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**LETTER TO THE EDITOR**

# Spectral determinant of Schrödinger operators on graphs

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**Abstract.** We study the spectral properties of the operator $(-\Delta + V(x))$ on a graph. ($\Delta$ is the Laplacian and $V(x)$ is some potential defined on the graph). In particular, we derive an expression for the spectral determinant that generalizes one previously obtained for the Laplacian operator.

For many years, the spectral properties of the Laplacian on graphs have interested physicists [1] as well as mathematicians [2]. Recently, a compact form for the determinant of the operator $(-\Delta+\gamma)$ has been obtained [3] ($\gamma$ is a constant). Our purpose in this letter is to generalize this expression to the operator $(H+\gamma)$, with $H = -\Delta + V(x)$. $V(x)$ is some potential defined at each point $x$ of the graph. The spectrum of such operators has already been considered in [4].

To introduce these results, let us consider a graph made of $V$ vertices linked by $B$ bonds. On each bond $(\alpha\beta)$, of length $l_{\alpha\beta}$, we define the coordinate $x_{\alpha\beta}$ that runs from 0 (vertex $\alpha$) to $l_{\alpha\beta}$ (vertex $\beta$). We will also use $x_{\beta\alpha} = l_{\alpha\beta} - x_{\alpha\beta}$. To avoid cumbersome notations, $\phi$ being some function defined on the graph, we will simply write $\phi(\alpha)$ for $\phi(x_{\alpha\beta=0})$, and $\int_{(\alpha\beta)}\phi$ for $\int_0^{l_{\alpha\beta}}\phi(x_{\alpha\beta})\,\mathrm{d}x_{\alpha\beta}$.

The spectrum of $H$ is determined by imposing continuity of the eigenfunctions and current conservation at each vertex.

In what follows, we will consider, for each bond, two independent solutions, $\psi_{\alpha\beta}$ and $\psi_{\beta\alpha}$, of the equation

$$(H+\gamma)\psi = 0. \tag{1}$$

These functions are chosen to satisfy

$$\psi_{\alpha\beta}(\alpha) = 1 \qquad \psi_{\alpha\beta}(\beta) = 0 \tag{2}$$

$$\psi_{\beta\alpha}(\alpha) = 0 \qquad \psi_{\beta\alpha}(\beta) = 1. \tag{3}$$

Their Wronskian may be presented as

$$W_{\alpha\beta} \equiv \psi_{\alpha\beta}\frac{\mathrm{d}\psi_{\beta\alpha}}{\mathrm{d}x_{\alpha\beta}} - \psi_{\beta\alpha}\frac{\mathrm{d}\psi_{\alpha\beta}}{\mathrm{d}x_{\alpha\beta}} = \frac{\mathrm{d}\psi_{\beta\alpha}}{\mathrm{d}x_{\alpha\beta}}(\alpha) = -\frac{\mathrm{d}\psi_{\alpha\beta}}{\mathrm{d}x_{\alpha\beta}}(\beta). \tag{4}$$

Let us recall the result of [3]. The authors established that

$$\det(-\Delta+\gamma) = \gamma^{\frac{V-B}{2}}\prod_{(\alpha\beta)}\sinh\left(\sqrt{(\gamma)}l_{\alpha\beta}\right)\det(M^0) \tag{5}$$

where $M^0$ is a $(V \times V)$ matrix with the elements

$$M^0_{\alpha\alpha} = \sum_{i=1}^{m_\alpha} \coth(\sqrt{\gamma} l_{\alpha\beta_i}) \tag{6}$$

$$\begin{aligned} M^0_{\alpha\beta} &= -\frac{1}{\sinh(\sqrt{\gamma} l_{\alpha\beta})} \qquad \text{if} \quad (\alpha\beta) \text{ is a bond} \\ &= 0 \quad \text{otherwise.} \end{aligned} \tag{7}$$

(The summation is taken over the $m_\alpha$ nearest vertices of $\alpha$.)

In this paper, we will show that

$$\det(H + \gamma) \equiv \det(-\Delta + V(x) + \gamma) = \prod_{(\alpha\beta)} \frac{1}{\frac{\mathrm{d}\psi_{\beta\alpha}}{\mathrm{d}x_{\alpha\beta}}(\alpha)} \det(M) \tag{8}$$

with the $(V \times V)$ matrix $M$:

$$M_{\alpha\alpha} = \sum_{i=1}^{m_\alpha} \frac{\mathrm{d}\psi_{\alpha\beta_i}}{\mathrm{d}x_{\alpha\beta_i}}(\alpha) \tag{9}$$

$$\begin{aligned} M_{\alpha\beta} = M_{\beta\alpha} &= \frac{\mathrm{d}\psi_{\beta\alpha}}{\mathrm{d}x_{\alpha\beta}}(\alpha) = W_{\alpha\beta} \qquad \text{if} \quad (\alpha\beta) \text{ is a bond} \\ &= 0 \quad \text{otherwise.} \end{aligned} \tag{10}$$

(All the $\psi$ functions appearing in (8)–(10) satisfy (1)–(3).) It is easy to see that (8)–(10) narrow down to (5)–(7) when $V(x) \equiv 0$. (This is actually true, up to an irrelevant multiplicative constant.)

We will now establish (8) by computing the Green function $G(x, y)$ on the graph

$$(\gamma + H)G(x, y) = \delta(x - y) \tag{11}$$

and using the relationship

$$\int_{\text{Graph}} G(x, x)\,\mathrm{d}x = \partial_\gamma \ln\det(H + \gamma). \tag{12}$$

So, let us construct this Green function.

If $x$ is located on the bond $(\alpha\beta)$ and $y$ on another bond, we have

$$G(x, y) = G(\alpha, y)\psi_{\alpha\beta}(x) + G(\beta, y)\psi_{\beta\alpha}(x). \tag{13}$$

Now, if $x$ and $y$ belong to the same bond, say $(ab)$, $G(x, y)$ must satisfy, when $\epsilon \to 0$

$$G(y - \epsilon, y) = G(y + \epsilon, y) \tag{14}$$

$$\left.\frac{\mathrm{d}G}{\mathrm{d}x}\right|_{x=y-\epsilon} = \left.\frac{\mathrm{d}G}{\mathrm{d}x}\right|_{x=y+\epsilon} + 1. \tag{15}$$

The result is

$$x \leqslant y \qquad G(x, y) = G(a, y)\psi_{ab}(x) + G(b, y)\psi_{ba}(x) + \frac{\psi_{ab}(y)\psi_{ba}(x)}{W_{ab}} \tag{16}$$

$$x \geqslant y \qquad G(x, y) = G(a, y)\,\psi_{ab}(x) + G(b, y)\,\psi_{ba}(x) + \frac{\psi_{ba}(y)\,\psi_{ab}(x)}{W_{ab}}. \tag{17}$$

($x < y$ means that point $x$ is closer to $a$ than $y$.)

Current conservation at vertex $\alpha$ reads

$$\sum_{i=1}^{m_\alpha} \left.\frac{\mathrm{d}G(x_{\alpha\beta_i}, y)}{\mathrm{d}x_{\alpha\beta_i}}\right|_{x_{\alpha\beta_i}=0} = 0. \tag{18}$$

If $y$ does not belong to a bond starting from $\alpha$, (13), (18) lead to

$$G(\alpha, y)\left(\sum_{i=1}^{m_\alpha} \frac{\mathrm{d}\psi_{\alpha\beta_i}}{\mathrm{d}x_{\alpha\beta_i}}(\alpha)\right) + \sum_{i=1}^{m_\alpha} G(\beta_i, y)\frac{\mathrm{d}\psi_{\beta_i\alpha}}{\mathrm{d}x_{\alpha\beta_i}}(\alpha) = 0. \tag{19}$$

On the other hand, when $y$ belongs to $(ab)$, we get, for the current conservation at vertex $a$ ((16), (18), (4)):

$$G(a, y)\left(\sum_{i=1}^{m_a} \frac{\mathrm{d}\psi_{a\mu_i}}{\mathrm{d}x_{a\mu_i}}(a)\right) + \sum_{i=1}^{m_a} G(\mu_i, y)\frac{\mathrm{d}\psi_{\mu_i a}}{\mathrm{d}x_{a\mu_i}}(a) + \psi_{ab}(y) = 0. \tag{20}$$

(The nearest neighbours of $a$ are called $\mu_i$, $i = 1, 2, \ldots, m_a$; $b$ is one of the $\mu_i$.)

Current conservation can be written in matrix form

$$M\mathcal{G} = L. \tag{21}$$

The matrix $M$ is defined in (9), (10). $\mathcal{G}$ and $L$ are two $(V \times 1)$ matrices:

$$\mathcal{G} = \begin{pmatrix} G(\alpha_1, y) \\ \vdots \\ G(a, y) \\ \vdots \\ G(b, y) \\ \vdots \\ G(\alpha_{V-2}, y) \end{pmatrix} \qquad L = \begin{pmatrix} 0 \\ \vdots \\ L_a = -\psi_{ab}(y) \\ \vdots \\ L_b = -\psi_{ba}(y) \\ \vdots \\ 0 \end{pmatrix}. \tag{22}$$

With the inverse matrix of $M$, $T \equiv M^{-1}$, one obtains for $G(a, y)$ and $G(b, y)$:

$$G(a, y) = T_{aa}L_a + T_{ab}L_b \tag{23}$$

$$G(b, y) = T_{ba}L_a + T_{bb}L_b. \tag{24}$$

After simple manipulations, (16) leads to

$$G(y, y) = T_{aa}(-\psi_{ab}^2(y)) + T_{bb}(-\psi_{ba}^2(y)) + \left(T_{ab} + T_{ba} - \frac{1}{W_{ab}}\right)(-\psi_{ab}(y)\psi_{ba}(y)). \tag{25}$$

To stick to (12), we must integrate $\psi_{ab}^2(y)$, $\psi_{ba}^2(y)$ and $\psi_{ab}(y)\psi_{ba}(y)$. Let us show that

$$\int_{(ab)} \psi_{ab}^2 = -\partial_\gamma \frac{\mathrm{d}\psi_{ab}}{\mathrm{d}x_{ab}}(a) \tag{26}$$

$$\int_{(ab)} \psi_{ba}^2 = \partial_\gamma \frac{\mathrm{d}\psi_{ba}}{\mathrm{d}x_{ab}}(b) \tag{27}$$

$$\int_{(ab)} \psi_{ab}\,\psi_{ba} = -\partial_\gamma \frac{\mathrm{d}\psi_{ba}}{\mathrm{d}x_{ab}}(a) = \partial_\gamma \frac{\mathrm{d}\psi_{ab}}{\mathrm{d}x_{ab}}(b) = -\partial_\gamma M_{ab}. \tag{28}$$

Indeed, starting with the equations

$$(H + \gamma)\psi_{ab} = 0 \tag{29}$$

$$(H + \gamma)\psi_{ba} = 0 \tag{30}$$

we take the derivative of (29) with respect to $\gamma$:

$$(H + \gamma)\partial_\gamma\psi_{ab} = -\psi_{ab}. \tag{31}$$

Obviously, $\partial_\gamma\psi_{ab}$ can be written in the form ($x_{ab} \equiv x$, $\frac{\mathrm{d}\psi}{\mathrm{d}x} \equiv \psi'$):

$$\partial_\gamma\psi_{ab}(x) = c(x)\psi_{ab}(x) + d(x)\psi_{ba}(x) \tag{32}$$

with

$$c(0) = d(l_{ab}) = 0. \tag{33}$$

This last point emerges from conditions (2), (3) that are satisfied whatever $\gamma$ is.

Determining the unknown functions $c(x)$ and $d(x)$ by standard methods, we impose the auxiliary condition

$$c'\psi_{ab} + d'\psi_{ba} = 0. \tag{34}$$

(29)–(32) and (34) lead to

$$c'\,\psi'_{ab} + d'\,\psi'_{ba} = \psi_{ab}. \tag{35}$$

Solving the above system, we get, with (33)

$$c(x) = -\int_0^x \frac{\psi_{ab}(u)\psi_{ba}(u)}{W_{ab}}\,\mathrm{d}u \tag{36}$$

$$d(x) = \int_{l_{ab}}^x \frac{\psi_{ab}^2(u)}{W_{ab}}\,\mathrm{d}u. \tag{37}$$

Using (32), (34), we arrive at

$$\partial_\gamma\psi'_{ab} = c\psi'_{ab} + d\psi'_{ba}. \tag{38}$$

Setting $x = 0$ in (36)–(38), we recover (26). With $x = l_{ab}$, we recover (28). Moreover, considering $\partial_\gamma\psi_{ba}$ instead of $\partial_\gamma\psi_{ab}$, we should prove that (27) holds.

Let us return to the computation of the trace of the Green function. Equations (25)–(28) give

$$\int_{(ab)} G(y,y) = T_{aa}\partial_\gamma\frac{\mathrm{d}\psi_{ab}}{\mathrm{d}x_{ab}}(a) + T_{bb}\partial_\gamma\frac{\mathrm{d}\psi_{ba}}{\mathrm{d}x_{ba}}(b) + T_{ab}\partial_\gamma M_{ba} + T_{ba}\partial_\gamma M_{ab} - \frac{\partial_\gamma\frac{\mathrm{d}\psi_{ba}}{\mathrm{d}x_{ab}}(a)}{W_{ab}}. \tag{39}$$

Summing over all the bonds and using (4) and (9), we obtain

$$\int_{\mathrm{Graph}} G(y,y) = \mathrm{Tr}(M^{-1}\partial_\gamma M) - \partial_\gamma\left(\sum_{(ab)}\ln\frac{\mathrm{d}\psi_{ba}}{\mathrm{d}x_{ab}}(a)\right). \tag{40}$$

Finally, with the observation that $\mathrm{Tr}(M^{-1}\partial_\gamma M) = \partial_\gamma \ln\det M$, it is easy to see that (12) leads to formula (8) (up to an inessential multiplicative constant).

To conclude, let us remark that, for more general boundary conditions than (18), i.e. for instance

$$\sum_{i=1}^{m_\alpha} \left.\frac{\mathrm{d}G(x_{\alpha\beta_i},y)}{\mathrm{d}x_{\alpha\beta_i}}\right|_{x_{\alpha\beta_i}=0} = \lambda_\alpha G(\alpha,y). \tag{41}$$

(8) still holds if we slightly modify the diagonal elements of $M$ ($M_{\alpha\alpha} \to M_{\alpha\alpha} - \lambda_\alpha$).

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