## Determinant of the Schrödinger Operator on a Metric Graph

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ABSTRACT. In the paper, we derive a formula for computing the determinant of a Schrödinger operator on a compact metric graph. This formula becomes very explicit in the case of the Laplacian with the Neumann boundary conditions.

#### 1. Introduction

Let G be a metric graph. This means that each edge of G is being considered as a segment of certain length. Throughout this paper, we assume that G has a finite number of edges, and the length of each edge is finite. We also assume that G is connected. Let V be the set of all vertices, and let E be the set of all edges. If  $e \in E$ , then l(e) is the length of the edge e. We allow multiple edges and loops. Though, in this paper, edges are not oriented, it is covenient to treat each edge as a pair of oppositely oriented edges. If an orientation of an edge is fixed, then one can talk about the initial and the terminal vertex of the edge, and one can fix a coordinate  $x_e$  on e that varies from 0 at the initial vertex to l(e) at the terminal vertex. If e is an edge then  $v \prec e$  will mean that v is an initial vertex of e. For two vertices, v and w, we denote by [v, w] the set of all edges connecting v and w. If v = w then [v, v] is the set of all loops incident to v. The degree of a vertex v is the number of oriented edges e such that  $v \prec e$ . Roughly speaking, the degree of a vertex is the number of edges that are incident to this vertex; however, each loop should be counted twice.

By  $C^{\infty}(G)$  we denote the set of continuous functions on G that belong to  $C^{\infty}$  on each closed edge;  $L^{2}(G)$  is the set of all functions on G that belong to  $L^{2}$  on each edge. One defines the  $L^{2}$ -norm of a function by

$$||f||^2 = \sum_{e \in E} \int_e |f(x_e)|^2 dx_e.$$

In the last formula, for each edge, one chooses an orientation; the result is clearly independent of these choices. The operator  $\Delta : C^{\infty}(G) \to L^2(G)$  is defined by the

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formula

$$(\Delta f)(x_e) = \frac{d^2 f(x_e)}{dx_e^2}$$

on each edge e. The result does not depend on the choice of an orientation of e. The space  $H^2(G)$  is defined as the closure of  $C^{\infty}(G)$  with respect to the norm

$$||f||_2^2 = ||f||^2 + ||\Delta f||^2.$$

Notice that Sobolev's embedding theorem implies that  $H^2(G)$ -functions belong to  $C^1$  on each closed edge. In addition, they are continuous on G. The operators r and j acting from  $H^2(G)$  to  $\mathbb{C}^{|V|}$  are defined by formulas

$$rf = (f(v))_{v \in V}; \quad jf = \left(\sum_{e \succ v} -\frac{\partial f}{\partial x_e}(v)\right)_{v \in V}.$$

In words, the operator r assigns to a function the vector of its values at vertices of the graph; the operator j assigns to a function the vector, each component of which is the total flux through the corresponding vertex.

Let q(x) be a continuous function on G that is smooth on each closed edge, and let A be a  $|V| \times |V|$  matrix. We define an operator  $H_A$  as an operator in  $L^2(G)$ that acts on functions by the formula

$$Hf(x) = -\Delta f(x) + q(x)f(x),$$

and the domain of which is

$$\mathcal{D}(H_A) = \{ f \in H^2(G) : (j + Ar)f = 0 \}$$

The boundary condition with A = 0 has several names; the most common ones are standard, Neumann, Kirchhoff. The corresponding operator will be denoted by  $H_0$ . The goal of this paper is to provide a formula for computing the determinant of the operator  $H_A$ . We will need the operator H with the Dirichlet boundary conditions rf = 0. This operator will be denoted by  $H_D$ . Notice that  $H_D$  is the direct sum of Schrödinger operators on edges with the Dirichlet conditions.

First, we have to recall the definition of the determinant. The operator  $H_A$  is an elliptic operator of order 2; its spectrum is discrete. In general,  $H_A$  is not self-adjoint, but the eigenvalues  $\lambda_k$  of  $H_A$  behave asymptotically like eigenvalues of  $H_0$ ; according to Weyl's law,

$$\lambda_k \sim \frac{\pi^2}{L^2} k^2$$

where  $L = \sum_{e} l(e)$  is the total length of the graph G. For almost all angles  $\theta$ ,  $0 < \theta < 2\pi$ , the ray

$$\Gamma_{\theta} = \{ z = re^{i\theta} : r > 0 \}$$

is free from eigenvalues  $\lambda_k$ . Such an angle will be called an admissible angle. One defines the  $\zeta$ -function of  $H_A$  by the formula

$$\zeta_{\theta}(z) = \sum_{\lambda_k \neq 0} \lambda_k^{-z};$$

the cut along  $\Gamma_{\theta}$  is used for determining values of complex powers. This  $\zeta$ -function is a holomorphic function in the half-plane  $\Re z > 1/2$ . It is known that  $\zeta_{\theta}(z)$  admits an analytic continuation to a meromorphic function in the whole complex plane that may have simple poles at the points (1/2) - n where n is a non-negative integer.

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According to Ray and Singer [RS], the modified determinant of the operator  $H_A$  is defined by the formula

$$\log \det' H_A = -\zeta_{\theta}'(0).$$

We use the adjective "modified" to emphasize that the zero eigenvalues of  $H_A$  are disregarded. If  $\theta_1 > \theta_2$  are two admissible angles then

$$\zeta_{\theta_1}'(0) - \zeta_{\theta_2}'(0) = 2\pi i m$$

where m is the number of eigenvalues  $\lambda_k$ , the argument of which lies between  $\theta_1$ and  $\theta_2$ . Therefore, the value of the modified determinant does not depend on the choice of an admissible angle. In what follows, the angle  $\theta$  will be supressed in notations. We define the determinant of  $H_A$  to be equal the modified determinant if  $H_A$  is invertible; otherwise, det  $H_A = 0$ .

To formulate the main theorem, we have to introduce the Dirichlet-to-Neumann operator. The Poisson operators  $P(\lambda)$  and  $Q_A(\lambda)$  map  $\mathbb{C}^{|V|}$  into  $C^{\infty}(G)$ . To a vector  $\alpha \in \mathbb{C}^{|V|}$ , they assign the solution of the equation

$$(H+\lambda)f = 0$$

that satisfy the boundary conditions  $rf = \alpha$ , for the operator  $P(\lambda)$ , and  $(j+Ar)f = \alpha$ , for the operator  $Q_A(\lambda)$ . Notice that the Poisson operators are defined not for all values of  $\lambda$ . Namely,  $P(\lambda)$  is defined if  $-\lambda$  does not belong to the spectrum of  $H_D$ , and  $Q_A(\lambda)$  is defined if  $-\lambda$  does not belong to the spectrum of  $H_A$ . Finally, the Dirichlet-to-Neumann operator

$$R(\lambda): \mathbb{C}^{|V|} \to \mathbb{C}^{|V|}$$

is defined as

$$R(\lambda) = jP(\lambda).$$

The main result of this paper is the following theorem.

THEOREM 1. Let d(v) be the degree of a vertex v. Then

(1.1) 
$$\det(H_A + \lambda) = \frac{1}{\prod_{v \in V} d(v)} \det(R(\lambda) + A) \det(H_D + \lambda).$$

The determinant of operators on quantum graphs has been studied in a number of papers, e.g. see [D1,2], [ACDMT]. Some of the formulas derived in that papers are similar to ours, though the normalization constants are different.

Let us make several remarks concerning formula (1.1). First, the operator  $R(\lambda)$  is not defined if  $\lambda = -\mu_k$  where  $\mu_k$  is a point of the Dirichlet spectrum for H. Suppose that a Dirichlet eigenvalue  $\mu_k$  has multiplicity  $m_k$ . Then, as  $\lambda \to -\mu_k$ , exactly  $m_k$  eigenvalues of  $R(\lambda)$  go to infinity, and det $(R(\lambda) + A)$  has a pole of order  $m_k$  at the point  $\mu_k$ . On the other hand, det $(H_D + \lambda)$  has a zero of order  $m_k$  at  $\lambda = -\mu_k$ . Therefore, the right hand side of (1.1) is an entire function.

The second remark is that the expression on the right in (1.1) is computable in the sense that to find its value one has to be able to perform two operations: solving ODEs and computing determinants of square matrices.  $R(\lambda)$  is a  $|V| \times |V|$ -matrix; to find its entries, one has to solve some ODEs. As it has already been mentioned, the operator  $H_D + \lambda$  is the direct sum of operators on closed edges; therefore,

(1.2) 
$$\det(H_D + \lambda) = \prod_{e \in E} \det(-\Delta + q(x_e) + \lambda)_D.$$

The determinant of a Schrödinger operator, with the Dirichlet boundary conditions, on a segment can be computed in the following way ([F1], [BFK1]): Let  $u(x_e)$  solve the initial value problem

(1.3) 
$$-u'' + (q(x_e) + \lambda)u = 0, \quad u(0) = 0, \quad u'(0) = 1.$$

Then

(1.4) 
$$\det(-\Delta + q(x_e) + \lambda)_D = 2u(l(e)).$$

Let us now treat one of the most important cases q(x) = 0, A = 0,  $\lambda = 0$ . This is the case of the determinant of the Neumann Laplacian on G. The determinant itself equals 0 because the Neumann Laplacian has a zero mode. The operator R(0)has a zero mode as well; it is

$$\beta = \frac{1}{\sqrt{|V|}}(1, \dots, 1).$$

Our goal is to compute the modified determinant of  $-\Delta_0$ . We will use the formula (1.1) with  $\lambda \neq 0$ , and take the limit  $\lambda \to 0$ . First,

$$\det'(-\Delta_0) = \lim_{\lambda \to 0} \frac{\det(-\Delta_0 + \lambda)}{\lambda}$$

Secondly, it follows from (1.3) and (1.4) that

$$\det(-\Delta_D) = 2^{|E|} \prod_{e \in E} l(e).$$

Therefore,

(1.5) 
$$\det'(-\Delta_0) = 2^{|E|} \frac{\prod_{e \in E} l(e)}{\prod_{v \in V} d(v)} \lim_{\lambda \to 0} \frac{\det R(\lambda)}{\lambda}.$$

As  $\lambda \to 0$ , one eigenvalue of  $R(\lambda)$  approaches 0; we denote it by  $\nu(\lambda)$ . One has

(1.6) 
$$\lim_{\lambda \to 0} \frac{\det R(\lambda)}{\lambda} = \dot{\nu}(0) \det' R(0)$$

where det'R(0) is the product of non-zero eigenvalues of R(0). By the "dot" we denote the derivative with respect to  $\lambda$ . The Rayleigh formula (e.g., see [K]) says that

(1.7) 
$$\dot{\nu}(0) = (\dot{R}(0)\beta,\beta) = \frac{1}{|V|} \sum_{v,w=1}^{|V|} \dot{R}(0)_{vw}.$$

Let v and w be two different vertices of G. Then

$$R(\lambda)_{vw} = \sum_{e \in [w,v]} u'_e(l(e))$$

Here the sum is taken over all edges that go from w to v, and  $u_e(x)$  is the solution of the boundary value problem

(1.8) 
$$u_e''(x) = \lambda u_e(x), \quad u_e(0) = 1, \quad u_e(l(e)) = 0$$

on the interval [0, l(e)]. When  $\lambda = 0$ ,

$$u_e(x) = \frac{l(e) - x}{l(e)}.$$

We differentiate (1.8) in  $\lambda$  and set  $\lambda = 0$ :

$$\dot{u}_e''(x) = u_e(x), \quad \dot{u}_e(0) = \dot{u}_e(l(e)) = 0.$$

The solution of the last problem is

(1.9) 
$$\dot{u}_e(x) = \frac{(l(e) - x)^3}{6l(e)} - \frac{l(e)}{6}((l(e) - x)),$$

and

$$\dot{u}_e'(l(e)) = \frac{l(e)}{6}.$$

We conclude that, for  $v \neq w$ ,

(1.10) 
$$\dot{R}(0)_{vw} = \sum_{e \in [w,v]} \frac{l(e)}{6}.$$

To find  $\dot{R}(0)_{vv}$ , one has to take into account both the edges connecting v and w, with  $w \neq v$ , and loops that start and terminate at v. The computation of a contribution of an edge [v, w] with  $v \neq w$  is the same as the computation from the previous paragraph; the only difference is that one has to take  $-\dot{u}'_e(0)$  where the function  $\dot{u}_e(x)$  is given by (1.9). The value is l(e)/3. For a loop, one has to solve the problem

$$u''_e(x) = \lambda u_e(x), \quad u_e(0) = u_e(l(e)) = 1$$

Its solution is

$$u_e(x) = \frac{\cosh(\sqrt{\lambda}(x - (l(e)/2)))}{\cosh(\sqrt{\lambda}l(e)/2)}$$

The contribution of the loop to  $R(\lambda)_{vv}$  equals

$$u'_e(l(e)) - u'_e(0) = 2\sqrt{\lambda} \tanh(\sqrt{\lambda}l(e)/2).$$

The  $\lambda$ -derivative of this function at  $\lambda = 0$  equals l(e). Therefore,

(1.11) 
$$\dot{R}(0)_{vv} = \sum_{e \in [v,w], v \neq w} \frac{l(e)}{3} + \sum_{e \in [v,v]} l(e).$$

From (1.10) and (1.11), we immediately conclude that

$$\sum_{v,w=1}^{|V|} \dot{R}(0)_{vw} = L = \sum_{e \in E} l(e).$$
(1.12)

Let us summarize our computations in

THEOREM 2. Let L be the total length of the graph G. Then

$$\det'(-\Delta_0) = 2^{|E|} \frac{L}{|V|} \frac{\prod_{e \in E} l(e)}{\prod_{v \in V} d(v)} \det' R(0).$$

Finally, we remark that the entries of the matrix R(0) are easily computable. One has

$$R(0)_{vw} = -\sum_{e \in [v,w]} \frac{1}{l(e)}$$

when  $v \neq w$ , and

$$R(0)_{vv} = \sum_{e \succ v; \text{ not } a \text{ loop}} \frac{1}{l(e)}.$$

# 2. Proof of Theorem 1

We introduce three functions

$$w_A(\lambda) = \log \det(H_A + \lambda),$$
  
 $w_D(\lambda) = \log \det(H_D + \lambda),$ 

and

$$\sigma_A(\lambda) = \operatorname{tr} \log(R(\lambda) + A).$$

To define the logarithms, we use an admissible angle that is suppressed in our notations. These functions are holomorphic functions of  $\lambda$  outside of the points  $-\lambda_k$  and  $-\mu_k$ . We recall that  $\{\lambda_k\}$  is the spectrum of  $H_A$  and  $\{\mu_k\}$  is the spectrum of  $H_D$ . The proof of theorem 1 consists of two parts (compare with [BFK1,2].) First, we will prove the following lemma.

LEMMA 1. One has

(2.1) 
$$\dot{w}_A(\lambda) = \dot{\sigma}_A(\lambda) + \dot{w}_D(\lambda).$$

Lemma 1 implies immediately that

(2.2) 
$$\det(H_A + \lambda) = c \det(R(\lambda) + A) \det(H_D + \lambda).$$

To find the value of the constant c in (2.2), we will study the asymptotic behavior of the functions  $w_A(\lambda)$ ,  $w_D(\lambda)$ , and  $\sigma_A(\lambda)$  as  $\lambda \to \infty$ . It follows from [F2] and [V] that both the functions  $w_A(\lambda)$  and  $w_D(\lambda)$  admit a complete asymptotic expansion as  $\lambda \to \infty$ . Moreover, constant terms in these expansions vanish. Therefore, the function  $\sigma_A(\lambda)$  also admits a complete asymptotic expansion as  $\lambda \to \infty$ . It  $c_0$  is the constant term in this expansion then

(2.3) 
$$c = e^{-c_0}$$
.

The second part of the proof of theorem 1 is computing the value of  $c_0$ .

PROOF OF LEMMA 1. One has

(2.4) 
$$\dot{\sigma}_A(\lambda) = \operatorname{tr}[(R(\lambda) + A)^{-1}\dot{R}(\lambda)] \\ = \operatorname{tr}[(R(\lambda) + A)^{-1}j\dot{P}(\lambda)].$$

Recall that  $P(\lambda)$  is a Poisson operator; it assigns the solution of the problem

(2.5) 
$$(H+\lambda)u = 0, \quad u(v) = \alpha_v$$

to a vector  $\alpha = \{\alpha_v\}, v \in V$ . One differentiates (2.5) with respect to  $\lambda$ :

$$(H+\lambda)\dot{u} + u = 0, \quad \dot{u}(v) = 0, \ v \in V.$$

Therefore,

(2.6) 
$$\dot{P}(\lambda) = -(H_D + \lambda)^{-1} P(\lambda).$$

The Poisson operator  $Q_A(\lambda)$  assigns the solution of the problem

(2.7) 
$$(H+\lambda)u = 0, \quad (j+Ar)u = \alpha$$

to a vector  $\alpha = \{\alpha_v\}, v \in V$ , and  $rQ_A(\lambda)$  gives the vector of values of the solution of (2.7) at the vertices; in other words, it maps the vector (j + Ar)u for a solution to  $(H + \lambda)u = 0$  into the vector ru. The operator  $R(\lambda) + A$  does exactly the opposite. Therefore,

(2.8) 
$$(R(\lambda) + A)^{-1} = rQ_A(\lambda).$$

We summarize (2.4), (2.6), and (2.8):

(2.9) 
$$\dot{\sigma}_A(\lambda) = -\operatorname{tr}[rQ_A(\lambda)j(H_D + \lambda)^{-1}P(\lambda)] \\ = -\operatorname{tr}[P(\lambda)rQ_A(\lambda)j(H_D + \lambda)^{-1}].$$

ŀ

In the last equality, we used the main property of the trace. There is an issue of whether the operator from the last line in (2.9) is of the trace class. We will see in a moment that it belongs to the trace class indeed. Notice that

$$P(\lambda)rQ_A(\lambda) = Q_A(\lambda).$$

Indeed, for a vector  $\alpha \in \mathbb{C}^{|V|}$ ,  $Q_A(\lambda)\alpha$  is a solution of the equation  $(H + \lambda)u = 0$ . If one takes the restriction of this solution to vertices, and then applies  $P(\lambda)$  to this restriction, one gets the same solution u(x). Therefore,

(2.10) 
$$\dot{\sigma}_A(\lambda) = -\text{tr}[Q_A(\lambda)j(H_D + \lambda)^{-1}].$$

We claim that

(2.11) 
$$Q_A(\lambda)j(H_D+\lambda)^{-1} = (H_D+\lambda)^{-1} - (H_A+\lambda)^{-1}.$$

It follows from (2.11) that the operator from the last line in (2.9) is of the trace class, and commuting operators under the trace in (2.9) is legitimate. Notice that  $r(H_D + \lambda)^{-1} = 0$ ; so

$$Q_A(\lambda)j(H_D + \lambda)^{-1} = Q_A(\lambda)(j + Ar)(H_D + \lambda)^{-1}$$

Let u(x) be a function on G, and

$$(H_D + \lambda)^{-1}u = g, \quad Q_A(\lambda)(j + Ar)(H_D + \lambda)^{-1}u = h.$$

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Then

$$(H+\lambda)g = u, \quad r(g) = 0,$$

and

$$(H+\lambda)h = 0, \quad (j+Ar)h = (j+Ar)g$$

For the difference, h - g, one gets

$$(H + \lambda)(h - g) = -u, \quad (j + Ar)(h - g) = 0.$$

Therefore,

 $h - g = -(H_A + \lambda)^{-1}u,$ 

and

$$h = (H_D + \lambda)^{-1}u - (H_A + \lambda)^{-1}u$$

This completes the proof of (2.11). The statement of the lemma follows from (2.10), (2.11) and

$$\dot{w}_*(\lambda) = \det(H_* + \lambda)^{-1}.$$

Here \* stands for either D or A.

Now, we turn to computing  $c_0$ , the constant term in the asymptotic expansion of  $\sigma_A(\lambda)$  as  $\lambda \to \infty$ .

LEMMA 2. Let D be a diagonal matrix with elements d(v) on the diagonal. Then

(2.12) 
$$R(\lambda) = \sqrt{\lambda}D + O(1)$$

as  $\lambda \to \infty$ .

Lemma 2 implies that

$$R(\lambda) + A = \sqrt{\lambda}D\left(1 + O\left(\lambda^{-1/2}\right)\right),$$

and, therefore,

$$\sigma_A(\lambda) = \frac{|V|}{2} \log \lambda + \log \det D + O(\lambda^{-1/2}).$$

We conclude that

$$c_0 = \log \det D = \sum_{v \in V} \log d(v).$$

The statement of Theorem 1.1 follows from (2.2), (2.3), and the last formula.

PROOF OF LEMMA 2. Let  $v, w \in V$ , and let  $e \in [v, w]$ . First, we assume that  $v \neq w$ . To compute the contribution of e to  $R(\lambda)_{vw}$  and its contribution to  $R(\lambda)_{ww}$ , one has to solve the boundary value problem

(2.13) 
$$-u'' + \lambda u + q(x)u = 0, \quad u(0) = 0, \quad u(l) = 1;$$

the contributions are -u'(0) and u'(l), respectively. We have suppressed e in notations: l = l(e),  $x = x_e$ . The solution of (2.13) can be looked for in the form

(2.14) 
$$u(x) = \frac{\sinh(\sqrt{\lambda}x)}{\sinh(\sqrt{\lambda}l)} + g(x)$$

where

(2.15) 
$$-g'' + (\lambda + q(x))g = -q(x)\frac{\sinh(\sqrt{\lambda}x)}{\sinh(\sqrt{\lambda}l)} = h(x), \quad g(0) = g(l) = 0.$$

The function h(x) is uniformly bounded as  $\lambda \to \infty$ ; therefore the  $L^2$  norm of g(x) is bounded as  $\lambda \to \infty$ . Actually,  $||g|| = O(1/\lambda)$ . One can re-write (2.15) in the form

$$-g'' + \lambda g = h(x) - q(x)g(x) = k(x), \quad g(0) = g(l) = 0;$$

the  $L^2$  norm of k(x) is uniformly bounded in  $\lambda$ . Then

$$g(x) = \int_0^l G(\lambda; x, y) k(y) dy$$

where  $G(\lambda; x, y)$  is the Green function of the operator  $-\Delta + \lambda$ , with the Dirichlet boundary conditions, on the interval [0, l]. One can easily compute it and check that  $|G_x(\lambda; x, y)| \leq 1$ . Therefore, the  $C^1$ -norm of g(x) is uniformly bounded in  $\lambda$ . Now, from (2.14) we conclude that u'(0) = O(1) and  $u'(l) = \sqrt{\lambda} + O(1)$  as  $\lambda \to \infty$ . To summarize, for  $v \neq w$ ,  $R(\lambda)_{vw} = O(1)$ , and the contribution of each edge  $e \in [v, w]$  to  $R(\lambda)_{ww}$  equals  $\sqrt{\lambda} + O(1)$ .

Now, let e be a loop incident to a vertex w. To compute the contribution of e to  $R(\lambda)_{ww}$ , one has to solve the boundary value problem

$$-u_1'' + \lambda u_1 + q(x)u - 1 = 0, \quad u_1(0) = u_1(l) = 1$$

the contribution of the loop e to  $R(\lambda)_{ww}$  equals  $u'_1(l) - u'_1(0)$ . One has  $u_1(x) = u(x) + \tilde{u}(x)$  where u(x) is the solution of (2.13), and  $\tilde{u}(l-x)$  solves a similar problem, with q(x) replaced by q(l-x). The analysis of the previous paragraph implies that

$$u_1'(l) - u_1'(0) = 2\sqrt{\lambda} + O(1)$$

as  $\lambda \to \infty$ .

Finally, up to terms that are bounded in  $\lambda$ , each edge that connects w with a different vertex contributes  $\sqrt{\lambda}$  to  $R(\lambda)_{ww}$ , and each loop incident to w contributes  $2\sqrt{\lambda}$  to  $R(\lambda)_{ww}$ . Therefore,  $R(\lambda)_{ww} = d(w)\sqrt{\lambda} + O(1)$ .

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