Spectral determinants and zeta functions of Schrödinger operators on metric graphs

J M Harrison 1, K Kirsten 1 and C Texier 2, 3

1 Department of Mathematics, Baylor University, Waco, TX 76798, USA
2 University Paris Sud; CNRS; LPTMS, UMR 8626, Bâtiment 100, F-91405 Orsay, France
3 University Paris Sud; CNRS; LPS, UMR 8502, Bâtiment 510, F-91405 Orsay, France

E-mail: jon_harrison@baylor.edu, klaus_kirsten@baylor.edu and christophe.texier@u-psud.fr

Received 2 November 2011, in final form 15 February 2012
Published 13 March 2012
Online at stacks.iop.org/JPhysA/45/125206

Abstract
A derivation of the spectral determinant of the Schrödinger operator on a metric graph is presented where the local matching conditions at the vertices are of the general form classified according to the scheme of Kostrykin and Schrader. To formulate the spectral determinant, we first derive the spectral zeta function of the Schrödinger operator using an appropriate secular equation. The result obtained for the spectral determinant is along the lines of the recent conjecture (Texier 2010 J. Phys. A: Math. Theor. 43 425203).

PACS numbers: 02.10.Ox, 02.30.Tb, 03.65.—w
Mathematics Subject Classification: 34B45, 81Q10, 81Q35

(Some figures may appear in colour only in the online journal)
the graph, namely the bond lengths \( \{ L_b \}_{b=1,\ldots,B} \) and the energy. The matrices \( \mathbb{A} \) and \( \mathbb{B} \) can thus be considered to define the graph topology as they record how the bonds are connected.

In particular, we will be concerned with the recent broad conjecture, introduced by one of the authors in [32], for the spectral determinant that is defined formally as

\[
S(\gamma) = \det[\gamma - \triangle + V(x)] = \prod_{j=0}^{\infty} (\gamma + E_j),
\]

where \( 0 < E_0 \leq E_1 \leq \cdots \) is the spectrum of the Schrödinger operator and \( \gamma \) is some spectral parameter; the condition on the positivity of the spectrum can be relaxed by accepting additional technicalities [21]. The first result for the spectral determinant of the Schrödinger operator on a graph with general vertex matching conditions was obtained by Desbois [9]; the method was, however, unable to determine the \( \gamma \)-independent prefactor of the determinant.

In order to regularize the formal definition of \( S(\gamma) \), we employ the spectral zeta function

\[
\zeta(s) = \sum_{j=0}^{\infty} (\gamma + E_j)^{-s}.
\]

The zeta function of the Schrödinger operator can be formulated by extending a technique introduced for graph Laplacians by some of the authors [17, 18]. Having derived the zeta function, the regularized spectral determinant is then defined by \( S(\gamma) = \exp(-\zeta'(0)) \). More precisely, we prove the following theorem along the lines of the conjecture.

**Theorem 1.** For the Schrödinger operator on a graph with local vertex matching conditions defined by a pair of matrices \( \mathbb{A} \) and \( \mathbb{B} \), with \( \mathbb{A} \mathbb{B}^\dagger = \mathbb{B} \mathbb{A}^\dagger \) and \( \text{rank}(\mathbb{A}, \mathbb{B}) = 2B \), and potential functions \( V_b(x_b) \in \mathbb{C}^\infty \) for \( b = 1, \ldots, B \), the spectral determinant is

\[
S(\gamma) = \left( \prod_{b=1}^{B} \frac{-2}{f'_b(L_b; \gamma)} \right) \det(\mathbb{A} + \mathbb{B}M(\gamma)) \frac{c_N\gamma^P}{c_N}. \]

\( f'_b(x; \gamma) \) and \( M(\gamma) \) are defined in terms of the solution to a boundary value problem on the interval \([0, L_b]\) described in section 4. \( c_N \) is the coefficient of the leading order \( t \to \infty \) asymptotic behaviour of \( \det(\mathbb{A} + \mathbb{B}M(t^2)) \), determined in section 5.1. Furthermore, the exponent \( P \) characterizes the \( t \to 0 \) behaviour of the determinant; \( P = 0 \) if \( \det(\mathbb{A} + \mathbb{B}M(0)) \neq 0 \), the generic case, otherwise \( \det(\mathbb{A} + \mathbb{B}M(\gamma)) \sim \gamma^P \) as \( \gamma \to 0 \).

The paper is organized as follows. In section 2, we define the terminology of the quantum graph model. Section 3 introduces the technique, followed subsequently, in the simple case of the Schrödinger operator on an interval with Dirichlet boundary conditions and a graph with Dirichlet conditions at the ends of every bond. To derive the zeta function of a general graph, we start from a secular equation whose solutions are \( \sqrt{E_j} \); an appropriate secular equation for the Schrödinger operator is identified in section 4. In section 5, we formulate the graph zeta function with general local matching conditions at the vertices. Finally, in section 6, we apply the results for the zeta function to prove theorem 1. The appendix shows the derivation of the \( t \to \infty \) asymptotics of the function \( f'_b(x; t^2) \).

2. The graph model

A graph \( G \) is a collection of vertices \( v = 1, \ldots, V \) and bonds \( b = 1, \ldots, B \). Each bond connects a pair of vertices \( b = (v, w) \) and we denote by \( o(b) = v \) the initial vertex of \( b \) and by \( t(b) = w \) the terminal vertex. \( \bar{b} = (w, v) \) will denote the reversed bond with the initial and
terminal vertices exchanged; therefore, \( o(b) = t(\bar{b}) \) and \( t(b) = o(\bar{b}) \). We consider undirected graphs with \( B \) undirected bonds, so \( b \) and \( \bar{b} \) refer to the same physical bond but the availability of two labels for each bond will be notationally convenient. \( m_v \) will denote the number of bonds meeting at a vertex \( v \), i.e. the valency of \( v \). To determine the valency \( b \) and \( \bar{b} \) refer to a single bond.

In order to define a metric graph, we associate with each bond \( b \) an interval \([0, L_b]\), where \( L_b \) is the length of \( b \) and \( x_b = 0 \) at \( o(b) \) and \( x_b = L_b \) at \( t(b) \). So, \( x_b \) is the distance to a point in the interval measured from the initial vertex \( o(b) \) and we also use \( x_{\bar{b}} = L_b - x_b \) for the distance to the same point measured from the terminal vertex of \( b \). The total length of \( G \) is denoted by \( L = \sum_{b=1}^{B} L_b \). A function \( \psi \) on \( G \) is defined by specifying the set of functions \( \{ \psi_b(x_b) \}_{b=1}^{B} \) on the collection of intervals. The redundancy of notation enforces the relation \( \psi_b(x_b) = \psi_{\bar{b}}(x_{\bar{b}}) = \psi_{\bar{b}}(L_b - x_b) \). The Hilbert space of \( G \) is consequently

\[
\mathcal{H} = \bigoplus_{b=1}^{B} L^2([0, L_b]).
\]  

Motivated by physical applications, we consider here Schrödinger operators on the metric graph. The eigenproblem on bond \( b \) is

\[
\left( \frac{d^2}{dx_b^2} + A_b \right) \psi_b(x_b) + V_b(x_b)\psi_b(x_b) = k^2\psi_b(x_b).
\]  

The set \( \{A_1, \ldots, A_B\} \) defines a vector potential on the graph constant on each bond\(^4\). For consistency, \( A_{\bar{b}} = -A_b \) as the direction is reversed when changing coordinate.

3. Dirichlet determinants

3.1. Laplace operator on a finite interval

We first analyse the determinant of the Laplace operator on a single finite interval \([0, L]\) with Dirichlet boundary conditions, a wire. The spectrum of the wire is \( E_j = \left( \frac{j\pi}{L} \right)^2 \) for \( j \in \mathbb{N}^* \) and we can compute the zeta function directly:

\[
\zeta_{\text{Dir}}(s) = \sum_{j=1}^{\infty} E_j^{-s} = \left( \frac{L}{\pi} \right)^2 \zeta_R(2s).
\]  

Differentiating,

\[
\zeta'_{\text{Dir}}(0) = 2\zeta_R'(0) + 2\zeta_R(0) \log(L/\pi) = -\log 2 - \log L,
\]  

where we have used \( \zeta_R(0) = -\frac{1}{2} \) and \( \zeta_R'(0) = -\frac{1}{2} \log(2\pi) \) \([16]\). We therefore obtain the spectral determinant for \( \gamma = 0 \):

\[
S_{\text{Dir}}(0) = \det(-\Delta) = \exp(-\zeta'_{\text{Dir}}(0)) = 2L,
\]  

which agrees with the formulation of the spectral determinant of the Laplace operator in \([18, 20, 32]\).

\(^4\) A vector potential \( A_b(x_b) \) that depends on the position on the bond can be made constant on each bond by a gauge transformation, so \( A_{\bar{b}} = \int_0^{L_b} \frac{d}{dx_b} A_b(x_b) \ dx_b \).
3.2. The Schrödinger operator on a finite interval

To compute the spectral determinant of the operator \(-\frac{d^2}{dx^2} + V(x)\) for \(x \in [0, L]\) with Dirichlet boundary conditions, let us introduce two useful bases for the solutions of the differential equation

\[
\left(-\frac{d^2}{dx^2} + V(x)\right) \psi(x) = k^2 \psi(x). \tag{8}
\]

The first basis was shown to be useful in [8, 9]: \(f(x; -k^2)\) is a solution of (8), such that \(f(0; -k^2) = 1\) and \(f(L; -k^2) = 0\), with the second linearly independent solution denoted \(\tilde{f}(\tilde{x}; -k^2)\), where \(\tilde{x} = L - x\) and \(\tilde{f}\) satisfies \(\tilde{f}(0; -k^2) = 1\) and \(\tilde{f}(L; -k^2) = 0\). For a symmetric potential, \(V(x) = V(L - x)\) and we have \(\tilde{f}(0; -k^2) = f(0; -k^2)\); note that in this case the two linearly independent solutions of the differential equation (8) are simply \(f(x; -k^2)\) and \(\tilde{f}(\tilde{x}; -k^2) = f(L - x; -k^2)\). An alternative basis was employed in [14]: \(u(x; -k^2)\) and \(\tilde{u}(\tilde{x}; -k^2)\) are the solutions satisfying \(u(0; -k^2) = 0\) and \(u'(0; -k^2) = 1\), where prime denotes derivation with respect to the spatial coordinate \(x\), i.e. first argument of the functions.

The relation between the two bases is given by

\[
u(L; -k^2) = 0. \tag{10}
\]

Note that the secular equation may be written in different forms, thanks to the relations \(u(L; -k^2) = \tilde{u}(L; -k^2) = -1/f'(L; -k^2) = -1/\tilde{f}'(L; -k^2)\), which hold for an arbitrary potential. However, \(u(x; y)\) and \(\tilde{u}(x; y)\) do not coincide in general (apart for a symmetric potential \(V(x) = V(L - x)\)); nevertheless \(u(L; y) = \tilde{u}(L; y)\) always holds. This may be shown by computing the Wronskian of the two solutions at the ends of the interval.

**Example 1.** For a free particle, where \(V(x) = 0\),

\[
f(x; -k^2) = \tilde{f}(x; -k^2) = \frac{\sin k(L - x)}{\sin kL} \quad \text{and} \quad u(x; -k^2) = \tilde{u}(x; -k^2) = \frac{1}{k} \sin kx. \tag{11}
\]

The Dirichlet spectrum is then given by solutions of the secular equation

\[
F(k) = u(L; -k^2) = \frac{-1}{f'(L; -k^2)} = \frac{1}{k} \sin kL = 0. \tag{12}
\]

**Example 2.** In the case of a linear potential \(V(x) = \omega x\), we find

\[
u(x; -k^2) = \frac{\pi}{\omega^{1/3}} [\text{Ai}(-\omega^{-2/3}k^2) \text{Bi}(\omega^{1/3}(x - k^2/\omega))] - \text{Bi}(-\omega^{-2/3}k^2) \text{Ai}(\omega^{1/3}(x - k^2/\omega))], \tag{13}
\]

\[
\tilde{u}(\tilde{x}; -k^2) = \frac{\pi}{\omega^{1/3}} [\text{Bi}(\omega^{1/3}(L - k^2/\omega)) \text{Ai}(\omega^{1/3}(x - k^2/\omega))] - \text{Ai}(\omega^{1/3}(L - k^2/\omega)) \text{Bi}(\omega^{1/3}(x - k^2/\omega))], \tag{14}
\]

with the Airy functions \(\text{Ai}(z)\) and \(\text{Bi}(z)\) [1]. The Dirichlet spectrum is given by solving the secular equation

\[
F(k) = \text{Ai}(-\omega^{-2/3}k^2) \text{Bi}(\omega^{1/3}(L - k^2/\omega)) - \text{Bi}(-\omega^{-2/3}k^2) \text{Ai}(\omega^{1/3}(L - k^2/\omega)) = 0. \tag{15}
\]
Example 3. Another interesting example is the case of a potential of the form \( V(x) = \phi(x)^2 + \phi'(x) \). The Hamiltonian
\[
H_S = -\frac{d^2}{dx^2} + \phi(x)^2 + \phi'(x)
\]
describes the so-called supersymmetric quantum mechanics [34]. In this case, exploiting the factorization \( H_S = Q^*Q \) with \( Q = -\frac{d}{dx} + \phi(x) \), it is possible to construct explicitly two linearly independent solutions of the differential equation \( H_S\psi = 0 \). We may choose \( \psi_0(x) = \exp \int_0^x \phi(y) dy \) and \( \psi_1(x) = \psi_0(x) \int_x^L \frac{dy}{\psi_0(y)^2} \). We obtain the two useful solutions for \( k = 0 \):
\[
u(x; 0) = \psi_0(0)\psi_0(x) \int_0^x \frac{dy}{\psi_0(y)^2} \quad \text{and} \quad \bar{u}(x; 0) = \psi_0(L)\psi_0(x) \int_x^L \frac{dy}{\psi_0(y)^2}
\]

We now explain the general method followed in [18] and in this paper. A secular equation \( F(k) = 0 \) can be related to the zeta function using the argument principle
\[
\zeta_{\Delta c}(s, \gamma) = \frac{1}{2\pi i} \int_{\gamma} (z^2 + \gamma)^{-s} \frac{d}{dz} \log(F(z)) dz,
\]
where the contour wraps around the positive real axis enclosing the roots of \( F(z) \), the solutions of the secular equation, and avoiding any poles; see figure 1(a).

In the present case, the function \( F(z) = u(L; -z^2) \) does not present poles. However, as there is some freedom in the choice of \( F(z) \), in the following section, it is convenient to choose a function \( F \) for the general graph that will possess poles. Transforming the contour \( \gamma \) to the imaginary axis \( z = it \) (see figure 1(b)), we obtain
\[
\zeta_{\Delta c}(s, \gamma) = \frac{\sin \pi s}{\pi} \int_{\gamma} (t^2 - \gamma)^{-s} \frac{d}{dt} \log(u(L; t^2)) dt,
\]
where, assuming \( F(0) \neq 0 \), the segment between \( i\sqrt{\gamma} \) and \(-i\sqrt{\gamma}\) does not contribute to the integral as \( F(z) = F(-z) \) (which follows from the symmetry of the secular equation); comments about the case \( F(0) = 0 \) follow in section 6. The analysis of the integral shows that this representation of the zeta function is valid in the strip \( 1/2 < \Re s < 1 \). The restriction to \( \Re s > 1/2 \) comes from the asymptotic behaviour of \( u(x; t^2) \) for \( t \to \infty \). The asymptotics of the function \( u(x; t^2) \) for \( t \to \infty \) were evaluated in [14]:
\[
\log u(L; t^2) \sim L \log 2t + O(t^0), \quad t \to \infty.
\]
An explicit example of such an expansion is provided in the appendix, see equation (A.9). To obtain a representation valid for $s \to 0$, we subtract and add the first two terms in the asymptotic expansion. Then, upon integration, we find

$$\zeta_{\text{Dir}}(s, \gamma) = \frac{\sin \pi s}{\pi} \int_0^{\infty} \left( t^2 - y^2 \right)^{-s} \frac{d}{dt} \left[ \log(u(L, t^2)) - tL + \log(2t) \right] dt$$

$$+ L \frac{\Gamma(s - 1/2)}{2\sqrt{\pi} \Gamma(s)} y^{-1-s} = \frac{1}{2} y^{-s},$$

valid in the strip $-1/2 < \Re s < 1$. Differentiating

$$\zeta'_{\text{Dir}}(0, \gamma) = -\log(u(L; \gamma)) - \log(2\sqrt{\gamma}) + \frac{1}{2} \log \gamma = -\log(2u(L; \gamma)).$$

Consequently, the zeta-regularized spectral determinant of a Dirichlet boundary conditions is [22]

$$S_{\text{Dir}}(\gamma) = \exp(-\zeta'_{\text{Dir}}(0, \gamma)) = 2u(L; \gamma) = \frac{-2}{f'(L; \gamma)}.$$

**Example 1.** In the absence of a potential, we obtain

$$S_{\text{Dir}}(\gamma) = \frac{2 \sinh \sqrt{\gamma}L}{\sqrt{\gamma}}.$$  

(24)

As $\gamma \to 0$, this expression agrees with (7).

**Example 2.** Using (13), the spectral determinant of $H = -\frac{d^2}{dx^2} + \omega x$, therefore, is

$$S_{\text{Dir}}(\gamma) = \frac{2\pi}{\omega^3/3} \left[ \text{Ai}(\omega^{-2/3} \gamma) \text{Bi}(\omega^{1/3}(L + \gamma/\omega)) - \text{Bi}(\omega^{-2/3} \gamma) \text{Ai}(\omega^{1/3}(L + \gamma/\omega)) \right].$$

(25)

**Example 3.** Using expression (17), we can obtain an explicit formula for the spectral determinant of the supersymmetric Hamiltonian for a vanishing spectral parameter:

$$S_{\text{Dir}}(0) = 2 \psi_0(0) \psi_0(L) \int_0^L \frac{dy}{\psi_0(y)^2},$$

(26)

i.e.

$$\det \left( -\frac{d^2}{dx^2} + \phi^2 + \phi' \right) = 2 e^{\phi(L)} \int_0^L e^{-2} \psi(t) \phi(t) dt dx.$$

(27)

Note that this explicit formula furnishes another way to obtain the determinant $\left( y - \frac{d^2}{dx^2} + V \right)$ in terms of one solution among a family of solutions of a Riccati equation $\phi(x) = \gamma - \phi(x)^2 + V(x)$. For example, in the free case, $V(x) = 0$, the Riccati problem is solved by $\phi(x) = \sqrt{\pi} \tanh \sqrt{\pi}(x + x_0)$: we can check that (27) leads to (24). Formula (27) may also be illustrated in the case $\phi(x) = \omega x$ (harmonic oscillator on a finite interval):

$$\det \left( -\frac{d^2}{dx^2} + \omega^2 x^2 + \omega \right) = \sqrt{\frac{\pi}{\omega}} e^{\lambda^2/2} \text{erf}(\sqrt{\omega} L),$$

(28)

where erf(x) is the error function [16]. The limit $L \to \infty$ of (28) is singular and does not approach either $\sqrt{\pi}/\omega$ or $\sqrt{\pi}/2\omega$, the determinant of the operator defined on $\mathbb{R}$ or $\mathbb{R}_+$, respectively. This is not unexpected as eigenfunctions on the interval [0, L] will not be square integrable in the limit $L \to \infty$. Eigenfunctions of high enough energy always feel the presence of the boundary conditions at both ends of the interval and thus differ significantly from the infinite space situation.
3.3. Dirichlet determinant of a graph

We are now also in a position to consider the case of a graph with Dirichlet boundary conditions at every vertex. The Dirichlet conditions describe a graph where all the bonds are decoupled, and consequently, the spectrum is simply the union of the Dirichlet spectra of the individual intervals. Since the zeta functions of each wire are additive and the determinants are multiplicative in this case, we recover a result of [32]

$$S_{\text{Dir}}(\gamma) = \prod_{b=1}^{B} \frac{-2}{f_b'(L_b; \gamma)}.$$  

(29)

To compare with the free case, we use (11) to obtain

$$S_{\text{Dir}}(\gamma) = 2B^{\gamma - B/2} \prod_{b=1}^{B} \sinh \sqrt{\gamma}L_b.$$  

Taking the limit $\gamma \to 0$, we see (29) reduces to the explicit formula

$$S_{\text{Dir}}(0) = 2B \prod_{b=1}^{B} L_b$$

that agrees with (7).

4. A secular equation of a Schrödinger operator with general matching conditions

For a general graph, let $f_b$ be the solution of the boundary value problem on the interval $[0, L_b]$:

$$\left(-\frac{d^2}{dx_b^2} + V_b(x_b)\right) f_b(x_b; \gamma) = \gamma^2 f_b(x_b; \gamma),$$  

(30)

such that $f_b(0; -\gamma^2) = 1$ and $f_b(L_b; -\gamma^2) = 0$. $f_b(x_b; -\gamma^2)$ will denote the complimentary solution on the same bond where the function vanishes at the initial vertex of $b$ and is unity at the terminal vertex, i.e. $f_\gamma(0; -\gamma^2) = 1$ and $f_\gamma(L_b; -\gamma^2) = 0$. $f_b$ and $f_\gamma$ are a pair of linearly independent functions on the interval satisfying the eigenvalue problem. Hence, the component of the wavefunction of the Schrödinger operator (4) with energy $\gamma$ on bond $b$ can then be written

$$\psi_b(x_b, -\gamma^2) = c_b f_b(x_b; -\gamma^2) e^{i\lambda_b x_b} + c_\gamma f_\gamma(x_b; -\gamma^2) e^{i\lambda_b x_b}.$$  

(31)

Matching conditions at the graph vertices are specified by a pair of $2B \times 2B$ matrices $A$ and $B$ via

$$A \psi + B \hat{\psi} = 0,$$  

(32)

where

$$\psi = (\psi_1(0), \ldots, \psi_B(0), \psi_1(L_1), \ldots, \psi_B(L_B))^T,$$  

(33)

$$\hat{\psi} = (D_1\psi_1(0), \ldots, D_B\psi_B(0), D_1\psi_1(L_1), \ldots, D_B\psi_B(L_B))^T.$$  

(34)

$D_b := \frac{d}{dx_b} - i\lambda_b$ is the covariant derivative, and in (33), we consider $\psi_b$ as a function of $x_b$, so $x_b = 0$ at $t(b)$ and $x_b = L_b$ at $t(b)$. $\hat{\psi}$ is therefore the vector of inward pointing covariant derivatives at the ends of the intervals.

The following theorem of Kostrykin and Schrader that classifies all matching conditions of self-adjoint realizations of the Laplace operator [24] also applies to the Schrödinger operator.

**Theorem 2.** The Laplace operator with matching conditions specified by $A$ and $B$ is self-adjoint if and only if $(A, B)$ has a maximal rank and $ABA^\dagger = BAB^\dagger$.  

Note that it is convenient to consider $f_b$ as a function of $x_b = L_b - x_b$.  

7
See [28], for an alternative unique classification scheme for general vertex matching conditions. Note that the general matching conditions we employ can be approximated by ornamenting the vertices of the graph with subgraphs whose vertices have δ-type matching conditions [6].

We consider only local matching conditions where the matrices $A$ and $B$ relate values of functions and their derivatives on the intervals where they meet at a vertex and where the matrices are independent of the metric structure of the graph, namely the bond lengths and the spectral parameter $k$. The restriction to matching conditions independent of the metric structure is necessary in order to employ the argument principle later.

Representing the components of an energy eigenfunction on $G$ following (31), we see that $\psi = (c_1, \ldots, c_B, c_T, \ldots, c_P)^T$ and $\hat{\psi} = M(-k^2)\psi$, where $M(-k^2)$ is the $2B \times 2B$ matrix

$$M_{ab} = \delta_{a,b} f_b^0(0; -k^2) - \delta_{a,b} f_b^0(L_b; -k^2) e^{ikL_b}.$$  

(35)

The vector $\hat{\psi}$ of coefficients of the two linearly independent solutions on each bond characterizes the wavefunction. Substituting into (32) we see that for $\hat{\psi}$ to define a wavefunction of energy $k^2$ satisfying the matching conditions, we require

$$\det(A + B M(-k^2)) = 0,$$  

(36)

which defines a secular equation for the graph Schrödinger operator.

**Example 1.** For a free particle, $V_0(x_b) = 0$ and we can write $f_b$ explicitly:

$$f_b(x_b; -k^2) = \frac{\sin kL_b - x_b}{\sin kL_b}, \quad \text{so} \quad f_b'(x_b; -k^2) = -\frac{k \cos k(L_b - x_b)}{\sin kL_b}. \quad (37)$$

Consequently, the matrix $M$ takes the form

$$M(-k^2) = -k \begin{pmatrix} \cot kL & -\csc kL \\ -\csc kL & \cot kL \end{pmatrix}, \quad (38)$$

where $\cot kL = \text{diag}(\cot kL_1, \ldots, \cot kL_B)$ and $\csc kL$ is defined similarly.

5. The zeta function of a Schrödinger operator with general matching conditions

Let us define the function

$$F(z) := \det(A + B M(-z^2))$$  

(39)

so the secular equation (36) reads $F(k) = 0$. As previously the zeta function is written as a contour integral

$$\zeta(s, \gamma) = \frac{1}{2\pi i} \int_C (z^2 + \gamma)^{-s} \frac{d}{dz} \log F(z) \, dz,$$  

(40)

where the contour $C$ encloses the zeros of $F$ and avoids its poles; see figure 1(a). Making a contour transformation to the imaginary axis (see figure 1(b)), the integral breaks into two parts

$$\zeta(s, \gamma) = \zeta_{\text{im}}(s, \gamma) + \zeta_{\text{re}}(s, \gamma),$$  

(41)

where we denote by $\zeta_{\text{im}}$ the integral along the imaginary axis and $\zeta_{\text{re}}$ the series that results from subtracting the residue $(\zeta_0^2 + \gamma)^{-s}$ at each pole $z_0$ of $F$. Writing $z = it$, the imaginary axis integral becomes

$$\zeta_{\text{im}}(s, \gamma) = \frac{\sin \pi s}{\pi} \int_{\gamma}^{\infty} (t^2 - \gamma)^{-s} \frac{d}{dt} \log F(it) \, dt,$$  

(42)

which converges in the strip $1/2 < \Re s < 1$.

As poles of $F$ lie at eigenvalues of the graph Schrödinger operator with Dirichlet boundary conditions, we see that $\zeta_{\text{re}}(s, \gamma) = \zeta_{\text{Dir}}(s, \gamma)$, which we evaluated previously. It remains to formulate the imaginary axis integral so that the zeta function given in (42) is well defined to the left of the line $\Re s = 1/2$. 




5.1. Large $t$ asymptotics of $F(it)$

To extend the zeta function to the left of the line $\Re s = 1/2$, we require the large $t$ asymptotics of $F(it) = \det(\mathbb{A} + BM(t^2))$. The $t \to \infty$ asymptotics of $f_b^i$ are analysed in the appendix where we find

$$f_b^i(0; t^2) \sim -t + \sum_{j=1}^{\infty} s_{b,j}(0)t^{-j},$$  \hspace{1cm} (43)

and $f_b^i(Lb; t^2)$ vanishes exponentially. The functions $s_{b,j}(x_0)$ are determined iteratively from the potential $V_b(x_0)$ via a recursion relation (A.4).

Using (43), we can write the expansion of $M(t^2)$ as $t \to \infty$ up to exponentially suppressed terms:

$$M_{ab} \sim \delta_{a,b} \left(-t + \sum_{j=1}^{\infty} s_{b,j}(0)t^{-j}\right).$$  \hspace{1cm} (44)

Hence,

$$F(it) = \det(\mathbb{A} + BM(t^2)) \sim \det(\mathbb{A} + B(-t\mathbf{I} + D(t))),$$  \hspace{1cm} (45)

where

$$D(t) = \sum_{j=1}^{\infty} t^{-j}\text{diag}\{s_{1,j}(0), \ldots, s_{b,j}(0), s_{\gamma,j}(0), \ldots, s_{\beta,j}(0)\}.$$  \hspace{1cm} (46)

The expansion of $F(it)$ fits with the free-particle case investigated in [18], where, in the absence of a potential, $D(t) = 0$ and $F(it) \sim \det(\mathbb{A} - t\mathbb{B})$.

Using (45) and the recursion relation (A.4), the expansion of $F(it)$ can be carried out to arbitrary order using a computer algebra package. In general, the expansion will take the form

$$F(it) \sim \det(\mathbb{A} + B(-t\mathbf{I} + D(t))) = \sum_{j=0}^{\infty} c_j t^{2B-j},$$  \hspace{1cm} (47)

where $c_0 = \det B$. We denote by $c_N$ the first nonzero coefficient in the expansion of $F(it)$, so $N = 0$ if $\det B \neq 0$. To evaluate the zeta-regularized spectral determinant, we need a representation of the zeta function valid about $s = 0$. To find this, we only require the leading order in the expansion. Subtracting and adding the leading order behaviour, we obtain an expression for the imaginary axis integral valid in the strip $-1/2 < \Re s < 1$:

$$\zeta_{im}(s, \gamma) = \frac{\sin \pi s}{\pi} \int_{\sqrt{2}}^{\infty} (t^2 - \gamma)^{-s} \frac{d}{dt} \log(F(it)t^{N-2B}/c_N) \, dt + \frac{1}{2} (2B - N)\gamma^{-s}. \hspace{1cm} (48)$$

Correspondingly,

$$\zeta'_{im}(0, \gamma) = \log c_N - \log \left(F(i\sqrt{2})\gamma^{0.2B}\right) - \frac{2B - N}{2} \log \gamma$$

$$= \log c_N - \log \det(\mathbb{A} + BM(\gamma)).$$  \hspace{1cm} (49)

6. Zeta-regularized spectral determinant

Collecting the results so far we can now formulate the spectral determinant, $S(\gamma) = \exp\left(-\zeta'_{im}(0, \gamma) - \zeta'_{im}(0, \gamma)\right)$, of a graph with general local vertex matching conditions, we obtain

$$S(\gamma) = \frac{S_{Dir}(\gamma)}{c_N} \det(\mathbb{A} + BM(\gamma)), \quad \text{where} \quad S_{Dir}(\gamma) = \prod_{b=1}^{B} \frac{-2}{f_b^i(Lb; \gamma)}.$$  \hspace{1cm} (50)
This is the statement of theorem 1. The $\gamma$-dependent part of this expression coincides with Desbois’ result [9] obtained by a different approach. If we choose Dirichlet matching conditions at the graph vertices, then $A = I_{2B}$ and $B$ is a matrix of zeros; see (32). Hence, $c_{2B} = 1$, which is the only nonzero term in the large $t$ expansion of $F(u)$, and $\det(A + BM(\gamma)) = 1$; consequently, (50) reduces to (29) as required.

$F(z)$ vanishing at zero. If $F(0) = 0$ the contour integral will pick up contributions associated with the behaviour at $z = 0$. While $F(0)$ does not vanish generically, when it does vanish it is straightforward to compensate for this by adjusting the function $F$. Assume $F(z) \sim z^{2P}$ as $z \to 0$ for $P \in \mathbb{N}$. We may define a new function $\tilde{F}(z) = F(z)/z^{2P}$. Then, $\tilde{F}(z) = 0$ is a secular equation but $F$ does not vanish at zero. Evaluating the zeta function using $\tilde{F}$, the procedure is identical and we find

$$S(\gamma) = \frac{S_{\text{Dir}}(\gamma)}{c_N \gamma^P} \det(A + BM(\gamma)).$$

The same technique was used, e.g., to evaluate the zeta function of the Laplacian on a star graph with Neumann-like matching conditions in [18]. To determine $P$ in a particular case, one requires the asymptotic expansion of $f_b(0, t^2)$ and $f_b(L_b, t^2)$ as $t \to 0$. We now discuss the spectral determinant in two particular cases.

Functions continuous at the vertices. We consider local vertex matching conditions for which the wavefunction is continuous at the vertices, namely the $\delta$-type conditions. At a vertex $v$, the local $\delta$-type matching conditions relate the functions and covariant derivatives at the ends of the intervals meeting at $v$. One explicit choice of $m_v \times m_v$ matrices to encode such matching conditions is

$$A_v = \begin{bmatrix} -\lambda_v & 0 & \cdots & 0 \\ -1 & 1 & 0 & \cdots \\ 0 & -1 & 1 & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 \end{bmatrix} \quad \text{and} \quad B_v = \begin{bmatrix} 1 & 1 & \cdots & 1 \\ 0 & 0 & \cdots & 0 \\ 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 \end{bmatrix},$$

where $\lambda_v$ is the strength of the coupling at $v$. We note that $\det(A_v - tB_v) = -(\lambda_v + m_v t)$. By relabelling the $2B$ ends of the intervals, we may write the matrices $A$ and $B$ describing matching conditions on the whole graph so the matrices $A_v$ and $B_v$ for $v = 1, \ldots, V$ appear as blocks on the diagonal. We recall that the factor $c_N$ appearing in the spectral determinant is the coefficient of the highest power of $t$ in the expansion of $\det(A + B(-tI + D(t)))$, where $D(t)$ is a diagonal matrix where each nonzero element is a series in inverse powers of $t$. Hence, we see that for a graph with $\delta$-type conditions at all the vertices and any potentials on the bonds

$$\det(A + BM(\gamma)) \sim \lim_{t \to \infty} \det(A + B(-tI + D(t))) \sim \lim_{t \to \infty} \left( \prod_v m_v \right) t^V + O(t^{V-1}).$$

Thus, we find $N = V$ and $c_V = \prod_v (\alpha_v)$. Consequently,

$$S(\gamma) = \left( \prod_{b \in B} \frac{-2}{f_b(L_b, \gamma)} \right) \det(A + BM(\gamma)) \prod_v (\alpha_v),$$

reproducing the result in [32]. Note that the choice of a wavefunction continuous at the vertices allows one to introduce vertex variables and simplify the spectral determinant by replacing $\det(A + BM(\gamma))$ by a matrix coupling vertices of a smaller dimension [2, 9, 32].

6 The even power is due to the symmetry of $F$. 
Functions whose derivative is continuous at the vertices. Another interesting case of matching conditions, studied in [31, 32], are the so-called $\delta'$-type matching conditions corresponding to a wavefunction whose derivative is continuous at the vertices [12]. A possible choice of matching matrices at a vertex $v$ is

$$A_v = \begin{pmatrix} 1 & 1 & \ldots & 1 & 1 \\ 0 & 0 & \ldots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \ldots & 0 & 0 \end{pmatrix} \quad \text{and} \quad B_v = \begin{pmatrix} -\mu_v & 0 & 0 & \ldots & 0 \\ -1 & 1 & 0 & \ldots & 0 \\ 0 & -1 & 1 & \ldots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \ldots & 1 \end{pmatrix}. \tag{55}$$

So, $\det(-\frac{1}{t}A_v + B_v) = - (\mu_v + \frac{1}{t}m_v)$, and therefore,

$$\det(\hat{A} + B \mathcal{M}(\gamma)) \sim \frac{t^{2B-V}}{\prod_v (-m_v)} \quad \text{for} \quad \mu_v = 0 \ \forall \ v. \tag{56}$$

The exponent $N = 2B - V$ and the coefficient $c_{2B-V} = \prod_v (-m_v)$. We again obtain (54).

Comparison with the conjecture of [32]. The zeta-regularized spectral determinant was obtained in [32] in the two particular cases considered above with a different method. Based on the observation that both sets of matching conditions led to equation (54), it was conjectured that this result is of greater generality (equation (61) of this reference). In light of this work, we now inject two observations.

- The matrices $\hat{A}$ and $B$ describing boundary conditions are not unique. Any transformation $(\hat{A}, B) \rightarrow (UA, UB)$, where $U$ is a matrix, such that $\det U \neq 0$, leaves the nature of the matching conditions invariant. Therefore, the general expression of the zeta-regularized spectral determinant should be invariant under such a transformation. It is clear that this is not the case for the form (54) conjectured in [32], whereas our main result theorem 1 is invariant.

- The conjecture was based on a continuity argument with respect to variations of $\hat{A}$ and $B$. However, in general, $c_N$ may depend on the particular choice of the matching conditions rather than simply the topology of the graph. In particular, it is not possible to rule out a priori that for a given choice of matching conditions and potentials a term in the series expansion (47) vanishes. We have seen in the previous pair of examples that the exponent $N$ does indeed vary with the nature of the matching conditions.

- Although the spectral determinant of a self-adjoint Schrödinger operator is real, this may not be apparent in the formulation presented in (51). The reason for this is the non-unique form used for the vertex matching conditions expressed through the matrices $\hat{A}$ and $B$. As the multiplication of $\hat{A}$ and $B$ by an invertible matrix $U$ provides another formulation of the same matching conditions, the phase of $\det (\hat{A} + B \mathcal{M}(\gamma))$ is arbitrary. However, the same phase appears in the asymptotic coefficient $c_N \rightarrow \det(U) c_N$.

Acknowledgments

The authors would like to thank Alain Comtet, Sebastian Eggers né Endres, Guglielmo Fucci, Frank Steiner and Yves Tourigny for stimulating discussions. KK is supported by National Science Foundation grant PHY-0757791. JMH was supported by the Baylor University summer sabbatical program.
Appendix. Large $t$ asymptotics of $f'(x; t^2)$

$f(x; t^2)$ is the solution of

$$\left(-\frac{d^2}{dx^2} + V(x) + t^2\right)f(x; t^2) = 0 \quad (A.1)$$
on the interval $[0, L]$ with $f(0; t^2) = 1$ and $f(L; t^2) = 0$. To find the asymptotics of $f'(x; t^2)$ in the limit $t \to \infty$, we let $\phi(x)$ be a general solution of (A.1) and call $S_i(x) = \frac{1}{\phi(x)} \log \phi(x)$. $S_i$ satisfies the differential equation

$$S_i'(x) = t^2 + V(x) - S_i^2(x). \quad (A.2)$$

Consequently, in the limit $t \to \infty$, $S_i$ has an expansion of the form

$$S_i(x) = \sum_{j=1}^{\infty} s_j(x) t^{-j}. \quad (A.3)$$

The functions $s_j(x)$ are determined by the recurrence relation

$$s_{j+1}(x) = \pm \frac{1}{2} \left(s_j'(x) + \sum_{k=0}^{j} s_k(x) s_{j-k}(x) \right), \quad (A.4)$$

where $s_{-1}(x) = \pm 1$, $s_0(x) = 0$ and $s_1(x) = \pm \frac{1}{2} V(x)$. The two alternative signs in the expansion produce exponentially growing and decaying solutions of (A.1). If we denote with $S_i^\pm(x)$, the functions with $s_{-1}(x) = \pm 1$, respectively, then we may write the large $t$ behaviour of $f(x; t^2)$ as a linear combination of the exponentially growing and decaying parts:

$$f(x; t^2) = A^+ \exp \int_0^x S_i^+(u) \, du + A^- \exp \int_0^x S_i^-(u) \, du. \quad (A.5)$$

Imposing the boundary conditions, we require $A^- = 1 - A^+$ and as it turns out

$$A^\pm = \frac{\mp \exp \int_0^L S_i^-(u) \, du \, \exp \int_0^L S_i^+(u) \, du - \exp \int_0^L S_i^-(u) \, du}{\exp \int_0^L S_i^+(u) \, du - \exp \int_0^L S_i^-(u) \, du}. \quad (A.6)$$

Consequently, differentiating (A.5) we find

$$f'(x; t^2) = \frac{S_i^-(x) \exp \left( \int_0^x S_i^+(u) \, du + \int_0^x S_i^+(u) \, du \right) - S_i^+(x) \exp \left( \int_0^x S_i^+(u) \, du + \int_0^x S_i^-(u) \, du \right) - \exp \int_0^L S_i^+(u) \, du - \exp \int_0^L S_i^-(u) \, du}{\exp \int_0^L S_i^+(u) \, du - \exp \int_0^L S_i^-(u) \, du}. \quad (A.7)$$

We are interested in the $t \to \infty$ asymptotics of both $f'(0; t^2)$ and $f'(L; t^2)$. From (A.7), we see that at $x = L$, $f'(x; t^2)$ vanishes exponentially. At $x = 0$, up to exponentially suppressed terms, we have the asymptotic relation

$$f'(0; t^2) \sim S_i^-(0) = -t + \sum_{j=1}^{\infty} s_j(0) t^{-j}. \quad (A.8)$$

Example. In the case of the linear potential $V(x) = \omega x$ considered earlier, the first eight functions $s_j$ in the expansion of $S_i^-$ constructed iteratively from the recurrence relation are shown below:

$$s_{-1}(x) = -1 \quad s_0(x) = 0 \quad s_1(x) = -\frac{\omega}{2} x$$

$$s_2(x) = -\frac{\omega}{2} x \quad s_3(x) = \frac{\omega^2}{2!} x^2 \quad s_4(x) = \frac{\omega^3}{2^2} x^3$$

$$s_5(x) = \frac{3\omega^2}{2^5} x - \frac{\omega^3}{2^3} x^3 \quad s_6(x) = -\frac{11\omega^3}{2^5} x^3.$$
Consequently,
\[ f'(0; t^2) \sim -t - \frac{\omega}{2t^2} + \frac{3\omega^2}{25t^5} + \cdots \quad (A.9) \]

References

[1] Abramowitz M and Stegun I A 1965 Handbook of Mathematical Functions With Formulas, Graphs, and Mathematical Tables (New York: Dover)
[2] Akkermans E, Comtet A, Desbois J, Montambaux G and Texier C 2000 Spectral determinant on quantum graphs Ann. Phys. 284 10–51
[3] Berkolaiko G and Keating J P 1999 Two-point spectral correlations for star graphs J. Phys. A: Math. Gen. 32 7827–41
[4] Bolte J and Endres S 2009 The trace formula for quantum graphs with general self-adjoint boundary conditions Ann. Henri Poincare 10 189–223 (arXiv:0805.3111)
[5] Carlson R 1999 Eigenvalue problems on directed graphs Trans. Am. Math. Soc. 99 4069–88
[6] Cheon T, Exner P and Turek O 2010 Approximation of a general singular vertex coupling in quantum graphs Ann. Phys. 325 548–78
[7] Comtet A, Desbois J and Texier C 2005 Functionals of the Brownian motion, localization and metric graphs J. Phys. A: Math. Gen. 38 R341–83
[8] Desbois J 2000 Spectral determinant of Schrödinger operators on graphs J. Phys. A: Math. Gen. 33 L63–7
[9] Desbois J 2001 Spectral determinant on graphs with generalized boundary conditions Eur. Phys. J. B 24 261–6
[10] Endres S and Steiner F 2010 The Berry–Keating operator on \( L^2(\mathbb{R}^+, dx) \) and compact quantum graphs with general self-adjoint realizations J. Phys. A: Math. Theor. 43 095204 (arXiv:0912.3183)
[11] Endres S and Steiner F 2011 An exact trace formula and zeta functions for an infinite quantum graph with a non-standard Weyl asymptotics J. Phys. A: Math. Theor. 44 185202
[12] Exner P 1995 Lattice Kronig–Penney models Phys. Rev. Lett. 74 3503
[13] Friedlander L 2006 Determinant of the Schrödinger operator on a metric graph Quantum Graphs and Their Applications (Contemporary Mathematics vol 415) ed G Berkolaiko, R Carlson, S A Fulling and P Kuchment (Washington, DC: American Mathematical Society) pp 151–60
[14] Fucci G, Kirsten K and Morales P 2011 Pistons modeled by potentials Cosmology, Quantum Vacuum and Zeta Functions: In Honour of Emilio Elizalde ed S D Odintsov, D Saez-Gomez and S Xambo-Descamps (Berlin: Springer) p 313 (arXiv:1106.0731)
[15] Gnutzmann S and Smilansky U 2006 Quantum graphs: applications to quantum chaos and universal spectral statistics Adv. Phys. 55 527–625
[16] Gradshteyn I S and Ryzhik I M 1994 Table of Integrals, Series and Products 5th edn (New York: Academic)
[17] Harrison J M and Kirsten K 2010 Vacuum energy, spectral determinant and heat kernel asymptotics of graph Laplacians with general vertex matching conditions Quantum Field Theory Under the Influence of External Conditions (QFEXT09) ed K A Milton and M Bordag (Singapore: World Scientific) pp 421–5 (arXiv:0912.0036)
[18] Harrison J M and Kirsten K 2011 Zeta functions of quantum graphs J. Phys. A: Math. Theor. 44 235301 (arXiv:0911.2509)
[19] Keating J P, Marklof J and Winn B 2003 Value distribution of the eigenfunctions and spectral determinants of quantum star graphs Commun. Math. Phys. 241 421–52
[20] Kirsten K and Loya P 2008 Computation of determinants using contour integrals Am. J. Phys. 76 60–4 (arXiv:0707.3755v1)
[21] Kirsten K and McKane A J 2004 Functional determinants for general Sturm–Liouville problems J. Phys. A: Math. Gen. 37 4649–70
[22] Kirsten K and McKane A J 2004 Functional determinants in the presence of zero modes Quantum Field Theory Under the Influence of External Conditions ed K A Milton (Paramus, NJ: Rinton) pp 146–51
[23] Kostrykin V, Pothoff J and Schrader R 2007 Heat kernels on metric graphs and a trace formula Adventures in Mathematics (Contemporary Mathematics vol 447) ed F Germinet and P D Hislop (Washington, DC: American Mathematical Society) pp 175–98
[24] Kostrykin V and Schrader R 1999 Kirchhoff’s rule for quantum wires J. Phys. A: Math. Gen. 32 595–630
[25] Kottos T and Smilansky U 1997 Quantum chaos on graphs Phys. Rev. Lett. 79 4794–7
[26] Kottos T and Smilansky U 1999 Periodic orbit theory and spectral statistics for quantum graphs Ann. Phys. 274 76–124
[27] Kuchment P 2002 Graph models of wave propagation in thin structures Waves Random Media 12 R1–24
[28] Kuchment P 2004 Quantum graphs: I. Some basic structures Waves Random Media 14 S107–28
[29] Kuchment P 2008 Quantum graphs: an introduction and a brief survey Analysis on Graphs and Its Applications (Proceedings of Symposia in Pure Mathematics vol 77) ed P Exner, J P Keating, P Kuchment, T Sunada and A Teplyaev (Washington, DC: American Mathematical Society) pp 291–312
[30] Roth J-P 1984 Le spectre du Laplacian sur un graphe Théorie du Potentiel (Lecture Notes in Maths vol 1096) ed G Mokobodzki and D Pinchon (Berlin: Springer) pp 521–39
[31] Texier C 2008 On the spectrum of the Laplace operator of metric graphs attached at a vertex: spectral determinant approach J. Phys. A: Math. Theor. 41 085207
[32] Texier C 2010 $\zeta$-regularised spectral determinants on metric graphs J. Phys. A: Math. Theor. 43 425203 (arXiv:1006.2163)
[33] Texier C and Montambaux G 2005 Quantum oscillations in mesoscopic rings and anomalous diffusion J. Phys. A: Math. Gen. 38 3455–71
[34] Witten E 1981 Dynamical breaking of supersymmetry Nucl. Phys. B 188 513