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Trace formulae for quantum graphs

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Abstract

Quantum graph models are based on the spectral theory of (differential) Laplace operators on metric graphs. We focus on compact graphs and survey various forms of trace formulae that relate Laplace spectra to periodic orbits on the graphs. Included are representations of the heat trace as well as of the spectral density in terms of sums over periodic orbits. Finally, a general trace formula for any self adjoint realisation of the Laplacian on a compact, metric graph is given.

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1 Introduction

The idea of a trace formula as a tool to investigate spectral problems in quantum mechanics goes back to Gutzwiller [Gut71]. He showed that, in the semiclassical limit, the spectral density of a quantum Hamiltonian can be approximated by a sum over the periodic orbits of an associated classical dynamical system. A related approach employing short wavelength approximations to the spectral density of Laplacians on domains in $\mathbb{R}^n$ is due to Balian and Bloch [BB72]. The first rigorous proofs of such trace formulae, for Laplacians on closed Riemannian manifolds, are due to Colin de Verdiere [CdV73] as well as Duistermaat and Guillemin [DG75]. Their proofs employ heat kernel and microlocal techniques, respectively, and they relate the spectrum of the Laplacian to the closed geodesics on the manifold.

Predecessors of these trace formulae exist for Laplacians on flat tori and on manifolds of constant negative sectional curvatures in the form of the Poisson summation formula and the Selberg trace formula [Sel56], respectively. In these particular cases harmonic analysis is used in the proofs, resulting in trace formulae that are identities rather than asymptotic expansions of the spectral densities as in the general case.

Kottos and Smilansky [KS99b] introduced quantum graphs as models that on the one hand mimick spectral properties of Laplacians on manifolds, and on the other hand are simpler to deal with. They found, in particular, that the associated trace formluae require no short wavelength asymptotics, although they appear to be closely analogous to trace formulae on manifolds with hyperbolic geodesic flows. This last observation is reflected in the eigenvalue correlations in quantum graphs, which Kottos and Smilansky found in their numerical studies to coincide with the expected eigenvalue correlations of random hermitian matrices. This coincidence is usually found in quantum systems with chaotic classical analogues [BGS84], and its appearance in quantum graphs is the principal motivation to study quantum graphs in the field of quantum chaos (see, e.g., [GS06]).

The first proof of a trace formula for a Laplacian on a finite metric graph was provided by Roth [Rot83], who considered the trace of the associated heat kernel. In his work, Roth realised the Laplacian as a self adjoint operator by imposing Kirchhoff boundary conditions in the vertices of the graph. Kottos and Smilansky considered the spectral density and the integrated spectral density, respectively, and allowed for generalised Kirchhoff boundary conditions. These can be modelled by placing δ-potentials on the vertices. Their proof is based on a secular equation involving a so-called S-matrix operating on a finite dimensional space of boundary values of functions and their derivatives. Gutkin and Smilansky [GS01] then applied this trace formula to solve the inverse spectral problem ("Can you hear the shape of a graph?") when this is restricted to metric graphs with rationally independent edge lengths. Kurasov and Nowaszyk [KN05, Kur07] refined this analysis and introduced a connection with the graph topology.

Generalised Kirchhoff boundary conditions are not the only choice that result in a self adjoint realisation of the Laplacian. Useful parameterisations of all self adjoint realisations have been provided by Kostrykin and Schrader [KS99a] and Kuchment [Kuc04], respectively. A certain class of such boundary conditions, later termed "non-Robin conditions", is characterised by an S-matrix that is independent of the wave number. This class includes the case of Kirchhoff boundary conditions, but not their generalisation used in [KS99b].

Kostrykin, Potthoff, and Schrader proved a trace formula for the heat kernel in the case of general non-Robin boundary conditions. A trace formula for a large class of test functions that applies to any self adjoint realisation of the Laplacian can be found in [BE07].

This paper is organised as follows: In Section 2 we review the construction of quantum graphs and explain the two parameterisations of boundary conditions leading to self adjoint realisations of the Laplacian. The S-matrix is introduced in Section 3, and a few of its most relevant properties are discussed. Section 4 is devoted to introducing the various forms of trace formulae in quantum graphs that relate to spectra of Laplacians to periodic orbits on the graph.

2 Quantum graphs

A quantum graph models the Schrödinger equation

$$\mathrm{i}\frac{\partial}{\partial t}\psi_t = -\Delta\psi_t \ , \tag{2.1}$$

where Δ is a suitable (differential) Laplace operator, on a finite, simple, metric graph $\Gamma = (\mathcal{V}, \mathcal{E})$. Here $\mathcal{V} = \{v_1, \ldots, v_V\}$ is a set of vertices and $\mathcal{E} = \{e_1, \ldots, e_E\}$ is a set of edges. Two vertices are called adjacent, if they are connected by an edge. The edge connecting adjacent vertices v_α and v_β are also denoted as (v_α, v_β). In this case v_α is the incident vertex and v_β is the terminal vertex of the edge. The degree d_v of the vertex v specifies the number of edges that meet in v. That way not only the connectedness of the graph is specified, but also an orientation of the edges is introduced. For the following, however, we do not always insist on this orientation, but will often tacitly employ the fact that the Laplacian, being a second order differential operator, is independent of edge orientations. A metric structure is introduced by assigning an interval $(0, l_j)$ to each edge e_j. Both the coordinates x_j and $\bar{x}_j = l_j - x_j$ can be used on the interval $(0, l_j)$.

Quantum mechanics requires to introduce a suitable Hilbert space: the quantum graph Hilbert space is that of square integrable functions on Γ. In this context a function on the graph is a collection $F = (f_1, \ldots, f_E)$ of functions $f_j : (0, l_j) \to \mathbb{C}$ on the edges. Therefore, one considers the following function spaces,

$$C^\infty(\Gamma) = \bigoplus_{j=1}^{E} C^\infty(0, l_j) \quad \text{and} \quad L^2(\Gamma) = \bigoplus_{j=1}^{E} L^2(0, l_j) \ . \tag{2.2}$$

The latter is a closed direct sum of Hilbert spaces, and the scalar product reads

$$\langle F, G \rangle := \sum_{j=1}^{E} \int_0^{l_j} \overline{f_j(x_j)}\, g_j(x_j)\ \mathrm{d}x_j \ . \tag{2.3}$$

The Schrödinger equation (2.1) requires a (differential) Laplacian, realised as a self adjoint operator on the quantum graph Hilbert space. As a differential expression the Laplacian is simply given by

$$-\Delta F := (-f_1'', \dots, -f_E'') \ , \tag{2.4}$$

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

$$\mathcal{D}_0 = \bigoplus_{j=1}^{E} H_0^2(0, l_j) \ . \tag{2.5}$$

Here each term in the direct sum consists of an L^2-Sobolev space of functions with vanishing boundary values. Obvious self adjoint extensions are provided by the direct sums of the Dirichlet- or Neumann-Laplacians, respectively, on the edges. The direct sum structure, however, does not reflect the connectivity of the graph. Moreover, the spectrum of such an operator would not show particularly interesting features as it is a union of the spectra of the individual operators on the edges. One might therefore prefer self adjoint extensions that involve the graph connectivity in that the boundary values of functions in their domains are related at vertices. A frequent choice of that kind is provided by Kirchhoff boundary conditions. In this case functions $F = (f_1, \dots, f_E)$ in the domain of the Laplacian are continuous in the vertices and satisfy

$$\sum_{e \ni v} f_e' = 0 \quad \text{for all} \quad v \in \mathcal{V} \ , \tag{2.6}$$

where the sum extends over all edges e of which v is either an initial or a terminal vertex.

A systematic approach to classify all self adjoint extensions can be based on von Neumann's theory of extensions. An alternative has been developed in detail by Kostrykin and Schrader [KS99a]. This provides a convenient parameterisation that is particularly useful for later purposes. In this context one introduces the boundary values

$$\begin{aligned} F_{bv} &= \big(f_1(0), \dots, f_E(0), f_1(L_1), \dots, f_E(L_E)\big) \ , \\ F_{bv}' &= \big(f_1'(0), \dots, f_E'(0), -f_1'(L_1), \dots, -f_E'(L_E)\big) \ , \end{aligned} \tag{2.7}$$

of functions and their derivatives, whereby the signs ensure that inward derivatives are considered at all edge ends. Boundary conditions on the functions in the domain of a given self adjoint operator are specified through a linear relation between boundary values of the form

$$AF_{bv} + BF_{bv}' = 0 \ . \tag{2.8}$$

Here $A, B \in \mathrm{M}(2E, \mathbb{C})$ are two matrices such that the matrix (A, B) consisting of the columns of A and B has maximal rank $2E$, and 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. This parameterisation is obviously not unique, since a multiplication of

(2.8) with $C \in \mathrm{GL}(2E, \mathbb{C})$ does not change the boundary conditions. Thus, $A' = CA$ and $B' = CB$ provide an equivalent characterisation of the same operator.

The linear relations (2.8) can in principle relate boundary values at any pair of vertices. We wish, however, the operator to respect the connectedness of the graph and therefore restrict to local boundary conditions. To this end we group edge ends in (2.7) according to the vertices they belong to. Local boundary conditions then lead to a block structure of the matrices A and B such that (2.8) only relates boundary values at the same vertex. The block matrices corresponding to the vertex v will be denoted as A_v and B_v, respectively. Then self adjointness is achieved, if for all $v \in \mathcal{V}$ the rank of (A_v, B_v) is $2d_v$ and $A_v B_v^*$ is self adjoint. As an example, the generalised Kirchhoff boundary conditions used by Kottos and Smilansky [KS99b] can be achieved by choosing

$$A_v = \begin{pmatrix} 1 & -1 & & \\ & \ddots & \ddots & \\ & & 1 & -1 \\ & & & \mu_v \end{pmatrix} \quad \text{and} \quad B_v = \begin{pmatrix} & & & \\ & & & \\ & & & \\ 1 & \cdots & \cdots & 1 \end{pmatrix} , \tag{2.9}$$

where only the non vanishing matrix entries are indicated. Here μ_v must be real. Whenever it vanishes, at that vertex the usual Kirchhoff conditions (2.6) are realised.

The non-uniquenes in the choice of the matrices A and B can be overcome by parameterising 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 [Kuc04] introduced the projector P onto the kernel of B and its orthogonal complement $Q = \mathbb{1} - P$ in $\mathbb{C}^{2E}$. He then defined the (self adjoint) endomorphism

$$L := \left(B|_{\mathrm{ran}\, B^*}\right)^{-1} AQ \tag{2.10}$$

of $\mathrm{ran}\, B^*$, and showed that the boundary conditions (2.8) are equivalent to

$$PF_{bv} = 0 \qquad \text{and} \qquad LQF_{bv} + QF'_{bv} = 0 \; . \tag{2.11}$$

There then exists a $C \in \mathrm{GL}(2E, \mathbb{C})$ such that $A' = CA = P + L$ and $B' = CB = Q$, implying that $L = A'B'^*$. A refinement of this construction can be found in [FKW07]. From (2.11) 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. Following a suggestion of Fulling we call these *non-Robin boundary conditions*, and all other cases *Robin boundary conditions*.

3 The S-matrix

One advantage of quantum graph models is that there exists a rigorous variant of the scattering approach to quantisation as pioneered by Smilansky [DS92]. In quantum billiards, e.g., this method provides a characterisation of Laplace eigenvalues in terms of a scattering matrix, or S-matrix, describing quantum mechanical scattering processes that locally mimic the quantum dynamics. As first demonstrated by Kottos and Smilansky [KS99b], in quantum graphs this approach allows to determine Laplace eigenvalues from a finite dimensional secular equation. This not only simplifies rigorous proofs considerably, but also reduces the numerical calculation of Laplace eigenvalues to finding zeros of a finite dimensional determinant.

Compact metric graphs of the kind under consideration do not allow for quantum mechanical scattering in the sense of scattering theory. The S-matrix involved in the scattering approach rather is an amalgam of local (vertex) S-matrices that describe scattering processes in the vicinity of a given vertex. Therefore, one first replaces each vertex with an infinite star, i.e., a graph with one vertex, $v \in \mathcal{V}$, attached with d_v half lines considered as infinitely long edges connected in this vertex. The resulting on-shell S-matrix of a given star, defined in the sense of quantum scattering theory, then provides a vertex S-matrix σ^v. In terms of the parameterisation of the boundary conditions described in Section 2 one then finds that

$$\sigma^v(k) = -(A_v + \mathrm{i}kB_v)^{-1}(A_v - \mathrm{i}kB_v) \ , \quad \text{for} \quad k \in \mathbb{R}\backslash\{0\} \ . \tag{3.1}$$

The conditions imposed on A_v and B_v in order to achieve self adjoint boundary conditions ensure that $A_v \pm \mathrm{i}kB_v$ are invertible and $\sigma^v(k)$ is unitary for all $k \in \mathbb{R}\backslash\{0\}$. As an example, the local S-matrix for a vertex with generalised Kirchhoff boundary conditions (2.6) has, according to (2.9), elements

$$\sigma^v_{e_i,e_j}(k) = -\delta_{ij} + \frac{1}{d_v} + \frac{1}{d_v}\frac{d_v k - \mathrm{i}\mu_v}{d_v k + \mathrm{i}\mu_v} \ . \tag{3.2}$$

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 its two edge ends. The resulting S-matrix of the whole graph then is

$$\begin{aligned} S(k) &= -\,(A + \mathrm{i}kB)^{-1}(A - \mathrm{i}kB) \\ &= -\,P - Q\,(L + \mathrm{i}k)^{-1}(L - \mathrm{i}k)\,Q \ , \quad k \in \mathbb{R}\backslash\{0\} \ . \end{aligned} \tag{3.3}$$

Again, $A \pm \mathrm{i}kB$ are invertible and $S(k)$ is unitary for all $k \in \mathbb{R}\backslash\{0\}$.

From the expressions (3.1)–(3.3) it appears that these S-matrices always depend on the wave number in a non-trivial way. However, Kirchhoff boundary conditions provide an immediate exception, since the choice $\mu_v = 0$ in (3.2) makes σ^v k-independent. A general characterisation of boundary conditions leading to k-independent S-matrices has been provided by Kostrykin and Schrader [KS06b, KPS07] in terms of the following equivalent conditions:

- $S(k)$ is self adjoint for one (and hence for all) $k \in \mathbb{R}\backslash\{0\}$,
- $AB^* = 0$, which is equivalent to $L = 0$,
- $\frac{1}{2}\big(S(k) - \mathbb{1}\big)$ is a projector; in fact, it is the projector P onto $\ker B$.

The second condition implies that the S-matrix is independent of k exactly in the case of non-Robin boundary conditions.

Further poperties of the S-matrix, which are relevant for Robin boundary conditions, are proved in [BE07].

Proposition 3.1. *Let A, B specify self adjoint boundary conditions for the Laplacian on Γ, then the S-matrix (3.3) has the following properties:*

1. *$S(k)$, $k \in \mathbb{R}\backslash\{0\}$, is differentiable and its derivative is*

$$S'(k) = -\frac{1}{2k}\big(S(k) - S(k)^*\big)\, S(k)\ . \tag{3.4}$$

2. *There exists $k_0 \geq 0$ such that for $k > k_0$ the following convergent expansion holds,*

$$S(k) = S_\infty + 2\sum_{n=1}^{\infty} \frac{1}{k^n}\,(\mathrm{i}QLQ)^n\ , \tag{3.5}$$

where $S_\infty = \mathbb{1} - 2P$.

3. *For $k < k_0$ the following convergent expansion holds,*

$$S(k) = S_0 - 2\sum_{n=1}^{\infty} k^n\,(-\mathrm{i}\tilde{Q}\tilde{L}\tilde{Q})^n\ . \tag{3.6}$$

Here $S_0 = \mathbb{1} - 2\tilde{Q}$ is the continuation of $S(k)$ to $k = 0$ and the quantities with a tilde emerge from those without under the replacement of A, B with $-B, A$.

In particular, the expression (3.4) for the derivative is consistent with the previously observed k-independence of self adjoint S-matrices. Moreover, the relations (3.4), (3.5) and (3.6) imply (convergent) expansions of the derivative of the S-matrix for large and for small k. Their leading orders read

$$S'(k) = -\frac{2\mathrm{i}}{k^2}\,QLQ + O(k^{-3}) \tag{3.7}$$

and

$$S'(k) = -2\mathrm{i}\,\tilde{Q}\tilde{L}\tilde{Q} + O(k)\ , \tag{3.8}$$

respectively. The latter relation also provides a continuation of $S'(k)$ to $k = 0$.

4 The trace formula

On a Riemannian manifold, a trace formula for the Laplacian relates the spectrum of $-\Delta$ to the length spectrum of closed geodesics. In a first step the trace of the wave group,

$$\mathrm{Tr}\,\mathrm{e}^{-\mathrm{i}t\sqrt{-\Delta}} + c.c. = 2\sum_{n} g_n \cos(k_n t)\ , \tag{4.1}$$

where the sum extends over the positive square roots k_n of the Laplace eigenvalues k_n^2 with multiplicities g_n, is identified as a Fourier integral operator. This defines a distribution with singular support in the length spectrum of closed geodesics (Poisson relation) [Cha74]. Its Fourier transform is the spectral density

$$d(k) = g_0\delta(k) + \sum_n g_n\big[\delta(k-k_n) + \delta(k+k_n)\big] \ . \tag{4.2}$$

Thereafter the singularities of (4.1) at the lengths of closed geodesics are analysed, and $t = 0$ is identified as the main contribution. Finally, a Fourier representation of the singularities leads to the trace formula [DG75], providing an asymptotic expansion of (4.2) in k^{-1}.

A slightly different approach employs the heat kernel associated with the Laplacian and therefore deals with the heat trace

$$\mathrm{Tr}\,\mathrm{e}^{t\Delta} = \sum_n g_n \mathrm{e}^{-k_n^2 t} \ . \tag{4.3}$$

By introducing complex variables t, the traces (4.1) and (4.3) seem to be similar. However, one has to be aware of certain subtleties in comparing both quantities, see [DG75] for a detailed discussion. Here we only wish to mention that the usual asymptotic expansion of the heat trace (4.3) is about $t = 0$, which to a certain extent corresponds to a short wavelength asymptotics. On the other hand, in the wave trace (4.1) $t = 0$ corresponds to the leading singularity only. It thus appears that the small-t asymptotics of the heat trace fails to include the contribution of periodic orbits (see, however, [BH94, FW07] for a more refined point of view). Without dwelling on further details we here wish to stress that, generally, the geometric (respectively dynamical) information contained in the short wavelength asymptotics of (4.1) is considerably finer than the information contained in the small-t asymptotics of (4.3).

Quantum graphs allow for both types of trace formulae, i.e., expressions representing (4.2) and (4.3). The first version of a trace formula is due to Roth, who proved a trace formula for the heat trace in the case of a Laplacian with Kirchhoff boundary conditions. This has recently been extended to the case of general non-Robin boundary conditions by Kostrykin, Potthoff, and Schrader.

Theorem 4.1 (Roth [Rot83]; Kostrykin, Potthoff, Schrader [KPS07]). *If the Laplacian on a compact metric graph is realised as a self adjoint operator such that the associated S-matrix is independent of the wave number k (non-Robin boundary conditions), the heat trace has the following representation,*

$$\mathrm{Tr}\,\mathrm{e}^{t\Delta} = \frac{\mathcal{L}}{2\sqrt{\pi t}} + \frac{1}{4}\,\mathrm{tr}\,S + \frac{1}{2\sqrt{\pi t}}\sum_p\sum_{r=1}^{\infty} A_{p,r}\, l_p\, \mathrm{e}^{-r^2 l_p^2/4t} \ , \tag{4.4}$$

where the sums extend over all primitive periodic orbits p of lengths l_p on the graph, and over their repetitions r, respectively. The quantities $A_{p,r}$ are defined in terms of the local S-matrix elements at the vertices visited by the r-fold repetitions of the primitive periodic orbits p, and $\mathcal{L} = l_1 + \cdots + l_E$ is the sum of all edge lengths on the graph.

Periodic orbits on a graph are understood as periodic sequences of edges such that the incident vertex of each edge is the terminal vertex of the preceding edge. Primitive orbits are those periodic orbits that are not multiple repetitions of other periodic orbits. In the case of Kirchhoff boundary conditions, $\frac{1}{4}\operatorname{tr} S = \frac{1}{2}(V-E)$, which is one half of the the Euler characteristic of the graph considered as a 1-complex and therefore is a purely topological quantity, see [KN05, Kur07, FKW07]. From Theorem 4.1 it is obvious that an expansion of the heat trace for small t only involves the first two terms on the right-hand side of (4.4), and hence the contributions of the periodic orbits escape such an asymptotic analysis. The trace formula, which in the case of quantum graphs is an identity, therefore provides much finer details of the geometry (or dynamics).

Kottos and Smilansky [KS99b] independently derived a trace formula for the spectral density (4.2), see also [KN05]. For Kirchhoff boundary conditions this reads

$$d(k) = \frac{\mathcal{L}}{\pi} + (V-E-1)\delta(k) + \frac{1}{2\pi}\sum_p \sum_{r=1}^{\infty} \big[A_{p,r}\, l_p\, \mathrm{e}^{\mathrm{i}kl_p} + \overline{A}_{p,r}\, l_p\, \mathrm{e}^{-\mathrm{i}kl_p} \big] \ . \tag{4.5}$$

As explained above, on a manifold the trace formula would usually be approached via the wave trace. In quantum graphs, however, the scattering approach is more direct and convenient. This approach, in fact, was the method used to prove (4.5). It can, moreover, be generalised in order to prove a trace formula for any self adjoint realisation of the Laplacian, including the case of Robin boundary condition where the S-matrix is k-dependent [BE07]. This will be described below.

The scattering approach is based on the observation that the Laplace eigenvalues can be characterised in terms of the zeroes of the (zeta-) function

$$\zeta(k) := (2\mathrm{i})^{-2E} \big(\det U(k)\big)^{-1/2} \det\big(\mathbb{1} - U(k)\big) = \prod_{j=1}^{2E} \sin\tfrac{\theta_j(k)}{2} \ , \tag{4.6}$$

where we have introduced the unitary matrix

$$U(k) := S(k)\, T(k) \ , \tag{4.7}$$

with eigenvalues $\mathrm{e}^{\mathrm{i}\theta_1(k)}, \dots, \mathrm{e}^{\mathrm{i}\theta_{2E}(k)}$. Whereas the S-matrix contributes to $U(k)$ information on the topology of the graph as well as on the boundary conditions for the Laplacian, the factor

$$T(k) = \begin{pmatrix} 0 & t(k) \\ t(k) & 0 \end{pmatrix} \quad \text{with} \quad t(k) = \begin{pmatrix} \mathrm{e}^{\mathrm{i}kl_1} & & \\ & \ddots & \\ & & \mathrm{e}^{\mathrm{i}kl_E} \end{pmatrix} \tag{4.8}$$

contains the metric information of Γ. In the definition (4.6) of the zeta function the choice of the prefactor is merely of convenience in that it makes this function real. The determinant, however, is the essential factor since its zeroes $k_n \in \mathbb{R}\backslash\{0\}$ exactly correspond to the non-zero eigenvalues k_n^2 of $-\Delta$. More precisely, results in [KS99b, KS06a] imply the following (see also [BE07]).

Proposition 4.2. *There exists $\lambda > 0$ such that the zeta function (4.6) can be continued as a meromorphic function into the strip $|\operatorname{Im} k| < \lambda$ with at most one pole at $k = 0$. In this strip, $k_n \neq 0$ is a zero of the zeta function with multiplicity g_n, iff k_n^2 is an eigenvalue of $-\Delta$ with the same multiplicity. Zero may be an eigenvalue of $-\Delta$ (with multiplicity g_0) as well as a zero of $\zeta(k)$ (with multiplicity N). In general, $g_0 \neq N$.*

To be more precise, if the matrix L (2.10) has a non-trivial positive part, λ is the smallest positive eigenvalue of L; otherwise it can be any positive number. The trace formula now follows from counting zeroes of the zeta function in the strip $|\operatorname{Im} k| < \lambda$. Let therefore be $0 < \kappa < \lambda$ and consider the strip

$$C_\kappa := \{k \in \mathbb{C};\ |\operatorname{Im} k| \leq \kappa\} \tag{4.9}$$

and a function $h : \mathbb{C} \to \mathbb{C}$ that is holomorphic in a neighbourhood of C_κ, such that

$$\frac{1}{2\pi \mathrm{i}} \int_{\partial C_\kappa} h(k) \, \frac{\zeta'}{\zeta}(k) \, \mathrm{d}k = N h(0) + \sum_{0 \neq k_n \in C_\kappa} g_n \, h(k_n) \ . \tag{4.10}$$

Here the sum on the right-hand side extends over all zeroes $k_n \in \mathbb{R}\backslash\{0\}$ of the zeta function with multiplicities g_n, corresponding to Laplace eigenvalues. The term with $k_0 = 0$ is counted with the multiplicity N of the zero of the zeta function at $k = 0$. The latter multiplicity may differ from that of the zero Laplace eigenvalue. In order to count contributions from $\pm k_n$ only once, we also require the function h to be even, $h(k) = h(-k)$.

In this count, the logarithmic derivative of the zeta function in (4.10) is calculated from (4.6). Its essential part comes from the determinant of $\mathbb{1} - U$, yielding

$$\frac{\mathrm{d}}{\mathrm{d}k} \log \det\bigl(\mathbb{1} - U(k + \mathrm{i}\kappa)\bigr) = - \sum_{n=0}^{\infty} \operatorname{tr}\bigl(U(k + \mathrm{i}\kappa)^n U'(k + \mathrm{i}\kappa)\bigr) \ , \tag{4.11}$$

and a corresponding result for $k - \mathrm{i}\kappa$. In order for the expansion of the logarithm that has been used to hold, one requires the (operator) norm of $U(k + \mathrm{i}\kappa)$ to be smaller than one. This is fulfilled, iff

$$0 \leq \kappa < \lambda \tanh \tfrac{\kappa l_{\min}}{2} \ . \tag{4.12}$$

Therefore, if L has a non-vanishing positive part, which can only occur in the case of Robin boundary conditions, (4.12) imposes a non-trivial condition on the shortest edge length. Eventually, one takes the limit $\kappa \to 0$ in (4.10), when (4.12) boils down to the condition $l_{\min} > 2/\lambda$.

Subsequently, the traces on the right-hand side of (4.11) are turned into sums over periodic orbits on the graph that consist of n edges. This representation of the traces is then used on the left-hand side of (4.10), and the summation and the integration are interchanged. The emerging sums over periodic orbits then converge, if the remaining (Fourier-) integrals decrease exponentially. In order to ensure this we first require the function h to be holomorphic in a strip of width 2σ, where $\sigma = \frac{1}{2l_{\min}} \log(2E)$. As a further condition one needs that in this strip the S-matrix has no poles, which is fulfilled once $\lambda \geq \sigma$. Moreover, the convergence of the sum on the right-hand side of (4.10) requires that the function h itself decreases sufficiently fast. We therefore now impose the following conditions on test functions to serve in the trace formula:

- h is even,
- h is holomorphic in a strip $|\operatorname{Im} k| < \sigma + \delta$ for some $\delta > 0$, where $\sigma = \frac{1}{2l_{\min}} \log(2E)$,
- $h(k) = O((1+|k|)^{-1-\varepsilon})$ for some $\varepsilon > 0$ in this strip.

We are now able to formulate the following general trace formula.

Theorem 4.3. *Let a compact, metric graph and a self adjoint realisation of the Laplacian on the graph be given, such that the condition* $l_{\min} > \max\{\frac{2}{\lambda}, \frac{1}{2\lambda}\log(2E)\}$ *is fulfilled, and let* h *be a test function satisfying the criteria outlined above. Then the following trace formula holds,*

$$\begin{aligned} \sum_{k_n \geq 0} g_n h(k_n) = \frac{\mathcal{L}}{2\pi}\hat{h}(0) + \left(g_0 - \tfrac{1}{2}N\right) h(0) - \frac{1}{4\pi}\int_{-\infty}^{+\infty} h(k)\, \frac{\operatorname{Im}\operatorname{tr} S(k)}{k}\, \mathrm{d}k \\ + \sum_p \sum_{r=1}^{\infty} \left[\hat{h} * \hat{A}_{p,r}(rl_p) + \hat{h} * \hat{\overline{A}}_{p,r}(rl_p)\right] . \end{aligned} \tag{4.13}$$

Here, $\hat{A}_{p,r}$ *is the Fourier transform of the amplitude function* $A_{p,r}$ *that has an expansion*

$$A_{p,r}(k) = \sum_{j\geq 0} a_{p,r}^{(j)}\, k^{-j} \ , \tag{4.14}$$

which converges for $k > k_0$*, where* k_0 *is the same quantity as in Proposition 3.1. In the case of non-Robin boundary conditions the amplitudes are independent of* k*, so that the convolutions in (4.13) degenerate into products.*

A proof of this theorem is given in [BE07], here we only want to add a few remarks:

1. In the case of non-Robin boundary conditions the Laplacian can have finitely many negative eigenvalues, see [Kuc04, KS06a]. In the complex k-plane these correspond to poles of the zeta function on the imaginary axis, which are not included in the domain C_κ of integration in (4.10). Their contribution hence is left out from this trace formula.
2. The amplitude functions arise from traces of powers of the S-matrix and its derivative, where the latter can be reduced to the S-matrix itself via the relation (3.4). Therefore, the expansion (4.14) is a direct consequence of Proposition 3.1.

3. The second term on the right-hand side of the trace formula accounts for different multiplicities of zero as a Laplace eigenfunction and a zero of the zeta function, respectively. For non-Robin boundary conditions this term is related to an index theorem for quantum graphs, see [FKW07].

4. The conditions imposed on the test functions h correspond directly to those required for test functions to be used in the Selberg trace formula [Sel56], in which case Weyl's law for the eigenvalue count requires h to decrease faster (by one power) than here. Moreover, $\sigma = 1/2$, which follows from Huber's law [Hub59] for the count of closed geodesics. This result can be seen as an analogue of the prime number theorem. Furthermore, in other (semiclassical) trace formulae a related condition, based on an appropriate count of periodic orbits, is imposed to ensure an absolute convergence of the sums over periodic orbits [SS90]. The quantity σ appearing there can be related to the topological pressure of the associated classical dynamical system [Bol99] and hence again to the (equi-) distribution of periodic orbits.

5. Under the conditions stated, the sums occurring in the trace formula (4.13) converge absolutely. Sometimes, however, one is interested in trace formulae that are only conditionally convergent (see, e.g., [BHW07]) so that the conditions to be imposed on the test functions can be relaxed [Win07].

Choosing the test function $h(k) = \mathrm{e}^{-k^2 t}$, $t > 0$, with Fourier transform $\hat{h}(l) = \sqrt{\pi/t}\,\mathrm{e}^{-l^2/4t}$, in the trace formula (4.13), one obtains a generalisation of Theorem 4.1 to any self adjoint realisation of the Laplacian. In the case of Robin boundary conditions, the fact that $\mathrm{Im}\,\mathrm{tr}\,S \neq 0$ then adds a term to the trace of the heat kernel that has an asymptotic expansion

$$\sum_{j \geq 0} \alpha_j \, t^{j+\frac{1}{2}} \ , \quad t \to 0 \ . \tag{4.15}$$

This additional term therefore neither influences the leading singular behaviour, nor the constant term in the expansion of the heat trace for $t \to 0$.

Apart from the trace formulae described above, quantum graph models have been investigated in a number of slightly different realisations. One can, e.g., replace the Laplacian by other operators that are relevant in quantum mechanics. This can, e.g., be a Pauli- or a Dirac-operator, describing spin-orbit coupling on a quantum graph. In that case the quantum graph Hilbert space is $L^2(\Gamma) \otimes \mathbb{C}^n$, and the construction of self adjoint realisations of the operators is largely similar to the case of the Laplacian [BH03], see also [Har07]. Functions on the graph now consist of n-component functions on the edges, where the n components reflect the presence of of the additional spin degree of freedom. For Pauli operators, $n = 2s + 1$, where $s = \frac{1}{2}, 1, \frac{3}{2}, \dots$ is the spin quantum number, and for Dirac operators $n = 2, 4$. In all cases the corresponding trace formula can be proven in very much the same manner as for Laplace operators, with results largely analogous to the trace formulae discussed above. The main difference is the occurrence of factors $\mathrm{tr}\, d_{p,r}$ in the sum over primitive periodic orbits and their repetitions. Here $d_{p,r}$ is a (spin-s representation of

a) SU(2) element describing the spin transport around the periodic orbit. For details see [BH03, Har07].

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