying that

$$L = A' B'^*.$$

A refinement of this construction can be found in [9]. From (2.7) one concludes that in cases where $L = 0$, the boundary conditions do not mix boundary values of the functions themselves with those of their derivatives. We call these *non-Robin boundary conditions*, and all other cases *Robin boundary conditions*.

Yet another description of the self adjoint realisations of the Laplacian employs the associated quadratic forms. As shown by Kuchment [24], given a realisation of the Laplacian as a self adjoint operator, the associated quadratic form

$$Q_\Delta[F] = \sum_{e=1}^E \int_0^{l_e} |f'_e(x)|^2 dx - \langle F_{bv}, L F_{bv} \rangle_{\mathbb{C}^{2E}} \quad (2.9)$$

has a domain that consist of all functions F on the graph, with components $f_e \in H^1(0, l_e)$, whose boundary values fulfil $P F_{bv} = 0$.

3. The S-matrix

In quantum graph models Laplace eigenvalues can be conveniently characterised in terms of zeros of finite dimensional determinants, and thus these models are amenable to powerful analytical as well as numerical methods. In quantum billiards a related method was pioneered by Doron and Smilansky [8] as the scattering approach to quantisation. In general, this method relies on semiclassical approximations. As first demonstrated by Kottos and Smilansky [21], however, in quantum graphs the scattering approach allows to determine Laplace eigenvalues exactly from a finite dimensional secular equation.

The scattering approach bears its name from the fact that it is based on scattering processes occurring when one opens up a given closed quantum system appropriately. In quantum graphs the procedure of opening up consists of replacing each vertex and its attached edges by an infinite star graph. This is the single, given vertex v with d_v infinite half lines attached that replace the edges of finite lengths. Carrying over the local boundary conditions at the vertices from the original closed quantum graph, one thus obtains V open quantum systems, which each possess an on-shell scattering matrix $\sigma^v(k)$. More precisely, this S-matrix is defined in terms of d_v functions $F^{(j)}$ on the infinite star graph associated with v , whose components on the d_v infinite edges are

$$f_i^{(j)}(x) := \begin{cases} \sigma_{ji}^v(k) e^{ikx}, & j \neq i \\ e^{-ikx} + \sigma_{jj}^v(k) e^{ikx}, & j = i \end{cases}.$$

One then requires each of these functions to fulfil the boundary conditions at v . In terms of the parameterisation of the boundary conditions described in Section 2.2 one then finds that

$$\sigma^v(k) = -(A_v + ikB_v)^{-1}(A_v - ikB_v), \quad \text{for } k \in \mathbb{R} \setminus \{0\}. \quad (3.1)$$

The conditions imposed on A_v and B_v in order to achieve self adjoint boundary conditions ensure that $A_v \pm ikB_v$ are invertible and that the vertex S-matrix $\sigma^v(k)$ is unitary for all $k \in \mathbb{R} \setminus \{0\}$, see [20].

The local scattering matrix associated with a vertex with Dirichlet or Neumann boundary conditions is $\sigma^v = -\mathbb{1}_{d_v}$ or $\sigma^v = \mathbb{1}_{d_v}$, respectively. In contrast, according to (2.5) generalised Kirchhoff boundary conditions lead to a vertex S-matrix with elements of the form [21]

$$\sigma_{ij}^v(k) = -\delta_{ij} + \frac{2k}{d_v k + i\mu_v}. \quad (3.2)$$

The local S-matrices of the entire graph can now be grouped together vertex by vertex. In that process all edges occur twice, namely associated with the vertex S-matrices of their two edge ends. It is hence useful to consider directed edges, and view the matrix elements of σ^v as describing transitions from a directed edge with terminal point v to a directed edge that has v as its initial point. As the list of all directed edges corresponds to listing their initial points, the transitions prescribed

by σ^v can also be performed on the boundary values (2.2). As a result one obtains the matrix

$$S(A, B; k) = -(A + ikB)^{-1}(A - ikB). \quad (3.3)$$

Again, $A \pm ikB$ are invertible and $S(A, B; k)$ is unitary for all $k \in \mathbb{R} \setminus \{0\}$. Moreover, (3.3) is invariant under the substitution of A, B by CA, CB for all $C \in \text{GL}(2E, \mathbb{C})$ and therefore is associated with the self adjoint realisations of the Laplacian [22].

We emphasise that, although (3.3) can be defined for any self adjoint realisation, the vertex S-matrices (3.1) can only be recovered from (3.3) in the case of local boundary conditions, i.e., when (2.4) is satisfied. Despite the fact that a closed quantum graph does not allow for quantum scattering in the usual sense, the quantity (3.3) is often referred to as the edge (or bond) S-matrix [21] of the quantum graph.

Furthermore, using the parametrisation (2.7) of boundary conditions and utilising (2.8) as well as the fact that $(L + ik)^{-1}$ commutes with $L - ik$, one obtains the representation

$$S(A, B; k) = -P - Q(L + ik)^{-1}(L - ik)Q, \quad k \in \mathbb{R} \setminus \{0\}, \quad (3.4)$$

for the edge S-matrix, see [22].

From the expressions (3.3) and (3.4) it appears that the S-matrix generally depends on the wave number k in a non-trivial way. However, certain boundary conditions lead to k -independent S-matrices. Obvious examples are Dirichlet and Neumann boundary conditions, as well as the usual Kirchhoff boundary conditions, i.e., (3.2) with $\mu_v = 0$. A general characterisation of such boundary conditions was provided in [18] in terms of the following equivalent conditions:

- $S(A, B; k)$ is k -independent.
- $S(A, B; k)$ is self adjoint for some, and hence for all, $k > 0$.
- $S(A, B; k) = \mathbb{1} - 2P$ for some, and hence for all, $k > 0$.
- $AB^* = 0$, i.e., $L = 0$.

The last point shows that k -independent S-matrices arise exactly in the case of non-Robin boundary conditions.

Below we are going to prove some properties of S-matrices that are relevant for the trace formula. In this context, for Robin boundary conditions an important role will be played by the spectrum $\sigma(L)$ of the self adjoint matrix L (2.6).

We shall make extensive use of the S-matrix extended to complex wave numbers k and therefore need the following.

Lemma 3.1. *Let A and B specify self adjoint boundary conditions for the Laplacian on the graph. Then the S-matrix (3.3) has the following properties:*

1. $S(A, B; k)$ can be continued into the complex k -plane as a meromorphic function, and has simple poles at the points of the set $i\sigma(L) \setminus \{0\}$.
2. $S(A, B; k)$ is unitary for all $k \in \mathbb{R}$.
3. $S(A, B; k)$ is invertible for all $k \in \mathbb{C} \setminus [\pm i\sigma(L) \setminus \{0\}]$, and its inverse is $S(A, B; -k)$.

Now choose $C(k) = (A + ikB)^{-1} \in \text{GL}(2E, \mathbb{C})$ and find that (see also [23])

$$C(k)A = -\frac{1}{2}(S(k) - \mathbb{1}) \quad \text{and} \quad C(k)B = -\frac{1}{2ik}(S(k) + \mathbb{1}). \quad (3.8)$$

Inserting this into (3.7) finally leads to

$$\begin{aligned} S'(k) &= \frac{1}{2k}(S(k) + \mathbb{1})(S(k) - \mathbb{1}) \\ &= -\frac{1}{2k}(S(k) - S(k)^*)S(k), \end{aligned} \quad (3.9)$$

which proves the statement for $k \in \mathbb{R} \setminus \{0\}$.

From Lemma 3.1 we infer that $S(k)$ is analytic in a neighbourhood of $k = 0$ and that the right-hand side of (3.9) has a removable singularity at $k = 0$; hence (3.9) extends to all real k . Since, moreover, $S(k)$ is unitary on \mathbb{R} and analytic on $\mathbb{C} \setminus [\pm i\sigma(L)]$, and $\frac{1}{k}$ as well as $S(k)^{-1}$ are also analytic on this set, the full statement of the lemma follows by analytic continuation. \square

From Lemma 3.1 we know that $S(k)$ is meromorphic with finitely many poles on the imaginary axis. One can therefore perform power series expansions of the S-matrix in large parts of the complex k -plane. Below we want to specify two such expansions, and to this end we exclude an annulus containing $i\sigma(L) \setminus \{0\}$. This annulus is characterised by the two radii

$$\lambda_{\min / \max} := \min / \max \{|\lambda|; \lambda \in \sigma(L) \setminus \{0\}\}.$$

Here we assume that $\sigma(L) \neq \{0\}$; otherwise $L = 0$ which is equivalent to the S-matrix being independent of k .

We are now in a position to provide the announced expansions of the S-matrix.

Lemma 3.3. *Let the same conditions as in Lemma 3.1 be given and assume that $L \neq 0$. Then the following power series expansions converge absolutely and uniformly in any closed subsets of the specified regions:*

1. For $|k| > \lambda_{\max}$,

$$S(A, B; k) = \mathbb{1} - 2P + 2 \sum_{n=1}^{\infty} \frac{1}{k^n} (iL)^n. \quad (3.10)$$

2. For $|k| < \lambda_{\min}$,

$$S(A, B; k) = -\mathbb{1} + 2\tilde{P} - 2 \sum_{n=1}^{\infty} k^n (i\tilde{L})^n, \quad (3.11)$$

where \tilde{P} and \tilde{L} emerge from P and L , respectively, by replacing A, B with $-B, A$.

Proof. For the first expansion we refer to the representation (3.5) of the S-matrix and employ the expansion

$$-\frac{\lambda_\alpha - ik}{\lambda_\alpha + ik} = \frac{1 + \frac{i}{k}\lambda_\alpha}{1 - \frac{i}{k}\lambda_\alpha} = 1 + 2 \sum_{n=1}^{\infty} \left(\frac{i\lambda_\alpha}{k}\right)^n, \quad \alpha = 1, \dots, d,$$

valid for $|k| > \lambda_\alpha$. Hence, for $|k| > \lambda_{\max}$ the S-matrix is $\mathbb{1} + 2 \sum_{n=1}^{\infty} \frac{1}{k^n} (iL)^n$ on $\text{ran } B^*$ and $-\mathbb{1}$ on $\text{ker } B$. Since $L = 0$ on $\text{ker } B$, the relation (3.10) follows.

For the second expansion we remark that from (3.3) one can readily deduce the relation $S(A, B; k) = -S(-B, A; \frac{1}{k})$ for $k \in \mathbb{R} \setminus \{0\}$, see [22]. Thus, (3.10) implies (3.11), and the domain $|k| < \lambda_{\min}$ of convergence, in which $S(k)$ is holomorphic, follows immediately. \square

Lemma 3.3 also provides limiting expressions for the edge S-matrix as $|k| \rightarrow \infty$ and $|k| \rightarrow 0$, respectively,

$$S_\infty = \mathbb{1} - 2P \quad \text{and} \quad S_0 = -\mathbb{1} + 2\tilde{P},$$

which we shall use subsequently.

Later we shall integrate expressions containing the S-matrix along contours in the upper complex half plane and, therefore, we need to estimate the norm of the S-matrix along the contours. To this end we introduce

$$\lambda_{\min}^+ := \begin{cases} \min\{\lambda \in \sigma(L); \lambda > 0\}, & \text{if } \exists \lambda_\alpha > 0 \\ \infty, & \text{else} \end{cases}, \quad (3.12)$$

and obtain the following.

Lemma 3.4. *Let $k \in \mathbb{R}$ and $0 < \kappa < \lambda_{\min}^+$, then*

$$\|S(k + i\kappa)\|, \|S(k - i\kappa)^{-1}\| \leq \max \left\{ 1, \frac{\lambda_{\min}^+ + \kappa}{\lambda_{\min}^+ - \kappa} \right\} \quad (3.13)$$

in the operator norm. Furthermore, if $\kappa > \lambda_{\max}$, then

$$\|S(k + i\kappa)\|, \|S(k - i\kappa)^{-1}\| \leq \frac{\kappa + \lambda_{\max}}{\kappa - \lambda_{\max}}. \quad (3.14)$$

Proof. From (3.5) one can read off the eigenvalues of $S(k + i\kappa)$ as ± 1 and $-(\lambda_\alpha + \kappa - ik)/(\lambda_\alpha - \kappa + ik)$, $\alpha = 1, \dots, d$. In absolute values the latter quantities, as functions of $k \in \mathbb{R}$, are maximised at $k = 0$. Now suppose that $\lambda_{\min}^+ > 0$ and let $0 < \kappa < \lambda_{\min}^+$. Then the largest quantity among the $|\lambda_\alpha + \kappa|/|\lambda_\alpha - \kappa|$ is the one on the right-hand side of (3.13). In the case $\lambda_{\min}^+ = \infty$ the upper bound is one. The proof for $S(k - i\kappa)^{-1}$ is completely analogous.

If $\kappa > \lambda_{\max}$ the same argument yields the bound (3.14). \square

4. The spectrum of the Laplacian

The scattering approach to the quantisation of a finite, metric graph utilises a secular equation based on the edge S-matrix of the graph. Here we closely follow the original approach as developed by Kottos and Smilansky [21] for the case of (generalised) Kirchhoff boundary conditions, which was later generalised by Kostrykin and Schrader [23]. To keep the presentation sufficiently self-contained, we reproduce the relevant results below. We begin, however, with some general properties of Laplace spectra and finish this section with some remarks on the eigenvalue zero.

4.1. Preliminaries on the spectrum

Given a Laplacian on a compact metric graph, one would naturally expect that its spectrum is discrete and has a finite lowest eigenvalue. Kuchment indeed proved [24] that any such self adjoint (negative) Laplacian is bounded from below, and that its resolvent is trace class. Thus, the spectrum is discrete and bounded from below. Subsequently, Kostrykin and Schrader [23] improved the lower bound. They showed that

$$-\Delta \geq -s^2, \quad (4.1)$$

where $s \geq 0$ is the unique solution of

$$s \tanh\left(\frac{sl_{\min}}{2}\right) = \lambda_{\max}^+, \quad (4.2)$$

with l_{\min} denoting the shortest edge length and

$$\lambda_{\max}^+ := \begin{cases} \max\{\lambda \in \sigma(L); \lambda > 0\}, & \text{if } \exists \lambda_\alpha > 0 \\ 0, & \text{else} \end{cases}. \quad (4.3)$$

Remark 4.1. As an aside we should like to mention that the lower bound (4.1) is optimal in the following sense: Consider a trivial example of a metric graph given by an interval I of length l , and a Laplacian with domain specified by the choice

$$A = \lambda \mathbb{1}_2 \quad \text{and} \quad B = \mathbb{1}_2,$$

where $\lambda > 0$, such that $L = \lambda \mathbb{1}_2$ and $\sigma(L) = \{\lambda\}$. (Equivalently, $P = 0$, $Q = \mathbb{1}_2$ and $L = \lambda \mathbb{1}_2$.) Hence, (2.7) leads to the Robin boundary conditions

$$\lambda \begin{pmatrix} f(0) \\ f(l) \end{pmatrix} + \begin{pmatrix} f'(0) \\ -f'(l) \end{pmatrix} = 0,$$

and this implies the quantisation condition

$$\left(\frac{\lambda - ik}{\lambda + ik}\right)^2 e^{2ikl} = 1. \quad (4.4)$$

The solution $k = i\kappa$, with $\kappa > \lambda > 0$, representing the lowest Laplace eigenvalue $-\kappa^2$ corresponds to a solution of the equation

$$\kappa \tanh\left(\frac{\kappa l}{2}\right) = \lambda.$$

This condition is equivalent to (4.2), demonstrating that the bound (4.1) is sharp for this ‘quantum graph’.

Kostrykin and Schrader also showed [23] that the number of negative Laplace eigenvalues is bounded by the number of positive eigenvalues of L (counted with their respective multiplicities). In the example above, the Robin Laplacian on an interval hence has at least one and at most two negative eigenvalues.

For the trace formula one requires an a priori estimate on the number of eigenvalues. This is well known for the Dirichlet and the Neumann Laplacian, and in the case of Kirchhoff boundary conditions can be found in [33]. The same asymptotic law, however, holds also in the general case.

Proposition 4.2. *Given a self adjoint realisation of the Laplacian on a compact metric graph, the number of its eigenvalues $k_j^2 \in \mathbb{R}$ (counted with their multiplicities) fulfils the following asymptotic law,*

$$N(K) := \#\{j; k_j^2 \leq K^2\} \sim \frac{\mathcal{L}}{\pi} K, \quad K \rightarrow \infty, \quad (4.5)$$

where $\mathcal{L} := l_{e_1} + \dots + l_{e_E}$ is the total length of the graph. In particular, the Laplacian has infinitely many eigenvalues that only accumulate at infinity.

Proof. We prove the asymptotic law employing a variational characterisation of the eigenvalues based on the quadratic form (2.9), as well as an analogue of the Dirichlet-Neumann bracketing (see [31]). To this end we introduce two comparison operators.

The first comparison operator is the direct sum of the Dirichlet operators on the edges, i.e., the Dirichlet-Laplacian of Section 2.2. The domain of the associated quadratic form is characterised by the condition $F_{bv} = 0$, and therefore is contained in the domain of (2.9). Moreover, on the Dirichlet-form domain both quadratic forms coincide. The comparison lemma devised in [31] hence implies that $N_D(K) \leq N(K)$. Here $N_D(K)$ is the counting function for the eigenvalues of the Dirichlet-Laplacian, which trivially fulfils the asymptotic law (4.5).

As our second comparison operator we choose the direct sum of Robin Laplacians on the edges (see the example above). This operator is characterised by $P_R = 0$, $Q_R = \mathbf{1}_{2E}$ and $L = \lambda \mathbf{1}_{2E}$ with some $\lambda \geq 0$. ($\lambda = 0$ in fact corresponds to Neumann Laplacians on the edges.) The boundary conditions are $\lambda F_{bv} + F'_{bv} = 0$, and thus they decouple the edges. The respective eigenvalue counting function $N_R(K)$ can be determined from (4.4) and clearly obeys the asymptotic law (4.5). The associated form domain, characterised by the condition $P_R F_{bv} = 0$, contains the domain of (2.9). Choosing $\lambda = \lambda_{\max}^+$, see (4.3), on the form domain of

(2.9) one finds $Q_R[F] \leq Q_\Delta[F]$. Therefore, the comparison lemma of [31] implies $N_R(K) \geq N(K)$.

Thus, $N_D(K) \leq N(K) \leq N_R(K)$ and the upper and the lower bounds both fulfil the same asymptotic law, which proves (4.5). The further statement follows immediately. \square

This result is independent of any details of the quantum graph, apart from its volume. This is analogous to the corresponding results for Laplacians on manifolds or domains. In general, the asymptotic growth of the number of eigenvalues is proportional to the volume of the manifold/domain and to K^D , where D is the dimension of the manifold/domain. This type of results is often referred to as ‘Weyl’s law’ [35], and insofar Proposition 4.2 is the quantum graph version of Weyl’s law.

4.2. The secular equation

Apart from the edge S-matrix, the scattering approach requires the metric information of the graph, which enters through

$$T(\mathbf{l}; k) := \begin{pmatrix} 0 & t(\mathbf{l}; k) \\ t(\mathbf{l}; k) & 0 \end{pmatrix} \quad \text{with} \quad t(\mathbf{l}; k) := \begin{pmatrix} e^{ikl_1} & & \\ & \ddots & \\ & & e^{ikl_E} \end{pmatrix}, \quad (4.6)$$

where $k \in \mathbb{C}$. Both matrices are then used to introduce

$$U(k) := S(A, B; k) T(\mathbf{l}; k). \quad (4.7)$$

The topological and the metric data entering $U(k)$ are hence clearly separated.

For real k the endomorphisms $S(k)$, $T(k)$ and $U(k)$ of \mathbb{C}^{2E} are obviously unitary. We therefore denote the eigenvalues of $U(k)$ by $e^{i\theta_1(k)}, \dots, e^{i\theta_{2E}(k)}$. Following Lemma 3.1 we conclude that $U(k)$ can be extended into the complex k -plane as a meromorphic function with poles at $i\sigma(L) \setminus \{0\}$. The determinant function

$$F(k) := \det(\mathbb{1} - U(k)), \quad (4.8)$$

on which the scattering approach is based (see [21]), hence is also meromorphic. Its poles are in $i\sigma(L) \setminus \{0\}$, but do not necessarily exhaust the entire set.

Proposition 4.3 (Kostykin, Schrader [23]). *The determinant function (4.8) is meromorphic on the complex plane with poles in the set $i\sigma(L) \setminus \{0\}$. Furthermore, let $k_n \in \mathbb{C} \setminus [i\sigma(L) \cup \{0\}]$ with $\text{Im } k_n \geq 0$, then k_n^2 is an eigenvalue of $-\Delta$, iff k_n is a zero of the function (4.8), i.e., $F(k_n) = 0$. Moreover, the spectral multiplicity g_n of the Laplace eigenvalue $k_n^2 > 0$ coincides with the multiplicity of the eigenvalue one of $U(k_n)$.*

Proposition 4.3 establishes a close connection between zeros of the determinant function (4.8) and Laplace eigenvalues. Notice that although Laplace eigenvalues occur as squares, k^2 , the function (4.8) is not invariant under a change of sign in its argument. There exists, however, a functional equation under the substitution $k \mapsto -k$.

Lemma 4.4. *For all $\mathbb{C} \setminus [\pm i\sigma(L) \setminus \{0\}]$ the following identity holds:*

$$F(k) = (-1)^M e^{2ik\mathcal{L}} \left(\prod_{\alpha=1}^d \frac{\lambda_\alpha - ik}{\lambda_\alpha + ik} \right) F(-k), \tag{4.9}$$

where $M = E + d + \dim \ker B$ and $\mathcal{L} = l_{e_1} + \dots + l_{e_E}$ is the sum of all edge lengths.

Proof. We decompose

$$\mathbb{1} - S(k)T(k) = -S(k)[\mathbb{1} - S(-k)T(-k)]T(k),$$

so that after taking determinants,

$$F(k) = (-1)^{2E} \det T(k) \det S(k) F(-k).$$

Using the definition (4.6) of $T(k)$ and the representation (3.5) of $S(k)$ then yields (4.9). \square

We remark that when $k^2 \in \mathbb{R}$ is a Laplace eigenvalue, then either $k \in \mathbb{R}$ when the eigenvalue is non-negative or, in the case of a negative eigenvalue, $k = \pm i\kappa$ with $\kappa > 0$. The relevant zeros of the determinant (4.8) are then $\pm k \in \mathbb{R}$ or $i\kappa$, respectively. Unless $\kappa \in \sigma(L)$ or $k = 0$, all Laplace eigenvalues are covered by Proposition 4.3. However, in order to count Laplace eigenvalues in terms of zeros of $F(k)$ with their correct multiplicities one has to establish a connection between the order of the zero and the multiplicity of one as an eigenvalue of $U(k)$. In the trace formula we shall need this connection for the non-negative eigenvalues and hence now consider the eigenphases $\theta(k)$ of $U(k)$, defined through

$$U(k)v(k) = e^{i\theta(k)}v(k) \quad \text{with} \quad \|v(k)\| = 1, \tag{4.10}$$

for $k \in \mathbb{R}$. We then recall that $U(k) = S(A, B; k)T(L; k)$ is analytic in $\mathbb{C} \setminus [i\sigma(L) \setminus \{0\}]$. According to analytic perturbation theory (see, e.g., [16]) its eigenvalues, for which we keep the notation $e^{i\theta(k)}$, are continuous on this set and differentiable apart from possibly isolated points. Since, however, $U(k)$ is real-analytic and normal for all $k \in \mathbb{R}$, we can apply a sharpened version of analytic perturbation theory (see [26]) to conclude that the eigenvalues are real analytic for all $k \in \mathbb{R}$ and that there exists a choice of eigenvectors with the same property.

The following statement is a generalisation of a result found in [5, 21] that is valid for k -independent S-matrices.

Lemma 4.5. *Let $\theta(k)$ be an eigenphase of $U(k)$, $k \in \mathbb{R}$, with associated normalised eigenvector $v(k) = (v_1(k), \dots, v_{2E}(k))^T$. Then*

$$\frac{d}{dk}\theta(k) = \sum_{i=1}^{2E} l_i |v_i(k)|^2 - 2 \left\langle v(k), \frac{L}{L^2 + k^2} v(k) \right\rangle_{\mathbb{C}^{2E}}. \tag{4.11}$$

Proof. Taking Lemma 3.2 into account we first observe that

$$\begin{aligned} U'(k) &= -\frac{1}{2k}(S(k) - S^*(k))S(k)T(k) + iS(k)T(k)D(\mathbf{l}) \\ &= -2i\frac{L}{L^2 + k^2}U(k) + iU(k)D(\mathbf{l}), \end{aligned} \quad (4.12)$$

where

$$D(\mathbf{l}) := \begin{pmatrix} D_1(\mathbf{l}) & 0 \\ 0 & D_1(\mathbf{l}) \end{pmatrix}, \quad D_1(\mathbf{l}) := \begin{pmatrix} l_1 & & \\ & \ddots & \\ & & l_E \end{pmatrix}. \quad (4.13)$$

We also employed the relation

$$-\frac{1}{2k}(S(k) - S^*(k)) = -2i\frac{L}{L^2 + k^2} \quad (4.14)$$

that follows from (3.4). This then yields

$$\begin{aligned} \left\langle v(k), \frac{d}{dk}[U(k)v(k)] \right\rangle &= -2i e^{i\theta(k)} \left\langle v(k), \frac{L}{L^2 + k^2}v(k) \right\rangle + i \langle U^*(k)v(k), D(\mathbf{l})v(k) \rangle \\ &\quad + \langle U^*(k)v(k), v'(k) \rangle \\ &= -2i e^{i\theta(k)} \left\langle v(k), \frac{L}{L^2 + k^2}v(k) \right\rangle + i e^{i\theta(k)} \langle v(k), D(\mathbf{l})v(k) \rangle \\ &\quad + e^{i\theta(k)} \langle v(k), v'(k) \rangle. \end{aligned} \quad (4.15)$$

On the other hand, taking the derivative on the right-hand side of (4.10) and then multiplying with $v(k)$ leads to

$$\left\langle v(k), \frac{d}{dk}[e^{i\theta(k)}v(k)] \right\rangle = i\theta'(k)e^{i\theta(k)} + e^{i\theta(k)} \langle v(k), v'(k) \rangle. \quad (4.16)$$

Comparing (4.15) and (4.16) proves the statement (4.11). \square

This lemma allows us to obtain an upper and a lower bound for the derivative of an eigenphase. Using l_{\max}/l_{\min} to denote the largest and the smallest edge length, respectively, and introducing

$$\lambda_{\min}^- := \begin{cases} \min\{|\lambda|; \lambda \in \sigma(L) \cap \mathbb{R}^-\}, & \text{if } \exists \lambda_\alpha < 0 \\ \infty, & \text{else} \end{cases},$$

in analogy to (3.12), we immediately get the following.

Corollary 4.6. *The derivative $\theta'(k)$ of an eigenphase $\theta(k)$ is bounded from above and below according to*

$$l_{\min} - \frac{2}{\lambda_{\min}^+} \leq \theta'(k) \leq l_{\max} + \frac{2}{\lambda_{\min}^-}. \quad (4.17)$$

In particular, if $l_{\min} > 2/\lambda_{\min}^+$ the derivatives of all eigenphases are always positive.

Proof. Obviously,

$$l_{\min} \leq \sum_{i=1}^{2E} l_i |v_i(k)|^2 \leq l_{\max},$$

since the eigenvector is supposed to be normalised. Moreover, after a diagonalisation of L , when WLW^* is diagonal with the eigenvalues λ_α on the diagonal, one obtains

$$\left\langle v(k), \frac{L}{L^2 + k^2} v(k) \right\rangle = \sum_{\alpha=1}^{2E} |w_\alpha(k)|^2 \frac{\lambda_\alpha}{\lambda_\alpha^2 + k^2},$$

where $w(k) = Wv(k)$. This first yields

$$-\frac{1}{\lambda_{\min}^-} \leq \left\langle v(k), \frac{L}{L^2 + k^2} v(k) \right\rangle \leq \frac{1}{\lambda_{\min}^+},$$

and then finally (4.17). \square

As an important consequence of this corollary we are now able to extend the statement of Proposition 4.3 as required to count eigenvalues in terms of zeros of the determinant function.

Proposition 4.7. *Let the metric structure of the graph be such that $l_{\min} > 2/\lambda_{\min}^+$. Then $k_n^2 > 0$ is an eigenvalue of the Laplacian with multiplicity g_n , if $\pm k_n \in \mathbb{R} \setminus \{0\}$ are zeros of the function $F(k)$ of order g_n .*

Proof. From Proposition 4.3 and Lemma 4.4 we know that the positive Laplace eigenvalues are in one-to-one correspondence with (pairs of) k values where $U(k)$ has an eigenvalue one, and the respective multiplicities coincide. It hence remains to establish that the order of the corresponding zeros of $F(k)$ are exactly these multiplicities: From the definition (4.8) of the function $F(k)$ one obtains

$$F(k) = \prod_{j=1}^{2E} \left(1 - e^{i\theta_j(k)}\right),$$

so Corollary 4.6 implies $\frac{d}{dk} (1 - e^{i\theta_j(k)}) = -i\theta_j'(k)e^{i\theta_j(k)} \neq 0$, and the claim follows immediately. \square

We remark that since the scattering approach to the proof of the trace formula is based on counting zeros of the function $F(k)$ on the real line with their multiplicities, the requirement $l_{\min} > 2/\lambda_{\min}^+$ is essential. Otherwise one might count Laplace eigenvalues with incorrect multiplicities. Whenever L has no positive part, however, the condition is empty. This is, e.g., the case for non-Robin boundary conditions.

4.3. The eigenvalue zero

In general, zero is a Laplace eigenvalue as well as a zero of the determinant (4.8), and in so far Proposition 4.3 also applies to $k_0 = 0$. The spectral multiplicity g_0 , however, typically is different from the degree of $k_0 = 0$ as a zero of $F(k)$. For Kirchhoff boundary conditions it has been shown in [17] that the degree of the zero is $E - V + 2$, whereas the zero Laplace eigenvalue is non-degenerate, i.e., $g_0 = 1$. Kurasov [25] subsequently linked this difference in the multiplicities to the topology of the graph by noticing that a suitable trace formula contains the quantity

$$1 - \frac{1}{2}(E - V + 2) = \frac{1}{2}(V - E),$$

and hence the Euler characteristic of the graph. This observation was generalised to yield an index theorem for any quantum graph with non-Robin boundary conditions by Fulling, Kuchment and Wilson [9]. One can view the t -independent term $\frac{1}{4} \text{tr } S = \frac{1}{2}(V - E)$ in the trace formula for the heat kernel (due to [29] for Kirchhoff boundary conditions and [18] for general non-Robin conditions) as a predecessor of this result. See also [2] for a more detailed discussion.

We here wish to give a further characterisation of the spectral multiplicity of the zero eigenvalue in the case of a general self adjoint realisation of the Laplacian. To this end we first introduce, for $k \in \mathbb{R} \setminus \{0\}$, the matrix

$$C(l; k) := \begin{pmatrix} \frac{l_1}{2^{\frac{1}{k}+l_1}} & & & \frac{2^{\frac{i}{k}}}{2^{\frac{1}{k}+l_1}} & & \\ & \ddots & & & \ddots & \\ & & \frac{l_E}{2^{\frac{1}{k}+l_E}} & & & \frac{2^{\frac{i}{k}}}{2^{\frac{1}{k}+l_E}} \\ \frac{2^{\frac{i}{k}}}{2^{\frac{1}{k}+l_1}} & & & \frac{l_1}{2^{\frac{1}{k}+l_1}} & & \\ & \ddots & & & \ddots & \\ & & \frac{2^{\frac{i}{k}}}{2^{\frac{1}{k}+l_E}} & & & \frac{l_E}{2^{\frac{1}{k}+l_E}} \end{pmatrix}, \tag{4.18}$$

in which all matrix entries not indicated are zero. This now enables us to formulate the following.

Proposition 4.8. *For any given self adjoint realisation of the Laplacian specified through A, B , zero is a Laplace eigenvalue, iff one is an eigenvalue of $S(A, B; k) C(l; k)$ for one, and hence any, $k \in \mathbb{R} \setminus \{0\}$. Moreover, the multiplicity of this eigenvalue one coincides with the spectral multiplicity g_0 of the zero Laplace eigenvalue.*

Proof. Eigenfunctions of the Laplacian corresponding to the eigenvalue zero must be of the form $F = (f_1, \dots, f_E)^T$ with

$$f_j(x) = \alpha_j + \beta_j x, \quad x \in [0, l_j]. \tag{4.19}$$

Hence, the boundary values (2.2) take the form

$$F_{bv} = (\alpha_1, \dots, \alpha_E, \alpha_1 + \beta_1 l_1, \dots, \alpha_E + \beta_1 l_E)^T,$$

$$F'_{bv} = (\beta_1, \dots, \beta_E, -\beta_1, \dots, -\beta_E)^T.$$

We now employ the boundary conditions (2.3) by using the expressions (3.8) for a possible choice of A and B . The result can be rearranged to yield

$$S(k)C_+(\mathbf{l}; k) \begin{pmatrix} \boldsymbol{\alpha} \\ \boldsymbol{\beta} \end{pmatrix} = C_-(\mathbf{l}; k) \begin{pmatrix} \boldsymbol{\alpha} \\ \boldsymbol{\beta} \end{pmatrix}, \tag{4.20}$$

where, for any $k \in \mathbb{R} \setminus \{0\}$, we have introduced

$$C_{\pm}(\mathbf{l}; k) := \begin{pmatrix} \mathbb{1}_E & \pm \frac{i}{k} \mathbb{1}_E \\ \mathbb{1}_E & \mp \frac{i}{k} \mathbb{1}_E + D_1(\mathbf{l}) \end{pmatrix},$$

with $D_1(\mathbf{l})$ as defined in (4.13). We also use the abbreviations

$$\boldsymbol{\alpha} := \begin{pmatrix} \alpha_1 \\ \vdots \\ \alpha_E \end{pmatrix} \quad \text{and} \quad \boldsymbol{\beta} := \begin{pmatrix} \beta_1 \\ \vdots \\ \beta_E \end{pmatrix}.$$

The matrices $C_{\pm}(\mathbf{l}, k)$ are invertible for all $k \in \mathbb{R} \setminus \{0\}$, with

$$C_{\pm}(\mathbf{l}; k)^{-1} = \begin{pmatrix} \frac{\pm \frac{i}{k} - l_1}{\pm 2 \frac{i}{k} - l_1} & & & \frac{\pm \frac{i}{k}}{\pm 2 \frac{i}{k} - l_1} & & \\ & \ddots & & & \ddots & \\ & & \frac{\pm \frac{i}{k} - l_E}{\pm 2 \frac{i}{k} - l_E} & & & \frac{\pm \frac{i}{k}}{\pm 2 \frac{i}{k} - l_1} \\ \frac{1}{\pm 2 \frac{i}{k} - l_1} & & & \frac{-1}{\pm 2 \frac{i}{k} - l_1} & & \\ & \ddots & & & \ddots & \\ & & \frac{1}{\pm 2 \frac{i}{k} - l_E} & & & \frac{-1}{\pm 2 \frac{i}{k} - l_1} \end{pmatrix}.$$

We now substitute

$$v(k) := C_-(\mathbf{l}; k) \begin{pmatrix} \boldsymbol{\alpha} \\ \boldsymbol{\beta} \end{pmatrix} \tag{4.21}$$

in (4.20) and obtain

$$S(k)C_+(\mathbf{l}; k)C_-(\mathbf{l}; k)^{-1}v(k) = v(k).$$

It is straight forward to check that $C_+(\mathbf{l}; k)C_-(\mathbf{l}; k)^{-1} = C(\mathbf{l}; k)$, compare (4.18). The linearly independent eigenvectors of SC corresponding to the eigenvalue one then yield, via (4.21) and (4.19), coefficients α_j and β_j for as many linearly independent Laplace eigenfunctions in $L^2(\Gamma)$. \square

We remark that the order N of $k_0 = 0$ as a zero of the function (4.8) is the multiplicity of the eigenvalue one of

$$U(0) = S_0 \begin{pmatrix} 0 & \mathbb{1}_E \\ \mathbb{1}_E & 0 \end{pmatrix},$$

which is in no obvious way related to the multiplicity of the eigenvalue one of $S(k)C(\mathbf{l}; k)$ that appears in Proposition 4.8. In the case of non-Robin boundary conditions, where the edge S-matrix is independent of k , however, Fulling, Kuchment and Wilson [9] were able to relate the different multiplicities in the form of an index theorem. They showed, in particular, that then

$$g_0 - \frac{1}{2}N = \frac{1}{4} \operatorname{tr} S.$$

As mentioned above, this term will reappear in the trace formula.

5. The trace formula

A trace formula expresses counting functions of Laplace eigenvalues in terms of sums over periodic orbits. Ideally, one would like to count Laplace eigenvalues k_n^2 , with their multiplicities g_n , in intervals I in the form

$$\operatorname{Tr} \chi_I(-\Delta) = \sum_{k_n^2 \in I} g_n. \quad (5.1)$$

The sharp cut-off provided by the characteristic function χ_I of the interval I , however, cannot be dealt with. One therefore replaces (5.1) with a smooth cut-off and, moreover, performs this count in terms of the associated wave numbers k_n , i.e., one seeks to find a representation for

$$\sum_n g_n h(k_n) \quad (5.2)$$

in terms of sums over periodic orbits. One ambition then is to find a sufficiently large class of test functions h . It turns out that the following one parameter family of test functions is particularly suited for these purposes.

Definition 5.1. For each $r \geq 0$ the space H_r consists of all functions $h : \mathbb{C} \rightarrow \mathbb{C}$ satisfying the following conditions:

- h is even, i.e., $h(k) = h(-k)$.
- For each $h \in H_r$ there exists $\delta > 0$ such that h is analytic in the strip $M_{r+\delta} := \{k \in \mathbb{C}; |\operatorname{Im} k| < r + \delta\}$.
- For each $h \in H_r$ there exists $\eta > 0$ such that $h(k) = O(\frac{1}{(1+|k|)^{1+\eta}})$ on $M_{r+\delta}$.

We stress that the trace formula will only take non-negative Laplace eigenvalues into account. Hence, the test functions in (5.2) will be evaluated at real arguments. We can therefore arrange the wave numbers $k_n > 0$ corresponding to Laplace eigenvalues k_n^2 in ascending order. Proposition 4.2 then readily implies the existence of a constant $C > 0$ such that

$$\sum_{0 < k_n \leq K} g_n |h(k_n)| \leq CK \sup_{k \in [0, K]} |h(k)|. \quad (5.3)$$

The third condition of Definition 5.1 now ensures that the sum in (5.2) converges absolutely when $h \in H_r$ with some $r \geq 0$. Since this sum constitutes one side of the trace formula, choosing test functions h from any of the spaces H_r is an appropriate prerequisite for the trace formula.

5.1. A precise eigenvalue count and the trace formula

The trace formula is based on an exact count of non-negative Laplace eigenvalues with, however, a smooth cut-off as in (5.2). Essentially, this sum is expressed in terms of a sum over periodic orbits on the graph. In order to perform such an eigenvalue count one relies on the connection between Laplace eigenvalues and zeros of the determinant function (4.8). More specifically, one chooses a test function $h \in H_r$ with some $r \geq 0$ as well as some $\varepsilon > 0$, which must be sufficiently small so that in the set $C_{\varepsilon,K} = \{k \in \mathbb{C}; |\operatorname{Im} k| \leq \varepsilon, |\operatorname{Re} k| \leq K\}$ the determinant function $F(k)$ has only (finitely many) real zeros related to non-negative Laplace eigenvalues (compare Proposition 4.3). Then, by the argument principle,

$$\frac{1}{2\pi i} \int_{\partial C_{\varepsilon,K}} \frac{F'}{F}(k) h(k) dk = N h(0) + 2 \sum_{0 < k_n \leq K} g_n h(k_n). \tag{5.4}$$

Here N and g_n are the multiplicities of $k_0 = 0$ and $k_n > 0$, respectively, as a zeros of $F(k)$. Following Proposition 4.7, g_n also is the multiplicity of the Laplace eigenvalue k_n^2 . The factor of two occurs since $k_n, -k_n \in C_{\varepsilon,K}$ and we have exploited the fact that $h(k)$ is even. Based on this relation the trace formula emerges when one expresses $F'(k)/F(k)$ in terms of a suitable series (eventually leading to a sum over periodic orbits), and performs the limit $K \rightarrow \infty$. The result of this procedure is summarised in the following statement.

Proposition 5.2. *Let $l_{\min} > 2/\lambda_{\min}^+$ and choose $h \in H_r$ with any $r \geq 0$. Then*

$$N h(0) + 2 \sum_{n=1}^{\infty} g_n h(k_n) = \sum_{l \in \mathbb{Z}} \frac{1}{2\pi i} \int_{-\infty}^{+\infty} \operatorname{tr}[\Lambda(k)U^l(k)] h(k) dk, \tag{5.5}$$

where

$$\Lambda(k) = -i \frac{2L}{L^2 + k^2} + iD(l). \tag{5.6}$$

Proof. Our strategy is to show that both sides of (5.5) equal

$$\lim_{\varepsilon \rightarrow 0^+} \frac{1}{2\pi i} \int_{-\infty}^{+\infty} \left[\frac{F'}{F}(k - i\varepsilon) h(k - i\varepsilon) - \frac{F'}{F}(k + i\varepsilon) h(k + i\varepsilon) \right] dk. \tag{5.7}$$

Beginning with the left-hand side, we have to show that in (5.4) the limit $K \rightarrow \infty$ can be taken, followed by $\varepsilon \rightarrow 0$. To this end we notice that the right-hand side of (5.4) is explicitly independent of ε , in the range described above that equation. Furthermore, from (5.3) we already know that the sum over k_n converges absolutely in the limit $K \rightarrow \infty$. In order to perform these limits on the left-hand side of (5.4), and thus producing (5.7), we have to estimate the contribution to the integral coming from the vertical parts of the contour.

Lemma 3.3 implies that for $k \in \mathbb{C}$ with $|k| > \lambda_{\max}$ the approximation $F(k) = F_\infty(k) + O(|k|^{-1})$ holds, where

$$F_\infty(k) := \det(\mathbf{1} - S_\infty T(k)). \tag{5.8}$$

Since F_∞ depends on k only through the matrix entries e^{ikl_e} of $T(k)$, see (4.6), it can be represented as

$$F_\infty(k) = 1 + \sum_{n=1}^b d_n e^{i\beta_n k}, \tag{5.9}$$

with some $b < \infty$. Moreover, $\beta_n > 0$ is a finite sum of edge lengths, and $d_n \in \mathbb{C}$ is an appropriate coefficient. The expression (5.9) is first defined for $k \in \mathbb{R}$, but can be readily extended to complex k . Since $S'(k) = O(|k|^{-2})$, see Lemma 3.2 and eq. (4.14), we also find $F'(k) = F'_\infty(k) + O(|k|^{-1})$. For sufficiently large $|k|$ one can therefore approximate $F'(k)/F(k)$ by $F'_\infty(k)/F_\infty(k)$. In order to estimate the latter we employ (5.9) to obtain

$$|F'_\infty(k)| \leq b d_{\max} \beta_{\max} e^{-\beta_{\min} \operatorname{Im} k}, \tag{5.10}$$

with $d_{\max} := \max\{|d_n|\}$ and $\beta_{\max/\min} := \max/\min\{\beta_n\}$. Note that this bound is independent of $\operatorname{Re} k$. Furthermore, we pick $k_{(0)} \in \mathbb{R}$ such that $F(k_{(0)}) \neq 0$ as well as $F_\infty(k_{(0)}) \neq 0$, and take advantage of the fact that $F_\infty(k)$, $k \in \mathbb{R}$, is an almost periodic function (see, e.g., [4]). One can hence construct a (strictly increasing) sequence $\{k_{(j)}; j \in \mathbb{N}_0\}$ with

$$|F_\infty(k_{(j)}) - F_\infty(k_{(0)})| < \frac{|F_\infty(k_{(0)})|}{2}, \quad j > 0. \tag{5.11}$$

Hence, in particular, $F_\infty(k_{(j)}) \neq 0$. The estimate (5.10), moreover, implies that

$$|F_\infty(k_{(j)}) - F_\infty(k_{(j)} + i\kappa)| < \frac{|F_\infty(k_{(0)})|}{4} \tag{5.12}$$

when $|\kappa|$ is sufficiently small. Therefore, when ε is small enough, the function $|F_\infty(k_{(j)} + i\kappa)|$, $-\varepsilon \leq \kappa \leq \varepsilon$, is uniformly bounded from below away from zero. Thus there exists $C_\varepsilon > 0$ such that

$$\left| \int_{k_{(j)} - i\varepsilon}^{k_{(j)} + i\varepsilon} \frac{F'_\infty(k)}{F_\infty(k)} h(k) \, dk \right| \leq C_\varepsilon \sup \{|h(k_{(j)} + i\kappa)|; \kappa \in (-\varepsilon, +\varepsilon)\}. \tag{5.13}$$

The third property of test functions required in Definition 5.1 then ensures that this integral vanishes as $k_{(j)} \rightarrow \infty$. A completely analogous reasoning applies when replacing $k_{(j)}$ with $-k_{(j)}$. Hence, as $K \rightarrow \infty$ the contributions coming from $[-K + i\varepsilon, -K - i\varepsilon]$ and $[K - i\varepsilon, K + i\varepsilon]$ to the integration along $\partial C_{\varepsilon, K}$ in (5.4) vanish, and the limits $\varepsilon \rightarrow 0$ and $K \rightarrow \infty$ can be interchanged.

It remains to prove the equality of (5.7) with the right-hand side of (5.5). In order to achieve this we first recall from Proposition 4.3 that the function $F(k)$ is holomorphic and zero-free in the strip $\{k \in \mathbb{C}; 0 < \operatorname{Im} k < \varepsilon_1\}$, where

$\varepsilon_1 := \min\{\lambda_{\min}^+, \kappa_1\}$ when $-\kappa_1^2$ is the largest negative eigenvalue of $-\Delta$; if $-\Delta \geq 0$ we set $\varepsilon_1 := \lambda_{\min}^+$. Hence,

$$\frac{F'}{F}(k + i\varepsilon) = \frac{d}{dk} \log \det(\mathbb{1} - U(k + i\varepsilon)) = -\operatorname{tr}\left((\mathbb{1} - U(k + i\varepsilon))^{-1}U'(k + i\varepsilon)\right),$$

when $0 < \varepsilon < \varepsilon_1$. Furthermore, following Lemma 3.13 we obtain the bound

$$\|U(k + i\varepsilon)\| \leq \|S(k + i\varepsilon)\| \|T(k + i\varepsilon)\| \leq \max\left\{1, \frac{\lambda_{\min}^+ + \varepsilon}{\lambda_{\min}^+ - \varepsilon}\right\} e^{-\varepsilon l_{\min}} \quad (5.14)$$

in the operator norm. Thus, when

$$\varepsilon < \lambda_{\min}^+ \tanh\left(\frac{\varepsilon l_{\min}}{2}\right), \quad (5.15)$$

the operator norm of $U(k + i\varepsilon)$ is less than one. If $l_{\min} > 2/\lambda_{\min}^+$ this condition is solvable, providing some ε_2 with $0 < \varepsilon_2 < \lambda_{\min}^+$ such that (5.15) is true for all $\varepsilon \in (0, \varepsilon_2)$. For such ε the expansion

$$(\mathbb{1} - U(k + i\varepsilon))^{-1} = \sum_{l=0}^{\infty} U(k + i\varepsilon)^l$$

holds. Moreover, a straight forward calculation based on the relation (4.12) produces $\operatorname{tr}[U(k)^l U'(k)] = \operatorname{tr}[\Lambda(k)U(k)^{l+1}]$, see (5.6). Therefore, after cyclic permutations under the trace,

$$\frac{F'}{F}(k + i\varepsilon) = -\sum_{l=1}^{\infty} \operatorname{tr}(\Lambda(k + i\varepsilon)U^l(k + i\varepsilon)) \quad (5.16)$$

is true for all $k \in \mathbb{R}$ and $\varepsilon \in (0, \varepsilon_3)$, where $\varepsilon_3 := \min\{\varepsilon_1, \varepsilon_2\}$.

Likewise, based on the relation

$$(\mathbb{1} - U(k - i\varepsilon))^{-1} = -(\mathbb{1} - U^{-1}(k - i\varepsilon))^{-1}U^{-1}(k - i\varepsilon)$$

that holds for $0 < \varepsilon < \lambda_{\min}^+$, we obtain

$$\frac{F'}{F}(k - i\varepsilon) = \sum_{l=0}^{\infty} \operatorname{tr}(\Lambda(k - i\varepsilon)U^{-l}(k - i\varepsilon)) \quad (5.17)$$

for $k \in \mathbb{R}$ and sufficiently small $\varepsilon > 0$.

We now want to use the representations (5.16) and (5.17) in (5.7), interchange integration and summations, and finally perform the limit $\varepsilon \rightarrow 0$. In order to achieve this we first notice that (for fixed ε) the estimate

$$\begin{aligned} |\operatorname{tr}(\Lambda(k \pm i\varepsilon)U^{\pm l}(k \pm i\varepsilon))| &\leq 2E\|\Lambda(k \pm i\varepsilon)U^{\pm l}(k \pm i\varepsilon)\| \\ &\leq 2E\|\Lambda(k \pm i\varepsilon)\| \|U^{\pm 1}(k \pm i\varepsilon)\|^l \end{aligned} \quad (5.18)$$

justifies to interchange integration and summation according to the dominated convergence theorem. Next, the contour of the integral

$$\int_{\operatorname{Im} k = \pm\varepsilon} \operatorname{tr}[\Lambda(k)U^{\pm l}(k)] h(k) dk \quad (5.19)$$

can be deformed into $\text{Im } k = \pm\delta$ with a sufficiently small $\delta > 0$; in particular, $\delta < r$. We then fix δ and find

$$\begin{aligned} & \left| \int_{\text{Im } k = \pm\epsilon} \text{tr} [\Lambda(k)U^{\pm l}(k)] h(k) \, dk \right| \\ & \leq \int_{-\infty}^{+\infty} |\text{tr}(\Lambda(k \pm i\delta)U^{\pm l}(k \pm i\delta))| |h(k \pm i\delta)| dk \\ & \leq 2E \left(\frac{\lambda_{\min}^+ + \delta}{\lambda_{\min}^+ - \delta} e^{-\delta l_{\min}} \right)^l \int_{-\infty}^{+\infty} \|\Lambda(k \pm i\delta)\| |h(k \pm i\delta)| dk, \end{aligned} \tag{5.20}$$

when using (5.14) and (5.18) with δ instead of ϵ . Since the conditions in Definition 5.1 apply, the integral on the right-hand side is finite and the positive constant raised to the power l is smaller than one. The sum on l hence possesses an absolutely convergent majorant, uniform in ϵ in the range indicated. Thus the summation and the limit $\epsilon \rightarrow 0$ can be interchanged. Furthermore, another application of the dominated convergence theorem allows to perform the limit $\epsilon \rightarrow 0$ of (5.19) inside the integral, finally proving (5.5). \square

In order to arrive at the trace formula itself, the sum on the right-hand side of (5.5) has to be reformulated as a sum over periodic orbits. The summation index l then denotes the topological length of the orbits and the trace of $\Lambda(k)U^l(k)$ is identified as a sum over the set \mathcal{P}_l of periodic orbits with topological length l . The term with $l = 0$ plays a special role and will be treated separately, whereas contributions with negative l are related to those with $-l$ in a simple way.

Before we state the trace formula, however, we introduce some notation: The ‘volume’ of the graph is the sum $\mathcal{L} = l_{e_1} + \dots + l_{e_E}$ of all edge lengths. Furthermore, if $h \in H_r$ is a test function, its Fourier transform is

$$\hat{h}(x) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} h(k) e^{ikx} \, dk.$$

We recall that the second and the third property required for h in Definition 5.1 guarantee that $\hat{h}(x) = O(e^{-rx})$ as $x \rightarrow \infty$. Moreover, the Fourier transform of a product $A(k)h(k)$ is the convolution of the respective Fourier transforms, i.e., it reads

$$\widehat{Ah}(x) = \int_{-\infty}^{+\infty} \hat{A}(x - y) \hat{h}(y) \, dy = \hat{A} * \hat{h}(x). \tag{5.21}$$

Below this convolution will often have to be understood in a distributional sense, as the functions $A(k)$, though being regular, not always decay sufficiently fast as $k \rightarrow \infty$.

We are now in a position to state the first variant of the trace formula.

Theorem 5.3. *Let Γ be a compact, metric graph with a self adjoint realisation $-\Delta(A, B; l)$ of the Laplacian, such that the condition $l_{\min} > 2/\lambda_{\min}^+$ is fulfilled.*

Furthermore, let $h \in H_r$ be a test function with an arbitrary $r \geq 0$. Then the following identity holds:

$$\sum_{n=0}^{\infty} g_n h(k_n) = \mathcal{L} \hat{h}(0) + (g_0 - \frac{1}{2}N) h(0) - \frac{1}{4\pi} \int_{-\infty}^{+\infty} h(k) \frac{\text{Im tr } S(k)}{k} dk + \sum_{l=1}^{\infty} \sum_{p \in \mathcal{P}_l} \left[(\hat{h} * \hat{A}_p)(l_p) + (\hat{h} * \hat{A}_p)(l_p) \right]. \tag{5.22}$$

Here \hat{A}_p is the Fourier transform of the amplitude function $A_p(k)$ associated with every periodic orbit p . This function is meromorphic with possible poles at the poles of the S -matrix, and has a Taylor expansion

$$A_p(k) = \sum_{j=0}^{\infty} a_p^{(j)} k^{-j} \tag{5.23}$$

that converges for $|k| > \lambda_{\max}$. In general, only the sum over the topological lengths l on the right-hand side of (5.22) converges absolutely, but not the entire double sum over periodic orbits.

Proof. We have to evaluate $\text{tr}[\Lambda(k)U^l(k)]$, and first notice that according to (4.6) and (4.7) the matrix entries of U are

$$U_{j_1 j_2} = S_{j_1 \omega_{j_2}} e^{ikl_{j_1}},$$

where

$$\omega_j := \begin{cases} j + E, & \text{if } 1 \leq j \leq E \\ j - E, & \text{if } E + 1 \leq j \leq 2E \end{cases}.$$

Hence, the indices j and ω_j correspond to the two edge ends of the j -th edge. Local boundary conditions then imply that $S_{j_1 \omega_{j_2}} \neq 0$ requires the edges with ends j_1 and ω_{j_2} to be adjacent. Therefore, when $l > 0$ the non vanishing terms in the multiple sum

$$\text{tr}(\Lambda U^l) = \sum_{j_0, \dots, j_l=1}^{2E} \Lambda_{j_0 j_1} S_{j_1 \omega_{j_2}} \dots S_{j_l \omega_{j_0}} e^{ik(l_{j_1} + \dots + l_{j_l})} \tag{5.24}$$

correspond to the closed paths of topological length l on the graph.

We then make use of the decomposition (5.6) of Λ and begin with the contribution of $\text{tr}[D(l)U^l(k)]$, which can be evaluated as in the case of Kirchhoff boundary conditions [21]: Due to the specific diagonal form of D the terms in (5.24) corresponding to closed paths related by cyclic permutations of their edges can be grouped together. This finally yields a sum over the periodic orbits of topological length l ,

$$\text{tr}[D(l)U^l(k)] = 2 \sum_{p \in \mathcal{P}_l} l_p^\# A_{1,p}(k) e^{ikl_p}.$$

According to (5.24), the functions $A_{1,p}(k)$ result from multiplying the local S -matrices of the vertices visited along the periodic orbit p . Moreover, $l_p^\#$ is the

primitive length of p , i.e., the length of the primitive periodic orbit associated with p . Due to the relation (5.21) we therefore obtain

$$\frac{1}{2\pi} \int_{-\infty}^{+\infty} \text{tr} [D(\mathbf{l})U^l(k)] h(k) dk = 2 \sum_{p \in \mathcal{P}_l} l_p^\# (\hat{h} * \hat{A}_{1,p})(l_p).$$

The case of negative l follows by noticing that

$$U^{-l}(k) = T^{-1}(k)S^{-1}(k) = T(-k)S(-k),$$

and thus

$$\text{tr} [D(\mathbf{l})U^{-l}(k)] = 2 \sum_{p \in \mathcal{P}_l} l_p^\# \bar{A}_{1,p}(k) e^{-ikl_p},$$

leading to

$$\begin{aligned} \frac{1}{2\pi} \int_{-\infty}^{+\infty} \text{tr} [D(\mathbf{l})(U^l(k) + U^{-l}(k))] h(k) dk \\ = 2 \sum_{p \in \mathcal{P}_l} l_p^\# [(\hat{h} * \hat{A}_{1,p})(l_p) + (\hat{h} * \hat{\bar{A}}_{1,p})(l_p)]. \end{aligned}$$

In order to calculate the contribution from $\text{tr}[\frac{L}{L^2+k^2}U^l(k)]$ we notice that

$$\begin{aligned} -2i \text{tr} \left[\frac{L}{L^2 + k^2} U^l \right] &= \text{tr}[S' T U^{l-1}] \\ &= \sum_{j_1, \dots, j_l=1}^{2E} S'_{j_1 \omega_{j_2}} S_{j_2 \omega_{j_3}} \dots S_{j_l \omega_{j_1}} e^{ik(l_{j_1} + \dots + l_{j_l})}. \end{aligned} \tag{5.25}$$

Again, the multiple sum can be viewed as a sum over the closed paths of topological length l , and the contributions of representatives of periodic orbits can be grouped together. Eventually, this leads to

$$-2 \text{tr} \left[\frac{L}{L^2 + k^2} U^l(k) \right] = 2 \sum_{p \in \mathcal{P}_l} A_{2,p}(k) e^{ikl_p}, \tag{5.26}$$

where the functions $A_{2,p}(k)$ emerge from multiplying local S-matrix elements and their derivatives along the closed paths as specified in (5.25). Negative l are dealt with as above, so that the contribution from $l \in \mathbb{Z} \setminus \{0\}$ to the sum on the right-hand side of (5.5) yields the sum on the right-hand side of (5.22), with $A_p(k) = l_p^\# A_{1,p}(k) + A_{2,p}(k)$.

The contribution coming from $l = 0$ finally is

$$\begin{aligned} \frac{1}{2\pi i} \int_{-\infty}^{+\infty} \text{tr} \Lambda(k) h(k) dk &= -\frac{1}{2\pi} \int_{-\infty}^{+\infty} \text{tr} \left(\frac{2L}{L^2 + k^2} \right) h(k) dk + \frac{\mathcal{L}}{\pi} \int_{-\infty}^{+\infty} h(k) dk \\ &= 2\mathcal{L} \hat{h}(0) - \frac{1}{2\pi} \int_{-\infty}^{+\infty} h(k) \frac{\text{Im tr } S(k)}{k} dk. \end{aligned}$$

Adding the contribution of the Laplace-eigenvalue zero to (5.5), after a rearrangement of the terms the result (5.22) follows. \square

As mentioned in Theorem 5.3, the double sum over periodic orbits in (5.22) does not converge absolutely when $h \in H_r$ with arbitrarily small $r \geq 0$. In the following we are going to show that an absolutely convergent periodic orbit sum can be achieved under sharpened conditions on the test function. In order to formulate these conditions we introduce the function

$$l(\kappa) := \frac{1}{\kappa} \log(2E) + \frac{2}{\kappa} \operatorname{artanh} \left(\frac{\kappa}{\lambda_{\min}^+} \right), \quad 0 < \kappa < \lambda_{\min}^+, \quad (5.27)$$

which attains its unique minimum at some $\sigma \in (0, \lambda_{\min}^+)$. Moreover, the minimum can be bounded from below as $l(\sigma) \geq (2 + \log(2E))/\lambda_{\min}^+$ so that, in particular, $l(\sigma) > 2/\lambda_{\min}^+$.

Theorem 5.4. *Let Γ be a compact, metric graph with a self adjoint realisation $-\Delta(A, B; l)$ of the Laplacian, such that the condition $l_{\min} > l(\sigma)$ is fulfilled. Furthermore, let $h \in H_r$ be a test function with an arbitrary $r \geq \sigma$. Then the following identity holds:*

$$\begin{aligned} \sum_{n=0}^{\infty} g_n h(k_n) &= \mathcal{L} \hat{h}(0) + \left(g_0 - \frac{1}{2}N\right) h(0) - \frac{1}{4\pi} \int_{-\infty}^{+\infty} h(k) \frac{\operatorname{Im} \operatorname{tr} S(k)}{k} dk \\ &+ \sum_{p \in \mathcal{P}} \left[(\hat{h} * \hat{A}_p)(l_p) + (\hat{h} * \hat{\bar{A}}_p)(l_p) \right]. \end{aligned} \quad (5.28)$$

The quantities appearing are the same as in Theorem 5.3. Here, however, the sum over periodic orbits converges absolutely.

Proof. The task is to analyse the convergence of the sum over periodic orbits in (5.28) more closely. In Theorem 5.3 we only considered the convergence of the sum over l . This was based on the estimate (5.20), which shall now be refined. To this end we refer to (5.24) and (5.25), and notice that $\operatorname{tr}[\Lambda(k)U^l(k)]$ is a sum consisting of $(2E)^l$ terms $s_{i_1 i_2}(k) \dots s_{i_l i_{l+1}}(k)h(k)$, each of which contains a product of l factors that are matrix elements of either $S(k)$, $iD(l)$, or $i\frac{2L}{L^2+k^2}$. These factors are all holomorphic in a strip $0 \leq \operatorname{Im} k < \lambda_{\min}^+$ and, following Lemma 3.4, in any strip $0 \leq \operatorname{Im} k \leq \kappa$ with $\kappa < \lambda_{\min}^+$, they are bounded from above in absolute value by a constant times $(\lambda_{\min}^+ + \kappa)/(\lambda_{\min}^+ - \kappa)$. Thus, in particular, for all $\kappa < \min\{\lambda_{\min}^+, r\}$ any product $s_{i_1 i_2}(k) \dots s_{i_l i_{l+1}}(k)h(k)$ is holomorphic for $0 \leq \operatorname{Im} k \leq \kappa$. Since here we are evaluating Fourier transforms at $l_{i_1} + \dots + l_{i_l} > 0$, we can apply a suitable version of the Paley-Wiener theorem that is concerned with Fourier transforms of holomorphic functions in vertical strips of the upper half plane. This is an obvious, slight variation of Theorem IX.14 in [30], and implies that there exists $C_\kappa > 0$ such

that

$$\begin{aligned} & \left| \int_{-\infty}^{+\infty} \text{tr}[\Lambda(k)U^l(k)] h(k) \, dk \right| \\ & \leq \sum_{i_1, \dots, i_l=1}^{2E} \left| \int_{-\infty}^{+\infty} s_{i_1 i_2}(k) \dots s_{i_l i_1}(k) h(k) e^{ik(l_{i_1} + \dots + l_{i_l})} \, dk \right| \\ & \leq C_\kappa \left(2E \frac{\lambda_{\min}^+ + \kappa}{\lambda_{\min}^+ - \kappa} e^{-\kappa l_{\min}} \right)^l = C_\kappa e^{\kappa l(l(\kappa) - l_{\min})}, \end{aligned} \tag{5.29}$$

where we made use of the function defined in (5.27). We hence conclude that under the conditions stated the sum over periodic orbits converges absolutely. In particular, $l_{\min} > l(\kappa)$ must be fulfilled. The latter condition is optimised for $\kappa = \sigma$, at which the function $l(\kappa)$ attains its minimum. For the above to hold, the condition $h \in H_r$ with $r \geq \sigma$ must be satisfied. \square

We remark that whenever an amplitude function $A_p(k)$ associated with a periodic orbit is independent of k , as it is always true for non-Robin boundary conditions, the convolution $\hat{h} * \hat{A}_p(l_p)$ degenerates into a product $A_p \hat{h}(l_p)$. In any case, the condition $r \geq \sigma$ imposed on the test function h ensures that $\hat{h} * \hat{A}_p(x) = O(e^{-\sigma|x|})$, which enables the absolute convergence of the periodic orbit sum.

5.2. The trace of the heat kernel

The first trace formula of a quantum graph, due to Roth [29], expresses the trace of the heat kernel for the Laplacian with Kirchhoff boundary conditions in terms of a sum over periodic orbits. This has recently been extended to all non-Robin boundary conditions by Kostykin, Pothhoff and Schrader [18]. An application of Theorem 5.4 now allows us to produce an appropriate trace formula for all self adjoint realisations of the Laplacian. In such a case, however, negative Laplace eigenvalues $-\kappa_n^2$, with multiplicities g_n^- , may occur so that the trace of the heat kernel,

$$\text{Tr} e^{\Delta t} := \sum_{-\kappa_n^2 < 0} g_n^- e^{\kappa_n^2 t} + \sum_{k_n^2 \geq 0} g_n e^{-k_n^2 t}, \quad t > 0,$$

does not follow immediately from Theorems 5.3 and 5.4. Instead, we consider

$$\text{Tr}_+ e^{\Delta t} := \sum_{k_n^2 \geq 0} g_n e^{-k_n^2 t}, \quad t > 0.$$

In the trace formula we hence have to choose the (entire holomorphic) function $h(k) = e^{-k^2 t}$, $t > 0$, which is in H_r for all $r \geq 0$. Its Fourier transform is $\hat{h}(x) = \frac{1}{\sqrt{4\pi t}} e^{-x^2/4t}$. We also introduce the functions

$$a_p(t) := \frac{1}{\sqrt{4\pi t}} \int_{-\infty}^{+\infty} \hat{A}_p(l_p - y) e^{-y^2/4t} \, dy$$

associated with the periodic orbits on the graph and obtain the following statement.

Theorem 5.5. *Let Γ be a compact, metric graph with a self adjoint realisation $-\Delta(A, B; l)$ of the Laplacian, such that the condition $l_{\min} > l(\sigma)$ is fulfilled. Then the following identity holds:*

$$\begin{aligned} \text{Tr}_+ e^{\Delta t} &= \frac{\mathcal{L}}{\sqrt{4\pi t}} + \left(g_0 - \frac{1}{2}N\right) - \frac{1}{2} \sum_{\alpha=1}^d \frac{\lambda_\alpha}{|\lambda_\alpha|} e^{\lambda_\alpha^2 t} \text{erfc}(|\lambda_\alpha|\sqrt{t}) \\ &+ 2 \sum_{p \in \mathcal{P}} \text{Re } a_p(t). \end{aligned} \tag{5.30}$$

Here d is the number of non vanishing eigenvalues λ_α of L (counted with their multiplicities) and

$$\text{erfc}(x) = \frac{2}{\sqrt{\pi}} \int_x^\infty e^{-y^2} dy, \quad x \geq 0,$$

is the error function complement. Moreover, as $t \rightarrow 0^+$ the trace of the heat kernel has a complete asymptotic expansion in powers of \sqrt{t} , whose leading terms read

$$\text{Tr } e^{\Delta t} = \frac{\mathcal{L}}{\sqrt{4\pi t}} + \gamma + O(\sqrt{t}), \quad t \rightarrow 0^+. \tag{5.31}$$

Here

$$\gamma = g_0 - \frac{N}{2} + \sum_n g_n^- - \frac{1}{2} \sum_j \gamma_{0,j} + \frac{1}{2} \sum_j \gamma_{p,j} - \frac{d_+ - d_-}{2},$$

where $\gamma_{0,j}$ and $\gamma_{p,j}$ are the orders of the finitely many, non zero, purely imaginary zeros and poles, respectively, of the determinant function F and d_\pm denotes the number of positive/negative eigenvalues of L .

Proof. We first observe that the expression (4.14) implies

$$\text{Im tr } S(k) = \text{tr } \frac{2kL}{L^2 + k^2} = 2k \sum_{\alpha=1}^d \frac{\lambda_\alpha}{\lambda_\alpha^2 + k^2};$$

then we employ the representation

$$\text{erfc}(|x|) = \frac{2|x|}{\pi} e^{-x^2} \int_0^\infty \frac{e^{-y^2}}{y^2 + x^2} dy, \quad x \in \mathbb{R}.$$

Hence the relation (5.30) is an immediate consequence of (5.28), when the test function h is chosen as indicated above.

In order to determine the small- t asymptotics we go back to the relation (5.4), in which we use the test function $h(k) = e^{-k^2 t}$, $t > 0$. We then deform the contour into $\partial C_{\beta,K}$, with $\beta > \max\{\lambda_{\max}, s\}$, where s from (4.2) is such that $-s^2$ yields a lower bound on the Laplace spectrum. Thus the contour now encloses all non real zeros and poles of the determinant function F and, therefore, in this process we pick up contributions from all poles of F'/F on the imaginary axis.

Having to perform the limit $K \rightarrow \infty$ with β kept fixed, we need to estimate the contribution coming from the vertical parts of the contour, i.e., for $|\text{Re } k| = K$ and $\varepsilon < |\text{Im } k| < \beta$. Firstly, $F(k)$ is a polynomial in the matrix entries of

$S(k)$ and $T(k)$. The latter are e^{ikl_ε} , whereas the k -dependence of the former is given by $(\lambda_\alpha - ik)/(\lambda_\alpha + ik)$, see (3.5). In the two strips $\varepsilon < |\operatorname{Im} k| < \beta$, with neighbourhoods of the poles at $i\lambda_\alpha$ removed, all matrix entries are bounded, and hence $F'(k)$ is of polynomial growth in k . Secondly, for sufficiently large $|k|$ we again approximate $F(k)$ by $F_\infty(k)$, see (5.8), and write $F_\infty(k) = \prod_{j=1}^{2E} (1 - u_j(k))$. Here $u_1(k), \dots, u_{2E}(k)$ are the eigenvalues of $S_\infty T(k)$, which satisfy

$$|u_j(k)| \leq \|S_\infty\| \|T(k)\| \leq e^{-\varepsilon l_{\min}} < 1,$$

for all k in the strips $\varepsilon < |\operatorname{Im} k| < \beta$. Thus, in these strips,

$$|F_\infty(k)| > (1 - e^{-\varepsilon l_{\min}})^{2E} > 0.$$

Thirdly, when $|K| > \beta$ the factor e^{-tk^2} is of the order e^{-tK^2} in the strips. Hence, the integrand of (5.4) on the vertical parts of the contour with $|\operatorname{Im} k| > \varepsilon$ is bounded by a polynomial times e^{-tK^2} . As $K \rightarrow \infty$, these parts of the contour therefore do not contribute to the integral. Hence, from (5.4) we obtain

$$\begin{aligned} N + 2 \sum_{n=1}^{\infty} g_n e^{-k_n^2 t} &= \sum_j \gamma_{p,j} e^{\kappa_{p,j}^2 t} - \sum_j \gamma_{0,j} e^{\kappa_{0,j}^2 t} \\ &+ \frac{1}{2\pi i} \int_{-\infty}^{+\infty} \left[\frac{F'}{F}(k - i\beta) e^{-(k-i\beta)^2 t} - \frac{F'}{F}(k + i\beta) e^{-(k+i\beta)^2 t} \right] dk. \end{aligned}$$

Here the non real zeros of F are denoted as $i\kappa_{0,j}$ and its poles as $i\kappa_{p,j}$; the respective orders are $\gamma_{0,j}$ and $\gamma_{p,j}$.

To proceed further we follow the argument leading from (5.14) to (5.16) and (5.17), as well as the subsequent discussion of interchanging integration and summation. As we are dealing with large β instead of small ε , due to (3.14) the estimate (5.14) is replaced by

$$\|U(k + i\beta)\| \leq \max \left\{ 1, \frac{\beta + \lambda_{\max}}{\beta - \lambda_{\max}} \right\} e^{-\varepsilon l_{\min}},$$

Hence, for $k \in \mathbb{R}$ and β sufficiently large analogous relations to (5.16) and (5.17) are obtained, eventually leading to

$$\begin{aligned} N + 2 \sum_{n=1}^{\infty} g_n e^{-k_n^2 t} &= \sum_j \gamma_{p,j} e^{\kappa_{p,j}^2 t} - \sum_j \gamma_{0,j} e^{\kappa_{0,j}^2 t} \\ &+ \sum_{l=1}^{\infty} \frac{1}{2\pi i} \int_{-\infty}^{+\infty} \operatorname{tr}[\Lambda(k + i\beta) U^l(k + i\beta)] e^{-(k+i\beta)^2 t} dk \\ &+ \sum_{l=0}^{\infty} \frac{1}{2\pi i} \int_{-\infty}^{+\infty} \operatorname{tr}[\Lambda(k - i\beta) U^{-l}(k - i\beta)] e^{-(k-i\beta)^2 t} dk. \end{aligned}$$

In the integrals with $l \neq 0$ we now replace β by β/\sqrt{t} , $0 < t \leq 1$, and change variables from k to $q = k\sqrt{t}$, yielding

$$I_l^\pm(t, \beta) := \frac{1}{2\pi i \sqrt{t}} \int_{-\infty}^{+\infty} \text{tr} \left[\Lambda \left(\frac{1}{\sqrt{t}}(q \pm i\beta) \right) U^{\pm l} \left(\frac{1}{\sqrt{t}}(q \pm i\beta) \right) \right] e^{-(q \pm i\beta)^2} dq.$$

These integrals can be bounded in analogy to (5.29),

$$|I_l^\pm(t, \beta)| \leq \frac{C_\beta}{\sqrt{t}} \left(2E \frac{\beta + \sqrt{t}\lambda_{\max}}{\beta - \sqrt{t}\lambda_{\max}} e^{-\beta l_{\min}/\sqrt{t}} \right)^l.$$

Summing over $l \neq 0$ then finally shows that these contributions can be estimated as being $O(\frac{1}{\sqrt{t}}e^{-\beta l_{\min}/\sqrt{t}})$.

The term with $l = 0$ can be calculated explicitly and yields the same contribution to the heat trace as the first term and the sum over $\sigma(L) \setminus \{0\}$ on the right-hand side of (5.30).

We add the contributions of negative Laplace eigenvalues and use that $\text{erfc}(x)$ has a complete asymptotic expansion in x , with $\text{erfc}(x) = 1 + O(x)$, as $x \rightarrow 0$. The expansion (5.31) then follows immediately. \square

At this point we recall that in the case of non-Robin boundary conditions $\gamma = g_0 - \frac{1}{2}N = \frac{1}{4} \text{tr } S$, which has also been given an interpretation as (one half of) a suitable Fredholm index. In this case, therefore, the constant term in the small- t asymptotics of the heat kernel has a topological meaning.

Finally, we should like to mention that a suitable Tauberian theorem (see, e.g., [15]) allows us to recover Weyl's law

$$N(K) \sim \frac{\mathcal{L}}{\pi} K, \quad K \rightarrow \infty,$$

see also Proposition 4.2, from the leading term in the expansion (5.31).

6. Conclusions

Our principal goal was to investigate spectra of general self adjoint realisations of Laplace operators on compact metric graphs, culminating in proofs of some trace formulae. In this context we achieved to allow for a large class of test functions, leading either to absolutely or conditionally convergent sums over periodic orbits, respectively, representing appropriate spectral functions of the Laplacian.

Previous work on quantum graph trace formulae [17, 18, 21, 29] was restricted to Laplacians with non-Robin boundary conditions. As compared to these cases there are some modifications we had to take care of. Firstly, non-Robin boundary conditions correspond to k -independent S-matrices and hence do not involve any derivatives of $S(k)$. This is in line with the fact that $L = 0$, so that in the trace formula the contribution (5.26) to the periodic orbit sum is absent. Moreover, since therefore $\lambda_{\min}^+ = \infty$, the restriction imposed on l_{\min} in the general case is void so that any set of lengths can be attributed to the edges. What still remains

to ensure an absolutely convergent periodic orbit sum in the case of non-Robin boundary conditions is the single requirement $h \in H_r$ with $r \geq (\log 2E)/l_{\min}$ on the test functions. This implies $\hat{h}(x) = O(e^{-r|x|})$, which in turn compensates for the growth in the number of periodic orbits entering the sum

$$\sum_{p \in \mathcal{P}, l_p \leq \ell} A_p \hat{h}(l_p),$$

when $\ell \rightarrow \infty$.

Another property of Laplacians with non-Robin boundary conditions is that they are non-negative. This fact is linked to the non-positivity of L which, as $L = 0$, is trivial. The determinant function (4.8) hence is entire holomorphic with only real zeros in the complex non-negative half plane, see Proposition 4.3.

As we have shown in Theorem 5.3 the condition on the test functions can be relaxed to $h \in H_r$ with any $r \geq 0$, so that $h(x) = O(e^{-\delta|x|})$ with some (arbitrarily small) $\delta > 0$, when one is willing to accept a conditionally convergent sum. This has to be understood in the sense given in (5.22), i.e., where the terms are arranged as a double sum over the topological lengths of the orbits and over the periodic orbits of fixed topological length. For non-Robin boundary conditions a refined analysis of convergence had produced even more relaxed conditions to be demanded from the test functions, see [36].

An important application of the trace formula for quantum graphs with non-Robin boundary conditions was to prove an inverse theorem, very much in the sense of Kac's famous question 'Can one hear the shape of a drum?' [14]. Gutkin and Smilansky [10] showed that under certain conditions, which include the requirement that the edge lengths be rationally independent, the Laplace spectrum determines the connectedness and the metric structure of a compact metric graph uniquely. In this sense isospectral quantum graphs are isomorphic. Gutkin and Smilansky made essential use of the trace of the wave group,

$$\mathrm{Tr} e^{-it\sqrt{-\Delta}} + c.c. = 2 \sum_{n=0}^{\infty} g_n \cos(k_n t), \quad t \neq 0,$$

which can, in the case of non-Robin boundary conditions, be expressed as a sum of δ -singularities at the lengths l_p of periodic orbits. Searching for these singularities then allows one to first identify the geometric length spectrum. In a second step a certain algorithm can be used to determine the connectedness and all individual edge lengths. After a slight modification this proof can now be taken over to the case of Robin boundary conditions almost verbatim. For this purpose one reads off from the trace formula (5.28) the distributional identity

$$\begin{aligned} \sum_{n=0}^{\infty} g_n \cos(k_n t) &= \mathcal{L} \delta(t) + g_0 - \frac{1}{2}N - \frac{1}{2} \sum_{\alpha=1}^d \frac{\lambda_\alpha}{|\lambda_\alpha|} e^{-|t\lambda_\alpha|} \\ &\quad + \sum_{p \in \mathcal{P}} \mathrm{Re} [\hat{A}_p(l_p - t) + \hat{A}_p(l_p + t)]. \end{aligned}$$

Since, in general, the periodic orbit amplitudes are functions of k , there are no longer pure δ -singularities present at the lengths of periodic orbits. For large k the amplitudes, however, possess the expansions (5.23) with leading terms $a_p^{(0)}$. These do not vanish since they stem from the corresponding leading term $S_\infty = \mathbb{1} - 2P$ of the S-matrix. Hence, the Fourier transforms \hat{A}_p of the amplitudes have leading singularities of δ -type at the lengths l_p of periodic orbits. Therefore, applying the algorithm of Gutkin and Smilansky to this wave trace enables one to identify the graph connectivity and the edge lengths in the same way as previously.

In summary, almost all spectral properties established so far for Laplacians on compact metric graphs with non-Robin boundary conditions carry over to arbitrary self adjoint realisations of the Laplacian. Therefore, there are many more quantum graphs model available that are suitable for further investigations in, e.g., the field of quantum chaos.

Acknowledgments

J. Bolte would like to thank Stephen Fulling for very helpful discussions. We are also grateful to an anonymous referee for useful hints.

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Communicated by Jens Marklof.

Submitted: May 20, 2008.

Accepted: January 6, 2009.