Inverse spectral problem for quantum graphs

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Abstract
The inverse spectral problem for the Laplace operator on a finite metric graph is
investigated. It is shown that this problem has a unique solution for graphs with
rationally independent edges and without vertices having valence 2. To prove
the result, a trace formula connecting the spectrum of the Laplace operator with
the set of periodic orbits for the metric graph is established.

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1. Introduction

Differential operators on metric graphs (quantum graphs) are a rather new and rapidly
developing area of modern mathematical physics. Such operators can be used to model
the motion of quantum particles confined to certain low-dimensional structures. This explains
recent interest in such problems due to possible applications to quantum computing and design
of nanoelectronic devices [1].

Quantum graphs are differential (self-adjoint) operators on metric graphs determined on
the functions satisfying certain boundary conditions at the vertices. Therefore, these operators
combine features of both ordinary and partial differential equations. On every edge, the
differential equation to solve is an ordinary differential equation which includes the spectral
parameter. On the other hand, the Cauchy problem on the whole graph is not solvable but for
special values of the spectral parameter and Cauchy data only. The main mathematical tool
used in this paper—the trace formula—supports this point of view. This formula establishes
the connection between the spectrum of the Laplace operator on a metric graph and *the length
spectrum*—the set of all periodic orbits on the graph. This is in complete analogy with the
semiclassical approach due to Guillemin and Melrose [19, 20] and the relations between the
spectrum of a Laplace operator on certain two-dimensional domains and operators on graphs
established in [6, 7]. Roth [31] has proven trace formula for quantum graphs using the heat
kernel approach. An independent way to derive trace formula using a scattering approach was
suggested by Gutkin, Kottos and Smilansky [21, 24]. We provide a mathematically rigorous

proof of this result. The trace formula is applied to reconstruct the graph from the spectrum of the corresponding Laplace operator. This procedure can be carried out in the case when the lengths of the edges are rationally independent and the graph has no vertices having valence 2. A rigorous proof of this fact is also provided in the current paper (theorem 2). We decided to restrict our consideration to the case of the so-called Laplace operator on metric graphs—the second derivative operator with natural or free boundary conditions at the vertices. The results proven in the current paper are stronger than those proposed in [21]: it is not required that the graph is simple, i.e. graphs with loops and multiple edges are allowed. We believe that our methods can now be extended to prove similar results for arbitrary quantum graphs with rationally independent edges.

Explicit examples constructed in [3, 21, 27] show that the inverse spectral and scattering problems for quantum graphs in general do not have a unique solution (if no restriction on the lengths of the edges is imposed).

The notion of quantum graphs was introduced in the 1980s by Gerasimenko and Pavlov [17, 18, 30]. Many important examples including graphs with higher dimensional inclusions were considered by Exner and Seba [13, 16] (see also two conference proceedings volumes [14, 15] collecting articles on this subject). The extension theory used in the current paper is similar to the one developed for multi-interval problems in [8–12]. One can find a recent reference list with historical remarks in the book [2] and volumes [25, 26] devoted entirely to quantum graphs.

The spectral problem for quantum graphs has been investigated recently by Naimark, Sobolev and Solomyak [28, 29, 32–35]. The inverse spectral problem was investigated by Gutkin and Smilansky [21] and for a special class of operators in [5]. The Borg–Levison theorem for Sturm–Liouville operators on trees was proven in [4]. The direct scattering problem was investigated by Kostrykin and Schrader [23]. The inverse scattering problem is discussed in [22, 27].

2. Basic definitions

Consider arbitrary finite metric graph Γ consisting of N edges. The edges will be identified with the intervals of the real line $\Delta_j = [x_{2j-1}, x_{2j}] \subset \mathbb{R}$, $j = 1, 2, \ldots, N$. Their length will be denoted by $d_j = |x_{2j} - x_{2j-1}|$. Let us denote by M the number of vertices that can be obtained by dividing the set $\{x_k\}_{k=1}^{2N}$ of endpoints into equivalence classes V_m, $m = 1, 2, \ldots, M$. The coordinate parametrization of the edges does not play any important role, therefore we are going to identify metric graphs having the same topological structure and the same lengths of the edges. More precisely this equivalence is described in [3, 27]. A graph Γ is called *clean* if it contains no vertices of valence 2. In what follows we are going to consider clean graphs only, since vertices of valence 2 can easily be removed by substituting the two edges joined at the vertex by one edge with length equal to the sum of the lengths of the two edges. This procedure is called *cleaning* [27].

To define the self-adjoint differential operator on Γ consider the Hilbert space of square integrable functions on Γ

$$\mathcal{H} \equiv L^2(\Gamma) = \oplus \sum_{j=1}^{N} L^2(\Delta_j) = \oplus \sum_{j=1}^{N} L^2[x_{2j-1}, x_{2j}]. \tag{1}$$

The Laplace operator on Γ is the sum of second derivative operators in each space $L^2(\Delta_j)$,

$$H = \oplus \sum_{j=1}^{N} \left(-\frac{\mathrm{d}^2}{\mathrm{d}x^2} \right)_{L^2(\Delta_j)}. \tag{2}$$

This differential expression does not determine the self-adjoint operator uniquely. Two differential operators in $L^2(\Gamma)$ are naturally associated with the differential expression (2): the minimal operator with the domain $\mathrm{Dom}(H_{\min}) = \oplus \sum_{j=1}^{N} C_0^{\infty}(\Delta_j)$ and the maximal operator $H_{\max}$ with the domain $\mathrm{Dom}(H_{\max}) = \oplus \sum_{j=1}^{N} W_2^2(\Delta_j)$, where W_2^2 denotes the Sobolev space.

All self-adjoint operators associated with (2) can be obtained by restricting the maximal operator to a subspace using certain boundary conditions connecting boundary values of the functions on Γ associated with the same vertex.

The functions from the domain $\mathrm{Dom}(H_{\max})$ are continuous and have continuous first derivatives on each edge Δ_j. The Hilbert space $\mathcal{H}$ introduced above does not reflect the connectivity of the graph. It is the boundary conditions that connect values of the function on different edges. Therefore, these conditions have to be chosen in a special way so that they reflect the connectivity of the graph. See [27] for a discussion on how the most general boundary conditions can be chosen. In the current paper, we restrict our consideration to the case of natural, or free, boundary conditions given by

$$\begin{cases} f(x_j) = f(x_k), & x_j, x_k \in V_m, \\ \sum_{x_j \in V_m} \partial_n f(x_j) = 0, & \end{cases} \quad m = 1, 2, \ldots, M, \qquad (3)$$

where $\partial_n f(x_j)$ denotes the normal derivative of the function f at the endpoint x_j. The functions satisfying these conditions are continuous at the vertices. In the case of the vertex with valence 2 conditions (3) imply that the function and its first derivative are continuous at the vertex, i.e. the vertex can be removed as described above.

The Laplace operator $H(\Gamma)$ on the metric graph Γ is the operator $H_{\max}$ given by (2) restricted to the set of functions satisfying boundary conditions (3). This operator is self-adjoint [27] and uniquely determined by the graph Γ. Therefore, the inverse spectral problem for $H(\Gamma)$ is to reconstruct the graph Γ from the set of eigenvalues.

The Laplace operator $H(\Gamma)$ can be considered as a finite rank (in the resolvent sense) perturbation of the operator $H_{\max}$ restricted to the set of functions satisfying Dirichlet boundary conditions at the vertices. This operator is equal to the orthogonal sum of the second derivative operators on the disjoined intervals and therefore has pure discrete spectrum. Hence the spectrum of the operator $H(\Gamma)$ is also pure discrete with unique accumulation point at $+\infty$. The quadratic form of the operator

$$\langle Hf, f \rangle = \sum_{j=1}^{N} \int_{x_{2j-1}}^{x_{2j}} (-f''(x))\overline{f(x)}\,\mathrm{d}x = \sum_{j=1}^{N} \int_{x_{2j-1}}^{x_{2j}} |f'(x)|^2\,\mathrm{d}x \geqslant 0$$

is non-negative and therefore the operator H is non-negative. Thus, the spectrum of H contains an infinite sequence of non-negative real numbers accumulating to $+\infty$. The kernel of the operator contains only constant functions on Γ (see lemma 1).

3. Trace formula

In this section, we establish the correspondence between the positive spectrum of the operator $H(\Gamma)$ and *the length spectrum* of the metric graph Γ—the set L of lengths of all periodic orbits of Γ. Our presentation follows essentially [21, 24], but we were able to correct a few minor mistakes making the presentation mathematically rigorous.

Let us establish the secular equation determining all positive eigenvalues of the operator H. Suppose that ψ is an eigenfunction for the operator corresponding to the positive spectral parameter $E = k^2 > 0$. Then this function is a solution to the one-dimensional Schrödinger equation on the edges $-\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} = k^2\psi$. The general solution to the differential equation on the

edge $\Delta_j = [x_{2j-1}, x_{2j}]$ with the length $d_j = |x_{2j} - x_{2j-1}|$ can be written in the basis of incoming waves as follows:

$$\psi(x) = a_{2j-1}\, e^{ik|x-x_{2j-1}|} + a_{2j}\, e^{ik|x-x_{2j}|}, \tag{4}$$

where a_m is the amplitude of the wave coming from the end point x_m.
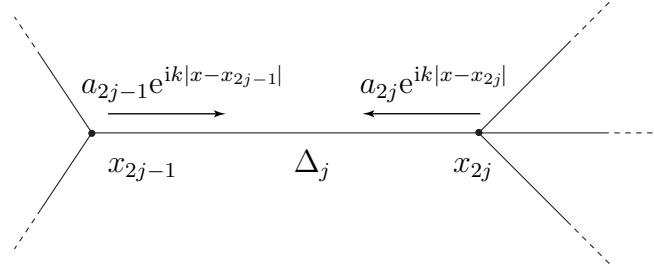
The same solution in the basis of outgoing waves possesses a similar representation

$$\psi(x) = b_{2j}\, e^{-ik|x-x_{2j}|} + b_{2j-1}\, e^{-ik|x-x_{2j-1}|},$$

where

$$\begin{pmatrix} b_{2j-1} \\ b_{2j} \end{pmatrix} = \begin{pmatrix} 0 & e^{ikd_j} \\ e^{ikd_j} & 0 \end{pmatrix} \begin{pmatrix} a_{2j-1} \\ a_{2j} \end{pmatrix}. \tag{5}$$

The following notation will be useful

$$e^j = \begin{pmatrix} 0 & e^{ikd_j} \\ e^{ikd_j} & 0 \end{pmatrix}.$$

If one introduces the $2N$-dimensional vectors of amplitudes of incoming and outgoing waves

$$\mathbf{a} = \left\{ \begin{pmatrix} a_{2j-1} \\ a_{2j} \end{pmatrix} \right\}_{j=1}^N; \qquad \mathbf{b} = \left\{ \begin{pmatrix} b_{2j-1} \\ b_{2j} \end{pmatrix} \right\}_{j=1}^N,$$

relation (5) can be written as

$$\mathbf{b} = \mathcal{E}\mathbf{a}, \qquad \text{where} \qquad \mathcal{E} = \left(\begin{array}{c|c|c} e^1 & 0 & \ldots \\ \hline 0 & e^2 & \ldots \\ \hline \vdots & \vdots & \ddots \end{array} \right) \tag{6}$$

is a block matrix composed of matrices e^j on the diagonal.

Consider any vertex $V_m = \{x_{l_1}, x_{l_2}, \ldots, x_{l_{v_m}}\}$ of valence $v_m = \mathrm{val}(V_m)$ connecting exactly v_m edges (counting multiplicities). Then knowing the amplitudes b_{l_j}, $j = 1, 2, \ldots, v_m$ of all waves $b_{l_j}\, e^{-ik|x-x_{l_j}|}$ approaching the vertex V_m, the amplitudes a_{l_j}, $j = 1, 2, \ldots, v_m$ of all waves $a_{l_j}\, e^{ik|x-x_{l_j}|}$ going out from the vertex can be calculated from the boundary conditions (3).

We introduce the notation

$$\mathbf{a}^m = \begin{pmatrix} a_{l_1} \\ a_{l_2} \\ \vdots \\ a_{l_{v_m}} \end{pmatrix}, \qquad \mathbf{b}^m = \begin{pmatrix} b_{l_1} \\ b_{l_2} \\ \vdots \\ b_{l_{v_m}} \end{pmatrix}.$$

Then the relation between the vectors $\mathbf{a^m}$ and $\mathbf{b^m}$ is described by a certain vertex scattering matrix σ^m determined by the boundary condition

$$\mathbf{a^m} = \sigma^m \mathbf{b^m}. \tag{7}$$

For natural boundary conditions the vertex scattering matrix does not depend on the energy

$$\sigma_{jk}^m = \begin{cases} \dfrac{2}{v_m}, & j \neq k, \\ \dfrac{2 - v_m}{v_m}, & j = k, \end{cases} \quad v_m \neq 1. \tag{8}$$

Observe that for $v_m = 2$ and $v_m = 1$ the scattering matrices are trivial and equal to[3] $\sigma = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ and $\sigma = 1$, respectively, which explains the reason to call the boundary conditions (3) free or natural (and the operator H the Laplace operator). For the same reason, we have to exclude vertices with valence 2 from our consideration and consider clean graphs only, since one cannot 'distinguish' vertices of valence 2 with natural boundary conditions from the other internal points of the edges. In the case $v_m = 1$ (loose endpoint), the boundary condition coincides with the Neumann condition.

The connection between the amplitudes $\mathbf{b}$ and $\mathbf{a}$ given by the vertex scattering matrices appears in a simple way if one considers the basis associated with the vertices

$$\begin{pmatrix} \mathbf{a}^1 \\ \mathbf{a}^2 \\ \vdots \\ \mathbf{a}^M \end{pmatrix} = \Sigma \begin{pmatrix} \mathbf{b}^1 \\ \mathbf{b}^2 \\ \vdots \\ \mathbf{b}^M \end{pmatrix}, \qquad \text{where} \quad \Sigma = \left(\begin{array}{c|c|c} \sigma^1 & 0 & \cdots \\ \hline 0 & \sigma^2 & \cdots \\ \hline \vdots & \vdots & \ddots \end{array} \right). \tag{9}$$

Then formulae (6) and (9) imply that the amplitudes $\mathbf{a}$ determine an eigenfunction of $H(\Gamma)$ for $E > 0$ if and only if $\mathbf{a} = \Sigma\mathcal{E}\mathbf{a}$, i.e. the matrix

$$U(k) = \Sigma\mathcal{E}(k) \tag{10}$$

has eigenvalue 1 and $\mathbf{a}$ is the corresponding eigenvector. Observe that the matrices Σ and $\mathcal{E}$ have simple representations in different bases associated with the vertices and edges respectively. Thus, the non-zero spectrum of the operator H can be calculated as zeroes of the following function:

$$f(k) = \det(U(k) - I) = 0 \tag{11}$$

on the positive axis. Let us denote the eigenvalues of the Laplace operator H in non-decreasing order as follows:

$$E_0 = k_0^2 = 0 < E_1 = k_1^2 \leqslant E_2 = k_2^2 \leqslant \dots.$$

Then the zeroes of the function $f(k)$ are situated at the points

$$k = 0, \pm\sqrt{E_1}, \pm\sqrt{E_2}, \dots.$$

(Lemma 1, see below, implies that $E_0 = 0$ has multiplicity 1). Together with the secular equation (11), we are going to consider the corresponding linear system

$$(U(k) - I)\mathbf{a} = 0, \tag{12}$$

which has non-trivial solutions if and only if (12) is satisfied.

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[3] Observe that in our parametrization, the scattering matrix $\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ corresponds to zero reflection coefficient and unit transition coefficient—no scattering occurs in that case.

Let us call by *spectral multiplicity* the multiplicity of the eigenvalue E of the operator H and by *algebraic multiplicity* the dimension of the linear space of solutions to equation (11).

The spectral and algebraic multiplicities of all non-zero eigenvalues of H coincide, since for $E \neq 0$ there is a one-to-one correspondence between **a** and $\psi(x)$ (see (4)).

Let us study the point $E = 0$ in more detail.

Lemma 1. *Let Γ be a connected metric graph with N edges. Then the point $E = 0$ is an eigenvalue for the Laplace operator H with the spectral multiplicity 1 and algebraic multiplicity $N + 1$.*

Proof. If $E = 0$ then the corresponding eigenfunction should satisfy the following equation $-\frac{d^2\psi}{dx^2} = 0$ on each edge. The solution to this equation is just a linear function. In addition, the function should satisfy the boundary conditions (3). To prove the first part of the lemma, it is enough to show that the unique eigenfunction is constant (having equal values on all edges). Assume that there is an eigenfunction which is not constant. Since such a function is linear on the edges it attains its maximum and minimum at the end points of the edges, i.e. at the vertices. Consider the vertex being the global maximum point for the function. Then the sum of the normal derivatives at this vertex is a sum of non-positive numbers but it is equal to zero. Therefore, all normal derivatives are equal to zero and the function is constant on all edges meeting at the vertex in question. It follows that the eigenfunction attains a maximum at all neighbouring vertices. Proceeding with the same argument and taking into account the continuity condition, we conclude that the function is constant on the whole graph since it is connected.

The general solutions to equation (12) are given by (4) on each edge. Now if $E = 0$ then $k = 0$ and using continuity of the eigenfunction at the vertices, the amplitudes a_j have to fulfil the relation $a_{2j-1} + a_{2j} = a_{2k-1} + a_{2k}$ where j, k are indices such that the edges Δ_j and Δ_k are connected. When the graph is connected there is always a path from Δ_1 to any other edge Δ_j. This system of equations is equivalent to the following system of $N - 1$ linearly independent equations: $a_1 + a_2 = a_{2j-1} + a_{2j}$, where $j = 2, \ldots, N$. Thus, the number of linearly independent solutions to (12) is equal to $2N - (N - 1) = N + 1$. Hence the algebraic multiplicity is $N + 1$. $\square$

Thus, the secular equation (11) gives all non-negative eigenvalues of $H(\Gamma)$ with correct multiplicities except for the point $E = 0$.

The function f is analytic in $\mathbb{C}$, because all elements of the finite matrix $U(k)$ are analytic functions of the variable k. Zeroes of this function cannot accumulate to any finite point, since f is analytic and it is not identically equal to zero. This gives another proof of the fact that the spectrum of the operator H is discrete.

Let us introduce the distribution u connected with the spectral measure

$$u \equiv \delta(k) + \sum_{n=1}^{\infty} (\delta(k - k_n) + \delta(k + k_n)).$$

For any test function $\varphi \in C_0^{\infty}(\mathbb{R})$, the value of the distribution $u[\varphi]$ can be calculated using the function f as follows:

$$u[\varphi] = \lim_{\varepsilon \to 0} \frac{1}{2\pi i} \int_{-\infty}^{\infty} \left(\frac{f'(k - i\varepsilon)}{f(k - i\varepsilon)} - \frac{f'(k + i\varepsilon)}{f(k + i\varepsilon)} \right) \varphi(k) \, dk - N\varphi(0), \qquad (13)$$

where the correction term $-N\varphi(0)$ appears due to the difference between the spectral and algebraic multiplicities at $E = 0$.

Since the function φ has compact support, say the interval $[a, b]$, the sum is in fact finite and thus it is sufficient to study the case when the support of φ contains only one zero of f, say a simple zero k_j. In this case we have

$$\int_{-\infty}^{\infty} \delta(k - k_j)\varphi(k)\,\mathrm{d}k = \lim_{\varepsilon \to 0} \frac{1}{2\pi\mathrm{i}} \int_a^b \left(\frac{f'(k - \mathrm{i}\varepsilon)}{f(k - \mathrm{i}\varepsilon)} - \frac{f'(k + \mathrm{i}\varepsilon)}{f(k + \mathrm{i}\varepsilon)} \right) \varphi(k)\,\mathrm{d}k$$

$$= \lim_{\varepsilon \to 0} \frac{1}{2\pi\mathrm{i}} \left(\int_a^{k_j - \chi} + \int_{k_j - \chi}^{k_j + \chi} + \int_{k_j + \chi}^b \right)(\ldots)\varphi(k)\,\mathrm{d}k,$$

where $\chi \ll 1$. The first and the third integrals have trivial limits

$$\lim_{\varepsilon \to 0} \left(\int_a^{k_j - \chi} + \int_{k_j + \chi}^b \right)(\ldots)\varphi(k)\,\mathrm{d}k = 0,$$

since $\frac{f'(k)}{f(k)}\varphi(k)$ is a continuous function outside $(k_j - \chi, k_j + \chi)$. We can split the middle integral into two as follows:

$$\lim_{\varepsilon \to 0} \frac{1}{2\pi\mathrm{i}} \varphi(k_j) \int_{k_j - \chi}^{k_j + \chi} (\ldots)\,\mathrm{d}k + \lim_{\varepsilon \to 0} \frac{1}{2\pi\mathrm{i}} \int_{k_j - \chi}^{k_j + \chi} (\ldots)(\varphi(k) - \varphi(k_j))\,\mathrm{d}k.$$

The integrand in the second integral is uniformly bounded, and therefore its absolute value is less than a constant times χ. The first integral can be transformed to the integral over a small circle around k_j, due to residue calculus equal to $\varphi(k_j)$. Therefore we have

$$\lim_{\varepsilon \to 0} \frac{1}{2\pi\mathrm{i}} \varphi(k_j) \int_{-\infty}^{\infty} \left(\frac{f'(k - \mathrm{i}\varepsilon)}{f(k - \mathrm{i}\varepsilon)} - \frac{f'(k + \mathrm{i}\varepsilon)}{f(k + \mathrm{i}\varepsilon)} \right) \mathrm{d}k = \varphi(k_j) = \delta(k - k_j)[\varphi].$$

If the support of φ contains several zeroes of f, then the following formula holds:

$$u[\varphi] = \frac{1}{2\pi\mathrm{i}} \int_{-\infty}^{\infty} [(\ln f(k - \mathrm{i}0))' - (\ln f(k + \mathrm{i}0))']\varphi(k)\,\mathrm{d}k - N\varphi(0). \qquad (14)$$

For any diagonalizable non-singular matrix A, the following equation holds modulo $2\pi\mathrm{i}$:

$$\ln \det A = \mathrm{Tr} \ln A. \qquad (15)$$

In the case when all entries of the matrix function $A = A(k)$ are differentiable we get the equality:

$$(\ln \det A(k))' = (\mathrm{Tr} \ln A(k))'. \qquad (16)$$

The matrix $A(k) = U(k) - I$ is diagonalizable for real k, since $U(k) = \Sigma\mathcal{E}(k)$ is unitary there. This property holds true in a certain neighbourhood of the real line, since the entries of $\mathcal{E}(k)$ are analytic functions.

Moreover, the matrix $U(k) - I = \Sigma\mathcal{E}(k) - I$ is non-singular outside the real axis because

 (i) for $\mathrm{Im}\, k > 0$, $\|U(k)\| = \|\mathcal{E}(k)\| < 1$, this implies that $\det(U - I) \neq 0$,
(ii) for $\mathrm{Im}\, k < 0$, $\|U^{-1}(k)\| = \|\mathcal{E}^{-1}(k)\| < 1$, this implies that $\det(U - I) = \det(U(I - U^{-1})) = \det U \cdot \det(I - U^{-1}) \neq 0$.

Formula (16) holds for $A(k) = U(k) - I$ and for $k \neq k_n$ from the neighbourhood of the real line.

With the function $f(k) = \det(U(k) - I)$ we have then

$$u[\varphi] + N\varphi(0) = \frac{1}{2\pi\mathrm{i}} \int_{-\infty}^{\infty} \{(\ln \det(U(k - \mathrm{i}0) - I))' - (\ln \det(U(k + \mathrm{i}0) - I))'\}\varphi(k)\,\mathrm{d}k$$

$$= \frac{1}{2\pi\mathrm{i}} \int_{-\infty}^{\infty} \{(\mathrm{Tr} \ln(U(k - \mathrm{i}0) - I))' - (\mathrm{Tr} \ln(U(k + \mathrm{i}0) - I))'\}\varphi(k)\,\mathrm{d}k$$

$$= \frac{1}{2\pi i} \int_{-\infty}^{\infty} \{\mathrm{Tr}(\ln(U(k-i0)-I))' - \mathrm{Tr}(\ln(U(k+i0)-I))'\}\varphi(k)\,dk$$

$$= \frac{1}{2\pi i} \int_{-\infty}^{\infty} \left\{\mathrm{Tr}\,\frac{U'(k-i0)}{U(k-i0)-I} - \mathrm{Tr}\,\frac{U'(k+i0)}{U(k+i0)-I}\right\}\varphi(k)\,dk.$$

Since $\|\mathcal{E}(k+i\varepsilon)\| < 1$, the norm $\|U(k+i\varepsilon)\|$ is also less than 1 and the geometric expansion can be used

$$\mathrm{Tr}\,\frac{U'(k+i\varepsilon)}{I-U(k+i\varepsilon)} = \mathrm{Tr}((I + U(k+i\varepsilon) + U^2(k+i\varepsilon) + \cdots)U'(k+i\varepsilon)).$$

In the lower half-plane $\mathrm{Im}(k - i\varepsilon) < 0$, $\|U^{-1}(k-i\varepsilon)\| < 1$ and we get

$$\mathrm{Tr}\,\frac{U'(k-i\varepsilon)}{U(k-i\varepsilon)-I} = \mathrm{Tr}\,\frac{1}{U(k-i\varepsilon)} \quad \frac{U'(k-i\varepsilon)}{I - U^{-1}(k-i\varepsilon)}$$

$$= \mathrm{Tr}\,U(k-i\varepsilon)^{-1}((I + U^{-1}(k-i\varepsilon) + U^{-2}(k-i\varepsilon) + \cdots)U'(k-i\varepsilon))$$

$$= \mathrm{Tr}((U^{-1}(k-i\varepsilon) + U^{-2}(k-i\varepsilon) + \cdots)U'(k-i\varepsilon)).$$

Putting together the last two expansions we have

$$u[\varphi] + N\varphi(0) = \frac{1}{2\pi i} \lim_{\varepsilon \to 0} \int_{-\infty}^{\infty} [\mathrm{Tr}((I + U(k+i\varepsilon) + \cdots)U'(k+i\varepsilon))$$

$$+ \mathrm{Tr}((U^{-1}(k-i\varepsilon) + U^{-2}(k-i\varepsilon) + \cdots)U'(k-i\varepsilon))]\varphi(k)\,dk.$$

Taking into account that the matrix Σ is independent of the energy one gets

$$U' = \Sigma \mathcal{E} i \mathcal{D} = iU\mathcal{D},$$

where $\mathcal{D} = \mathrm{diag}[d_1, d_1, d_2, d_2, d_3, d_3, \ldots]$ (in the basis associated with the edges). Substitution into the previous formula implies

$$u[\varphi] + N\varphi(0) = \frac{1}{2\pi i} \lim_{\varepsilon \to 0} \int_{-\infty}^{\infty} [\mathrm{Tr}((I + U(k+i\varepsilon) + U^2(k+i\varepsilon) + \cdots)U(k+i\varepsilon)i\mathcal{D})$$

$$+ \mathrm{Tr}((U^{-1}(k-i\varepsilon) + U^{-2}(k-i\varepsilon) + \cdots)U(k-i\varepsilon)i\mathcal{D})]\varphi(k)\,dk. \tag{17}$$

In the last formula one can exchange the $\lim_{\varepsilon \to 0}$ and the integral sign, since the sum under the integral is absolutely converging. To prove that one can use the fact that the test function φ has compact support and is infinitely many times differentiable and therefore its Fourier transform decays faster than any polynomial, i.e. in particular the following estimate holds

$$\left|\int_{-\infty}^{\infty} e^{i(k+i\varepsilon)d}\varphi(k)\,dk\right| \leqslant \frac{C}{d^{N+1}}, \qquad |d| > 1,$$

where C is a certain positive constant. Entries of the matrices $U(k)$ are exponential functions $e^{i(k+i\varepsilon)d_j}$. Therefore, the entries of the matrix $U^m(k+i\varepsilon)$ are equal to sums of exponentials $e^{i(k+i\varepsilon)\sum_{j=1}^m d_{\alpha_j}}$, where $\vec{\alpha} = (\alpha_1, \alpha_2, \ldots, \alpha_m)$ is an m-dimensional vector with non-negative integer coordinates less or equal to N. The number of all such vectors is less than m^{N-1}. Then the product of matrices $U^m(k)\mathcal{D}$ can be written as a finite sum with less than m^{N-1} items

$$U^m(k+i\varepsilon)\mathcal{D} = \sum_{\vec{\alpha}} B_{\vec{\alpha}}\,e^{i(k+i\varepsilon)\sum_{j=1}^m d_{\alpha_j}},$$

where the norms of the constant matrices $B_{\vec{\alpha}}$ are not greater than the norm of the matrix $U^m(k+i\varepsilon)\mathcal{D}$ equal to $\max\{d_j\}$. Therefore, the traces $|\mathrm{Tr}\,B_{\vec{\alpha}}|$ are less than $2N\max\{d_j\}$. Then

every item containing positive powers of U can be estimated as

$$\left| \int_{-\infty}^{\infty} \mathrm{Tr}[U^m(k+i\varepsilon)\mathcal{D}]\varphi(k)\,\mathrm{d}k \right| = \left| \int_{-\infty}^{\infty} \mathrm{Tr} \left[\sum_{\vec{\alpha}} B_{\vec{\alpha}}\, \mathrm{e}^{i(k+i\varepsilon)\sum_{j=1}^{m} d_{\alpha_j}} \right] \varphi(k)\,\mathrm{d}k \right|$$

$$\leqslant \sum_{\vec{\alpha}} 2N \max\{d_j\} \left| \int_{-\infty}^{\infty} \mathrm{e}^{i(k+i\varepsilon)\sum_{j=1}^{m} d_{\alpha_j}} \varphi(k)\,\mathrm{d}k \right|$$

$$\leqslant m^{N-1} 2N \max\{d_j\} \frac{C}{m^{N+1}(\min\{d_j\})^{N+1}} \leqslant \frac{K}{m^2}, \tag{18}$$

where K is another constant. Estimating the sum of negative powers of U in a similar way the following formula is now proven

$$u[\varphi] = \frac{1}{2\pi i} \int_{-\infty}^{\infty} \mathrm{Tr}((\cdots + U^{-1}(k) + I + U(k) + \ldots)i\mathcal{D})\varphi(k)\,\mathrm{d}k - N\varphi(0),$$

i.e.

$$u = \frac{1}{2\pi i} \mathrm{Tr}[(\ldots + U^{-1}(k) + I + U(k) + \ldots)i\mathcal{D}] - N\delta(k). \tag{19}$$

To calculate the trace, let us introduce the orthonormal basis of incoming waves to be $e_1 = (1, 0, 0, \ldots), e_2 = (0, 1, 0, \ldots), \ldots, e_{2N} = (\ldots, 0, 0, 1)$. By a *periodic orbit* we understand any oriented closed path on Γ. Note that the orbit so defined does not have any starting point. With any such (continuous) periodic orbit p one can associate the *discrete periodic orbit* consisting of all edges that the orbit comes across. Also let:

- $\mathcal{P}$ be the set of all periodic orbits for the graph Γ,
- $l(p)$ be the geometric length of a periodic orbit p,
- $n(p)$ be the discrete length of p—the number of edges that the orbit comes across,
- $\mathcal{P}_m^n$ be the set of all periodic orbits going through the point x_m into the interval $\Delta_{[\frac{m+1}{2}]}$, where $[\cdot]$ denotes the integer part, and having discrete length n,
- $\mathrm{prim}(p)$ denotes a primitive periodic orbit, such that p is a multiple of $\mathrm{prim}(p)$
- $d(p) = n(p)/n(\mathrm{prim}(p))$ is the degree of p.

The geometric length of an orbit is equal to the sum of lengths of the edges composing the orbit (with multiplicities of course). When the orbit goes from one edge to another it passes through a vertex and we will need to take into account the corresponding scattering coefficients. Then let us denote by $\mathcal{T}(p)$ the set of all scattering coefficients along the orbit p.

The right-hand side of (19) can be divided into three parts: identity, all positive powers of U and all negative powers of U. The first part gives

$$\frac{1}{2\pi} \mathrm{Tr}(I\mathcal{D}) = \frac{2\mathcal{L}}{2\pi} = \frac{\mathcal{L}}{\pi},$$

where $\mathcal{L} = d_1 + d_2 + \cdots + d_N$ is the total length of the graph Γ.

The contribution from all other terms can be calculated using corresponding periodic orbits. Let us consider for example the contribution from U^4:

$$\frac{1}{2\pi} \mathrm{Tr}(U^4\mathcal{D}) = \frac{1}{2\pi} \sum_{n=1}^{2N} \langle U^4 \mathcal{D} e_n, e_n \rangle.$$

Using that $\mathcal{D}e_n = d_{[\frac{n+1}{2}]}e_n$ and definition (10), the trace can be calculated

$$\frac{1}{2\pi} \mathrm{Tr}(U^4\mathcal{D}) = \frac{1}{2\pi} \sum_{n=1}^{2N} d_{[\frac{n+1}{2}]} \langle U^4 e_n, e_n \rangle$$

$$= \frac{1}{2\pi} \sum_{n=1}^{2N} d_{[\frac{n+1}{2}]} \sum_{p \in \mathcal{P}_n^4} \left(\prod_{\sigma_{ij}^m \in \mathcal{T}(p)} \sigma_{(ij)}^m \right) \mathrm{e}^{ikl(p)}.$$

Now we will sum all positive powers

$$\frac{1}{2\pi} \operatorname{Tr}[(U^1 + U^2 + U^3 + \cdots)\mathcal{D}] = \frac{1}{2\pi} \sum_{s=1}^{\infty} \sum_{n=1}^{2N} \langle U^s \mathcal{D} e_n, e_n \rangle$$

$$= \frac{1}{2\pi} \sum_{s=1}^{\infty} \sum_{n=1}^{2N} d_{[\frac{n+1}{2}]} \sum_{p \in \mathcal{P}_n^s} \left(\prod_{\sigma_{ij}^m \in \mathcal{T}(p)} \sigma_{ij}^m \right) e^{ikl(p)}$$

$$= \frac{1}{2\pi} \sum_{p \in \mathcal{P}} l(\operatorname{prim}(p)) \left(\prod_{\sigma_{ij}^m \in \mathcal{T}(p)} \sigma_{ij}^m \right) e^{ikl(p)}.$$

Similarly we have for negative powers

$$\frac{1}{2\pi} \operatorname{Tr}[(\cdots + U^{-3} + U^{-2} + U^{-1})\mathcal{D}] = \frac{1}{2\pi} \sum_{p \in \mathcal{P}} l(\operatorname{prim}(p)) \left(\prod_{\sigma_{ij}^m \in \mathcal{T}(p)} \overline{\sigma_{ij}^m} \right) e^{-ikl(p)}.$$

For the sake of simplicity one can introduce

$$\mathcal{A}_p = l(\operatorname{prim}(p)) \left(\prod_{\sigma_{ij}^m \in \mathcal{T}(p)} \sigma_{ij}^m \right), \qquad \mathcal{A}_p^* = l(\operatorname{prim}(p)) \left(\prod_{\sigma_{ij}^m \in \mathcal{T}(p)} \overline{\sigma_{ij}^m} \right). \tag{20}$$

Thus we have proved the following trace formula (21), which is a rigorous counterpart of the formula derived by Gutkin, Kottos and Smilansky in [21, 24].

Theorem 1 (trace formula). *Let $H(\Gamma)$ be the Laplace operator on a finite connected metric graph Γ, then the following two trace formulae establish the relation between the spectrum $\{k_j^2\}$ of $H(\Gamma)$ and the set of periodic orbits $\mathcal{P}$, the number of edges N and the total length $\mathcal{L}$:*

$$u(k) \equiv \delta(k) + \sum_{n=1}^{\infty} (\delta(k - k_n) + \delta(k + k_n))$$

$$= -N\delta(k) + \frac{\mathcal{L}}{\pi} + \frac{1}{2\pi} \sum_{p \in \mathcal{P}} (\mathcal{A}_p e^{ikl(p)} + \mathcal{A}_p^* e^{-ikl(p)}), \tag{21}$$

and

$$\hat{u}(l) \equiv 1 + \sum_{n=1}^{\infty} \left(e^{-ik_n l} + e^{ik_n l} \right) = -N + 2\mathcal{L}\delta(l) + \sum_{p \in \mathcal{P}} (\mathcal{A}_p \delta(l - l(p)) + \mathcal{A}_p^* \delta(l + l(p))) \tag{22}$$

where $\mathcal{A}_p$, $\mathcal{A}_p^*$ are independent of the energy complex numbers given by (20).

The second formula (22) is just a Fourier transform of (21). If the graph is not clean, then the coefficients $\mathcal{A}_p$ containing reflections from the vertices of valence 2 are equal to zero. If the graph is clean, then (8) implies that all coefficients $\mathcal{A}_p$ are different from zero, but it may happen that the singular support of $\hat{u}(l)$ does not contain lengths of all periodic orbits (see the following section).

4. The inverse spectral problem

In this section we are going to apply formula (22) to prove that the inverse spectral problem has a unique solution for clean finite connected metric graphs, provided the lengths of the edges are rationally independent.

The set L of lengths of all periodic orbits is usually called the length spectrum. In principle, formula (22) allows one to recover the length spectrum (of periodic orbits) from the energy spectrum (of the Laplace operator H). But this relation is not straightforward and we are able to prove it in certain special cases only (see the following section). Formula (22) implies directly that the spectrum of a graph allows one to recover the lengths l of all periodic orbits from the *reduced length spectrum* $L' \subset L$ defined as

$$L' = \left\{ l : \left(\sum_{\substack{p \in \mathcal{P} \\ l(p)=l}} \mathcal{A}_p \right) \neq 0 \right\}. \tag{23}$$

Lemma 2. *Let Γ be a connected finite clean metric graph with rationally independent lengths of edges. The reduced length spectrum L' contains at least the following lengths:*

- *the shortest orbit formed by any interval Δ_j only (i.e. d_j or $2d_j$ depending on whether Δ_j forms a loop or not);*
- *the shortest orbit formed by any two neighbouring edges Δ_j and Δ_k only (i.e. $2(d_j + d_k), d_j + 2d_k, 2d_j + d_k, d_j + d_k$ depending on how these edges are connected to each other).*

Proof. Note that if the graph is clean and there is a unique periodic orbit p_0 of a certain length $l(p_0)$ then the corresponding sum degenerates and is different from zero:

$$\sum_{\substack{p \in \mathcal{P} \\ l(p)=l(p_0)}} \mathcal{A}_p = \mathcal{A}_{p_0} \neq 0. \tag{24}$$

If there are several, say r, orbits having the same length as p_0 and all $\mathcal{A}$-coefficients are equal, then the sum is different from zero:

$$\sum_{\substack{p \in \mathcal{P} \\ l(p)=l(p_0)}} \mathcal{A}_p = r\mathcal{A}_{p_0} \neq 0. \tag{25}$$

- In the case Δ_j is a loop, there are two orbits of length d_j with equal coefficients $\mathcal{A}$. If Δ_j does not form a loop, then the shortest orbit is unique and has length $2d_j$.
- Suppose that neither Δ_j nor Δ_k forms a loop and they do not form a double edge. Then the shortest possible length of an orbit formed by Δ_j and Δ_k is $2(d_j + d_k)$ and such orbit is unique.

  Suppose that exactly one of the two neighbouring edges, say Δ_j, forms a loop. Then there are two orbits having the shortest possible length $d_j + 2d_k$ and the corresponding $\mathcal{A}$-coefficients are equal.

  Suppose that Δ_j and Δ_k form a double edge. Then there are two orbits with the shortest possible length $d_j + d_k$ and the corresponding $\mathcal{A}$-coefficients are equal.

  Suppose that both Δ_j and Δ_k form loops. Then the number of orbits having the shortest length $d_j + d_k$ is four and the $\mathcal{A}$-coefficients are equal.

All possible cases have been considered. $\qquad\square$

We are going to show now that the knowledge of the reduced length spectrum together with the total length of the graph is enough to reconstruct the graph. The first step in this direction is to recover the lengths of the edges from the total length of the graphs and the set L'. The following result can be proven by refining the method of Gutkin–Smilansky [21].

Lemma 3. *Let the lengths of the edges of a clean finite connected metric graph Γ be rationally independent. Then the total length $\mathcal{L}$ of the graph and the reduced length spectrum L' (defined by (23)) determine the lengths of all edges and whether these edges form loops or not.*

Proof. Consider the finite subset L'' of $L' \subset L$ consisting of all lengths less than or equal to $2\mathcal{L}$

$$L'' = \{l \in L' : l \leqslant 2\mathcal{L}\}.$$

This finite set contains at least one of the numbers d_j or $2d_j$. Therefore, there exists a basis $s_1, s_2, \ldots, s_N$, such that every length $l \in L''$ (as well as from L) can be written as a half-integer combination of s_j

$$l = \frac{1}{2}\sum_{j=1}^{N} n_j s_j, \qquad n_j \in \mathbb{N}.$$

Such a basis is not unique, especially if the graph has loops. Any two bases $\{s_j\}$ and $\{s'_j\}$ are related as follows: $s_j = n_j s'_{i_j}, n_j = \frac{1}{2}, 1, 2$, where $i_1, i_2, \ldots, i_N$ is a permutation of $1, 2, \ldots, N$. Then among all possible bases, consider a basis with the shortest total length $\sum_{j=1}^{N} s_j$.

The total length of the graph $\mathcal{L}$ can also be written as a sum of s_j with the coefficients equal to 1 or 1/2

$$\mathcal{L} = \sum_{j=1}^{N} \alpha_j s_j, \qquad \alpha_j = 1, 1/2. \tag{26}$$

The coefficients in this sum are equal to 1 if s_j is equal to the length of a certain edge Δ_j, i.e. when the edge forms a loop. The coefficient 1/2 appears if s_j is equal to double the length of an edge. In this case the edge does not form a loop. Therefore, the lengths of the edges up to permutation can be recovered from (26) using the formula $d_j = \alpha_j s_j, j = 1, 2, \ldots, N$. To check whether an edge Δ_j forms a loop or not it is enough to check whether d_j belongs to L' or not. $\square$

Once the lengths of all edges are known, the graph can be reconstructed from the reduced length spectrum. Lemma 2 implies that looking at the reduced length spectrum L' one can determine whether any two edges Δ_j and Δ_k are neighbours or not (have at least one common end point): the edges Δ_j and Δ_k are neighbours if and only if L' contains at least one of the lengths $d_j + d_k, 2d_j + d_k, d_j + 2d_k$, or $2(d_j + d_k)$.

Lemma 4. *Every clean finite connected metric graph Γ can be reconstructed from the set $D = \{d_j\}$ of the lengths of all edges and the reduced length spectrum L'—the subset of all periodic orbits determined by (23), provided that d_j are rationally independent.*

Proof. Let us introduce the set of edges $E = \{\Delta_j\}_{j=1}^{N}$ uniquely determined by $D = \{d_j\}$. We shall prove the lemma for simple graphs first. A graph is called *simple* if it contains no loops and no multiple edges. From an arbitrary graph one can obtain a simple graph by cancelling all loops and choosing only one edge from every multiple one:

(i) If $d_k \in L'$ then the corresponding edge is a loop. Then remove Δ_k from E and all lengths containing d_k from L'.

(ii) If $d_k + d_j \in L'$ then there exists a double edge composed of Δ_j and Δ_k (since the loops have already been removed). Then remove either Δ_j or Δ_k from E and also all lengths containing the chosen length from L.

The new subsets $E^* \subset E$ containing $N^* \leqslant N$ elements and $L^* \subset L'$ obtained in this way correspond to a simple subgraph $\Gamma^* \subset \Gamma$ which can be obtained from Γ by removing all loops and reducing all multiple edges. One obtains different Γ^* by choosing different edges to be left during the reduction.

The reconstruction will be done iteratively and we will construct an increasing finite sequence of subgraphs such that $\Gamma_1 \subset \Gamma_2 \subset \cdots \Gamma_{N^*} = \Gamma^*$. The corresponding subsets of edges will be denoted by E_k.

For $k = 1$ take the graph Γ_1 consisting of one edge, say Δ_1. By looking at L' pick up any edge, say Δ_2, which is a neighbour of Δ_1. Attach it to any endpoint of Δ_1 to get the graph Γ_2.

Suppose that connected subgraph Γ_k consisting of k edges ($k \geqslant 2$) is reconstructed. Pick up any edge, say Δ_{k+1}, which is a neighbour of at least one of the edges in Γ_k. Let us denote by E_k^{nbh} the subset of E_k of all edges which are neighbours of Δ_{k+1}. We have to identify one or two vertices in Γ_k to which the new Δ_{k+1} is attached. Every such vertex is uniquely determined by listing the edges joined at this vertex, since the subgraph Γ_k is simple, connected and contains at least two edges. Therefore, we have to separate E_k^{nbh} into two classes of edges attached to each endpoint of Δ_{k+1}. (One of the two sets can be empty, which corresponds to the case that the edge Δ_{k+1} is attached to Γ_k at one vertex only.)

Take any two edges from E_k^{nbh}, say Δ' and Δ''. The edges Δ' and Δ'' belong to the same class if and only if:

- Δ' and Δ'' are neighbours themselves and
- $d' + d'' + d_{k+1} \notin L'$, i.e. the edges Δ', Δ'' and Δ_{k+1} do not build a cycle. Note that if Δ', Δ'' and Δ_{k+1} form a cycle, then there are two periodic orbits having length $d' + d'' + d_{k+1}$ and the corresponding $\mathcal{A}$-coefficients are equal, which implies that $d' + d'' + d_{k+1} \in L'$.

In this way we either separate E_k^{nbh} into two classes of edges or E_k^{nbh} consists of edges joined at one vertex. In the first case the new edge Δ_{k+1} connects the two unique vertices determined by the subclasses. In the second case Δ_{k+1} is attached by one endpoint to Γ_k at the vertex uniquely determined by E_k^{nbh}. Since the graphs with different orientations of the edges are equivalent it does not matter which particular end point of the interval Δ_{k+1}, x_{2k+1} or x_{2k+2}, is attached to the chosen vertex of Γ_k.

Denote the graph obtained in this way by Γ_{k+1}.

Since the graph Γ^* is connected and finite after N^* steps one arrives at $\Gamma_{N^*} = \Gamma^*$.

It remains to add all loops and multiple edges to reconstruct the initial graph Γ. Suppose that the reconstructed subgraph Γ^* is not trivial, i.e. consists of more than one edge. Then every vertex is uniquely determined by listing all edges joined at it. Check first to which vertex the loop Δ_n is connected by checking if periodic orbits of the length $d_n + 2d_j$ belong to L' or not. All such edges Δ_j determine the unique vertex to which Δ_n should be adjusted. To reconstruct multiple edges check whether $d_m + d_j$ is from L', where $\Delta_j \in E^*$. Substitute all such edges Δ_j with corresponding multiple edges.

In the case Γ^* is trivial, the proof is an easy exercise. $\qquad\square$

Our main result can be obtained as a straightforward implication of lemmas 3 and 4.

Theorem 2. *The spectrum of a Laplace operator on a metric graph determines the graph uniquely, provided that*

- *the graph is clean, finite and connected,*
- *the edge lengths are rationally independent.*

Proof. The spectrum of the operator determines the left-hand side of the trace formula (21). Formula (22) shows that the spectrum of the graph determines the total length of the graph and

the reduced length spectrum. Lemma 3 implies that the lengths of all edges can be extracted from these quantities under the conditions of the theorem. It follows from lemma 4 that the whole graph can be reconstructed provided that its edges are rationally independent and it is clean, finite and connected. □

One can easily remove the condition that the graph is connected. The result can be generalized to include more general differential operators on the edges and boundary conditions at the vertices. Rigorous proofs of these results will be a subject of a forthcoming publications.

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