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Spectral determinant on graphs with generalized boundary conditions

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Abstract. The spectral determinant of the Schrödinger operator $(-\Delta + V(x))$ on a graph is computed for general boundary conditions. (Δ is the Laplacian and $V(x)$ is some potential defined on the graph). Applications to restricted random walks on graphs are discussed.

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1 Introduction

The study of spectral properties of the Laplacian operator on finite graphs began about fifty years ago. Many different domains are interested in the knowledge of those properties – let us simply mention organic molecules [1], superconducting networks [2], vibrational properties of fractal structures [3], weakly disordered systems [4] and, more recently, quantum chaos [5]. Of course, mathematicians [6] are also interested in that subject.

Let us come back, for the moment, to the physics of disordered systems. In [7], the authors emphasized the central role played by the spectral determinant of the Laplacian in the computation of the weak localization corrections. By constructing the Green's function on the graph, they obtained a compact form for this determinant. (See also [8] where a path integral approach is developed; in particular, a trace formula for the Laplacian on a graph [6] is recovered.)

Recently, the result of [7] was generalized [9,10] to the spectral determinant $\det(H+\gamma)$ $(\equiv S(\gamma))$ with $H = -\Delta + V(x)$. $V(x)$ is some external potential defined in each point x of the graph and γ is a constant (spectral parameter). In [10], the computation was done with the help of a path integral representation of the spectral determinant and also using time-dependent harmonic oscillator properties. Schrödinger operators have also been considered in [11] where the scattering matrix is computed for graphs made of one-dimensional wires connected to external leads.

All this was done assuming continuity of the eigenfunctions at each vertex.

Nevertheless, this "natural"(!) assumption is highly questionable.

For instance, in [12,13], the authors argue that the reduction of a realistic system of coupled tubes to a graph model is far from being obvious. In particular, serious problems arise from the finite thickness of the tubes, the geometry of the connection regions and also from eventually applied external fields. Analyzing in details a model of junction (what they call the "geometric-scatterer junction"), they suggest that it would be more appropriate to consider general boundary conditions on the resulting graph.

This is the point of view we will take up in this paper when computing the spectral determinant[1]. Moreover, we will show that "playing" with the boundary conditions allows us to study some properties of closed random walks on any graph. For instance, it is possible to count the number of such walks when the number of backtrackings on each of them is fixed [15–17].

The paper is organized as follows. In Section 2, we set up the notations that will be used throughout the paper. Section 3 will be devoted to the computation of the spectral determinant $S(\gamma)$ for general boundary conditions. Another expression for $S(\gamma)$ will be derived in Section 4 for permutation-invariant conditions. Applications to countings of restricted random walks on any graph will be discussed at the end of this section. Finally, a short conclusion will be given in Section 5.

2 Definitions and notations

We consider a graph $\mathcal{G}$ made of V vertices, numbered from 1 to V, linked by B bonds of finite lengths. The coordination of vertex α is m_α ($\sum_{\alpha=1}^{V} m_\alpha = 2B$).

On each bond $[\alpha\beta]$, of length $l_{\alpha\beta}$, we define the coordinate $x_{\alpha\beta}$ that runs from 0 (vertex α) to $l_{\alpha\beta}$ (vertex β). We will also use $x_{\beta\alpha} = l_{\alpha\beta} - x_{\alpha\beta}$.

[1] Spectral properties of graphs with general – even random – boundary conditions imposed at the vertices have already been studied in the context of quantum chaos [14].

To avoid cumbersome notations, Φ being some function defined on the graph, we will simply write $\int_{[\alpha\beta]} \Phi$ for $\int_0^{l_{\alpha\beta}} \Phi(x_{\alpha\beta})\, \mathrm{d}x_{\alpha\beta}$.

An arc $(\alpha\beta)$ is defined as the oriented bond from α to β. Each bond $[\alpha\beta]$ is therefore associated with two arcs $(\alpha\beta)$ and $(\beta\alpha)$. In the sequel, we will consider the following ordering of the $2B$ arcs: $(1\alpha_1)(1\alpha_2)\ldots(1\alpha_{m_1})(2\beta_1)\ldots(2\beta_{m_2})\ldots$

Concerning the eigenfunctions ϕ of H on the graph, we define on each link $[\alpha\beta]$:

$$\phi_{(\alpha\beta)} \equiv \lim_{x_{\alpha\beta}\to 0} \phi(x_{\alpha\beta}) \quad ; \quad \phi_{(\beta\alpha)} \equiv \lim_{x_{\beta\alpha}\to 0} \phi(x_{\beta\alpha}) \quad (1)$$

$$\phi'_{(\alpha\beta)} \equiv \lim_{x_{\alpha\beta}\to 0} \frac{\mathrm{d}\phi(x_{\alpha\beta})}{\mathrm{d}x_{\alpha\beta}} \quad ; \quad \phi'_{(\beta\alpha)} \equiv \lim_{x_{\beta\alpha}\to 0} \frac{\mathrm{d}\phi(x_{\beta\alpha})}{\mathrm{d}x_{\beta\alpha}} \quad (2)$$

($\phi'_{(\alpha\beta)}$ is the outgoing derivative at vertex α along the arc $(\alpha\beta)$).

For the Green's function $G(x,y)$ ($x \in [\alpha\beta]$, y anywhere on the graph), we similarly define:

$$\begin{aligned} G_{(\alpha\beta)}(y) &\equiv \lim_{x_{\alpha\beta}\to 0} G(x_{\alpha\beta}, y) \quad ; \\ G_{(\beta\alpha)}(y) &\equiv \lim_{x_{\beta\alpha}\to 0} G(x_{\beta\alpha}, y) \qquad (3) \\ G'_{(\alpha\beta)}(y) &\equiv \lim_{x_{\alpha\beta}\to 0} \frac{\mathrm{d}G(x_{\alpha\beta}, y)}{\mathrm{d}x_{\alpha\beta}} \quad ; \\ G'_{(\beta\alpha)}(y) &\equiv \lim_{x_{\beta\alpha}\to 0} \frac{\mathrm{d}G(x_{\beta\alpha}, y)}{\mathrm{d}x_{\beta\alpha}}. \qquad (4) \end{aligned}$$

With the above quantities, we can build the four $(2B \times 1)$ vectors ϕ, ϕ', $G(y)$ and $G'(y)$, respectively of components $\phi_{(\alpha\beta)}$, $\phi'_{(\alpha\beta)}$, $G_{(\alpha\beta)}(y)$ and $G'_{(\alpha\beta)}(y)$.

In those conditions, the generalized boundary conditions for the operator H on the graph can be written:

$$C\,\phi \;+\; D\,\phi' \;=\; 0 \qquad (5)$$

where C and D are two $(2B \times 2B)$ constant matrices that don't depend on γ.

In [18], the authors established the conditions for the operator H to be self-adjoint: CD^+ must be self-adjoint and the $(2B \times 4B)$ matrix (C, D) must have maximal rank $2B$.

Local boundary conditions connect, for each vertex α, the $\phi_{(\alpha\beta_i)}$'s to the $\phi'_{(\alpha\beta_j)}$'s, $i, j = 1, \ldots, m_\alpha$. For such conditions, C and D can be chosen block-diagonal, the square block C_α (or D_α) being of dimension m_α. If, in addition, we assume that, for each vertex α, the conditions are invariant in any permutation of the nearest neighbours of α, we can write:

$$C_\alpha = c_\alpha \mathbf{1} + t_\alpha F_\alpha \qquad (6)$$

$$D_\alpha = d_\alpha \mathbf{1} + w_\alpha F_\alpha \qquad (7)$$

where $\mathbf{1}$ is the unit matrix and F_α is a matrix with all its elements equal to 1. The constants c_α, d_α, t_α and w_α characterize the boundary conditions in α.

Remark that c_α and d_α can't both vanish because of the maximal rank condition[2].

It is easy to realize that the quantity $c_\alpha \phi_{(\alpha\beta_i)} + d_\alpha \phi'_{(\alpha\beta_i)}$ doesn't depend on i, *i.e.* it is the same for all the arcs starting at α. To conclude this section, let us mention the two limiting cases:

i) $d_\alpha = 0$ that ensures the continuity of ϕ at vertex α (thus $\phi(\alpha)$ is defined) and leads to

$$\sum_{j=1}^{m_\alpha} \phi'_{(\alpha\beta_j)} = -\left(\frac{c_\alpha + m_\alpha t_\alpha}{w_\alpha}\right) \phi(\alpha) \equiv \lambda_\alpha \phi(\alpha)$$

($\lambda_\alpha = 0$ corresponds to Neumann boundary conditions).

ii) $c_\alpha = 0$. In that case, all the outgoing derivatives in α are equal.

Now, we turn to the computation of the spectral determinant $S(\gamma)(\equiv \det(H+\gamma))$ of the operator $H = -\Delta + V(x)$ defined on the graph with boundary conditions given by (5).

3 General boundary conditions

As in [7,9], we construct the Green's function $G(x,y)$ on the graph:

$$(\gamma + H)\, G(x,y) = \delta(x-y) \qquad (8)$$

and use the relationship:

$$\int_{\mathrm{Graph}} G(x,x)\mathrm{d}x = \partial_\gamma \ln \det(H+\gamma). \qquad (9)$$

In this section, we will consider, for each bond $[\alpha\beta]$, two independent solutions, $\psi_{\alpha\beta}$ and $\psi_{\beta\alpha}$, of the equation:

$$(H+\gamma)\,\psi = 0. \qquad (10)$$

Those functions are chosen to satisfy:

$$\psi_{\alpha\beta}(\alpha) = 1 \quad ; \quad \psi_{\alpha\beta}(\beta) = 0 \qquad (11)$$

$$\psi_{\beta\alpha}(\alpha) = 0 \quad ; \quad \psi_{\beta\alpha}(\beta) = 1. \qquad (12)$$

Their Wronskian may be presented as:

$$\begin{aligned} W_{\alpha\beta} &\equiv \psi_{\alpha\beta}\frac{\mathrm{d}\psi_{\beta\alpha}}{\mathrm{d}x_{\alpha\beta}} - \psi_{\beta\alpha}\frac{\mathrm{d}\psi_{\alpha\beta}}{\mathrm{d}x_{\alpha\beta}} \\ &= \frac{\mathrm{d}\psi_{\beta\alpha}}{\mathrm{d}x_{\alpha\beta}}(\alpha) = -\frac{\mathrm{d}\psi_{\alpha\beta}}{\mathrm{d}x_{\alpha\beta}}(\beta) = W_{\beta\alpha}. \qquad (13) \end{aligned}$$

[2] Moreover, this condition imposes that, at least, one of the two matrices, C_α or D_α, is invertible and can be set equal to $\mathbf{1}$ because of the homogeneity of condition (5). Finally, self-adjointness of CD^+ implies that only two real parameters are, actually, necessary to characterize the boundary conditions at each vertex α [19]. This will appear explicitly in Section 4.2 where our results are expressed in terms of the two parameters η_α and ρ_α defined in equations (61, 62).

We also define:

$$\psi'_{\alpha\beta}(\alpha) \equiv \frac{\mathrm{d}\psi_{\alpha\beta}}{\mathrm{d}x_{\alpha\beta}}(x_{\alpha\beta}=0) \quad ;$$
$$\psi'_{\beta\alpha}(\beta) \equiv \frac{\mathrm{d}\psi_{\beta\alpha}}{\mathrm{d}x_{\beta\alpha}}(x_{\beta\alpha}=0)\cdot \tag{14}$$

So, let us construct this Green's function $G(x,y)$. We first suppose that y belongs to some link $[ab]$.

If x is located on another bond $[\alpha\beta]$, we have:

$$G(x,y) = G_{(\alpha\beta)}(y)\,\psi_{\alpha\beta}(x) + G_{(\beta\alpha)}(y)\,\psi_{\beta\alpha}(x). \tag{15}$$

Taking the derivative in α and using (13, 14), we get:

$$G'_{(\alpha\beta)}(y) = G_{(\alpha\beta)}(y)\,\psi'_{\alpha\beta}(\alpha) + G_{(\beta\alpha)}(y)\,W_{\alpha\beta}. \tag{16}$$

On the other hand, if x belongs to the same bond $[ab]$ as y, $G(x,y)$ must satisfy, when $\epsilon \to 0$:

$$G(y-\epsilon,y) = G(y+\epsilon,y) \tag{17}$$
$$\left.\frac{\mathrm{d}G}{\mathrm{d}x}\right|_{x=y-\epsilon} = \left.\frac{\mathrm{d}G}{\mathrm{d}x}\right|_{x=y+\epsilon} + 1\cdot \tag{18}$$

This leads to:

$$x \le y \quad G(x,y) = G_{(ab)}(y)\,\psi_{ab}(x) + G_{(ba)}(y)\,\psi_{ba}(x) + \frac{\psi_{ab}(y)\,\psi_{ba}(x)}{W_{ab}} \tag{19}$$
$$x \ge y \quad G(x,y) = G_{(ab)}(y)\,\psi_{ab}(x) + G_{(ba)}(y)\,\psi_{ba}(x) + \frac{\psi_{ba}(y)\,\psi_{ab}(x)}{W_{ab}} \tag{20}$$

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

For the derivative in a, we obtain:

$$G'_{(ab)}(y) = G_{(ab)}(y)\,\psi'_{ab}(a) + G_{(ba)}(y)\,W_{ab} + \psi_{ab}(y). \tag{21}$$

Equations (16, 21) can be written in matrix form:

$$G'(y) = NG(y) - L(y) \tag{22}$$

where N is a $(2B \times 2B)$ square matrix with elements:

$$N_{(\alpha\beta)(\mu\eta)} = \delta_{\alpha\mu}\delta_{\beta\eta}\psi'_{\alpha\beta}(\alpha) + \delta_{\alpha\eta}\delta_{\beta\mu}W_{\alpha\beta} \tag{23}$$

and $L(y)$ is a $(2B \times 1)$ vector:

$$L(y)_{(\alpha\beta)} = -\left(\delta_{\alpha a}\delta_{\beta b}\psi_{ab}(y) + \delta_{\alpha b}\delta_{\beta a}\psi_{ba}(y)\right). \tag{24}$$

Equation (22) together with the boundary condition (5) lead to:

$$G(y) = T\,L(y) \tag{25}$$
with the square matrix $$T = (C+DN)^{-1}D. \tag{26}$$

We deduce:

$$G_{(ab)}(y) = T_{(ab)(ab)}L(y)_{(ab)} + T_{(ab)(ba)}L(y)_{(ba)} \tag{27}$$
$$G_{(ba)}(y) = T_{(ba)(ab)}L(y)_{(ab)} + T_{(ba)(ba)}L(y)_{(ba)} \tag{28}$$

and, after simple manipulations:

$$G(y,y) = T_{(ab)(ab)}\left(-\psi^2_{ab}(y)\right) + T_{(ba)(ba)}\left(-\psi^2_{ba}(y)\right) + \left(-T_{(ab)(ba)} - T_{(ba)(ab)} + \frac{1}{W_{ab}}\right)\left(\psi_{ab}(y)\,\psi_{ba}(y)\right)\cdot \tag{29}$$

To take the trace of G, we must first integrate $\psi^2_{ab}(y)$, $\psi^2_{ba}(y)$ and $\psi_{ab}(y)\psi_{ba}(y)$ on $[ab]$. We have shown in [9] that:

$$\int_{[ab]} \psi^2_{ab} = -\partial_\gamma \psi'_{ab}(a) \tag{30}$$
$$\int_{[ab]} \psi^2_{ba} = -\partial_\gamma \psi'_{ba}(b) \tag{31}$$
$$\int_{[ab]} \psi_{ab}\,\psi_{ba} = -\partial_\gamma W_{ab}. \tag{32}$$

Thus:

$$\int_{[ab]} G(y,y) = T_{(ab)(ab)}\partial_\gamma\psi'_{ab}(a) + T_{(ba)(ba)}\partial_\gamma\psi'_{ba}(b) + \left(T_{(ab)(ba)}+T_{(ba)(ab)}\right)\partial_\gamma W_{ab} - \frac{1}{W_{ab}}\partial_\gamma W_{ab}\cdot \tag{33}$$

Now, we sum over all the bonds. With the definitions of the matrices N and T, we obtain (C and D don't depend on γ):

$$\int_{\mathrm{Graph}} G(y,y) = \mathrm{Tr}\left((C+DN)^{-1}\partial_\gamma(C+DN)\right) - \partial_\gamma\left(\sum_{[ab]}\ln W_{ab}\right)\cdot \tag{34}$$

Finally, with the observation that $\mathrm{Tr}((C+DN)^{-1}\partial_\gamma(C+DN)) = \partial_\gamma \ln\det(C+DN)$, we get the spectral determinant (up to an inessential multiplicative constant):

$$S(\gamma) \equiv \det(H+\gamma) = \prod_{[\alpha\beta]}\frac{1}{W_{\alpha\beta}}\ \det(C+DN)\cdot \tag{35}$$

where $\prod_{[\alpha\beta]}\dots$ means product over all the bonds.

The expression (35) is valid for quite general (even non-local) boundary conditions[3].

It is worthwhile to mention that equation (35) can be, heuristically, recovered by a path integral approach (see [8] ([10]) for the Neumann case without (with) an external potential). We will not use this way in the present work.

Coming back to (35) and introducing the matrix R:

$$R \equiv (\sqrt{\gamma}\mathbf{1}+N)(\sqrt{\gamma}\mathbf{1}-N)^{-1} \tag{36}$$

[3] For local coupling, C and D are block-diagonal matrices. N is always block-diagonal but not built with the same blocks as C and D. Thus, no further simplification appears in that case when evaluating $\det(C+DN)$ in equation (35).

we get:

$$\det(H+\gamma) = \prod_{[\alpha\beta]} \frac{1}{W_{\alpha\beta}} \; \frac{1}{\det(\mathbf{1}+R)} \times \det(C-\sqrt{\gamma}D)\; \det(\mathbf{1}-QR) \quad (37)$$

$$Q = (\sqrt{\gamma}D - C)^{-1}(\sqrt{\gamma}D + C). \quad (38)$$

Let us remark that, for the free case ($V(x) \equiv 0$), the matrix R is quite simple. Indeed, in that case:

$$N_{(\alpha\beta)(\mu\eta)} = \delta_{\alpha\mu}\delta_{\beta\eta} \coth \sqrt{\gamma} l_{\alpha\beta} + \delta_{\alpha\eta}\delta_{\beta\mu} \left(\frac{-1}{\sinh \sqrt{\gamma} l_{\alpha\beta}} \right) \quad (39)$$

$$R_{(\alpha\beta)(\mu\eta)} = \delta_{\alpha\eta}\delta_{\beta\mu} \mathrm{e}^{-\sqrt{\gamma} l_{\alpha\beta}}. \quad (40)$$

The matrix R couples any arc $(\alpha\beta)$ to its time-reversed $(\beta\alpha)$. Those considerations will show useful at the end of this paper.

Now, let us show that, for permutation-invariant boundary conditions (and $V(x) \neq 0$), the spectral determinant can be expressed in terms of a vertex $(V \times V)$ matrix.

4 Permutation-invariant boundary conditions

The boundary conditions are now given by equations (6, 7).

4.1 With an external potential

To compute the spectral determinant, we will proceed as before but, this time, we will consider, for each bond, two other independent solutions, $\chi_{\alpha\beta}$ and $\chi_{\beta\alpha}$, of the equation $(H+\gamma)\,\chi = 0$. They are chosen, now, to satisfy the following conditions:

$$c_\alpha \chi_{\alpha\beta}(\alpha) + d_\alpha \frac{\mathrm{d}\chi_{\alpha\beta}}{\mathrm{d}x_{\alpha\beta}}(\alpha) = 1 \quad (41)$$

$$c_\beta \chi_{\alpha\beta}(\beta) + d_\beta \frac{\mathrm{d}\chi_{\alpha\beta}}{\mathrm{d}x_{\beta\alpha}}(\beta) = 0 \quad (42)$$

$$c_\alpha \chi_{\beta\alpha}(\alpha) + d_\alpha \frac{\mathrm{d}\chi_{\beta\alpha}}{\mathrm{d}x_{\alpha\beta}}(\alpha) = 0 \quad (43)$$

$$c_\beta \chi_{\beta\alpha}(\beta) + d_\beta \frac{\mathrm{d}\chi_{\beta\alpha}}{\mathrm{d}x_{\beta\alpha}}(\beta) = 1. \quad (44)$$

As before, we will set:

$$\frac{\mathrm{d}\chi_{\alpha\beta}}{\mathrm{d}x_{\alpha\beta}}(\alpha) \equiv \chi'_{\alpha\beta}(\alpha) \quad ; \quad \frac{\mathrm{d}\chi_{\beta\alpha}}{\mathrm{d}x_{\beta\alpha}}(\beta) \equiv \chi'_{\beta\alpha}(\beta).$$

The Wronskian of $\chi_{\alpha\beta}$ and $\chi_{\beta\alpha}$ writes:

$$\mathcal{W}_{\alpha\beta} \equiv \chi_{\alpha\beta}\frac{\mathrm{d}\chi_{\beta\alpha}}{\mathrm{d}x_{\alpha\beta}} - \chi_{\beta\alpha}\frac{\mathrm{d}\chi_{\alpha\beta}}{\mathrm{d}x_{\alpha\beta}} = \mathcal{W}_{\beta\alpha}. \quad (45)$$

With equations (41–44), we get the useful relations:

$$c_\alpha \mathcal{W}_{\alpha\beta} = \frac{\mathrm{d}\chi_{\beta\alpha}}{\mathrm{d}x_{\alpha\beta}}(\alpha) \quad ; \quad d_\alpha \mathcal{W}_{\alpha\beta} = -\chi_{\beta\alpha}(\alpha). \quad (46)$$

Let us show what happens for the Green's function $G(x,y)$. We still assume $y \in [ab]$.

For $x \in [\alpha\beta] \neq [ab]$, we write:

$$G(x,y) = B_{(\alpha\beta)}(y)\chi_{\alpha\beta}(x) + B_{(\beta\alpha)}(y)\chi_{\beta\alpha}(x) \quad (47)$$

where the quantities $B_{(\alpha\beta)}(y)$ are to be determined.

Of course, if $x \in [ab]$, an additional term of the form "$\chi_{ab}\chi_{ba}/\mathcal{W}_{ab}$" must appear (see Eqs. (19, 20)).

Nevertheless, with the boundary conditions (6,7), it can be shown that, for any vertex α, the quantity $B_{(\alpha\beta_i)}(y)$ where β_i is a nearest neighbour of α, does not depend on i. In those conditions, we can set: $B_{(\alpha\beta_i)}(y) \equiv B_\alpha(y)$ and write for the Green's function:

i) $x \in [\alpha\beta] \neq [ab]$

$$G(x,y) = B_\alpha(y)\chi_{\alpha\beta}(x) + B_\beta(y)\chi_{\beta\alpha}(x); \quad (48)$$

ii) $x \in [ab]$

$$x \leq y \quad G(x,y) = B_a(y)\chi_{ab}(x) + B_b(y)\chi_{ba}(x) + \frac{\chi_{ab}(y)\chi_{ba}(x)}{\mathcal{W}_{ab}} \quad (49)$$

$$x \geq y \quad G(x,y) = B_a(y)\chi_{ab}(x) + B_b(y)\chi_{ba}(x) + \frac{\chi_{ba}(y)\chi_{ab}(x)}{\mathcal{W}_{ab}}. \quad (50)$$

The boundary conditions lead to the equation:

$$M\,B \;=\; \mathcal{L} \quad (51)$$

where M is a $(V \times V)$ matrix with elements:

$$M_{\alpha\alpha} = 1 + t_\alpha \left(\sum_{i=1}^{m_\alpha} \chi_{\alpha\beta_i}(\alpha) \right) + w_\alpha \left(\sum_{i=1}^{m_\alpha} \chi'_{\alpha\beta_i}(\alpha) \right) \quad (52)$$

$$M_{\alpha\beta} = (c_\alpha w_\alpha - t_\alpha d_\alpha)\mathcal{W}_{\alpha\beta} \quad \text{if } [\alpha\beta] \text{ is a bond} \quad (53)$$
$$= 0 \quad \text{otherwise.}$$

B and $\mathcal{L}$ are two $(V \times 1)$ vectors of components:

$$B_\alpha = B_\alpha(y) \quad (54)$$

$$\mathcal{L}_\alpha = -\left(\delta_{\alpha a}\chi_{ab}(y)(c_a w_a - d_a t_a) + \delta_{\alpha b}\chi_{ba}(y)(c_b w_b - d_b t_b)\right). \quad (55)$$

Solving (51) and taking the trace of G with the relations [9]:

$$d_a \int_{[ab]} \chi_{ab}^2 = \partial_\gamma \chi_{ab}(a) \quad (56)$$

$$d_b \int_{[ab]} \chi_{ba}^2 = \partial_\gamma \chi_{ba}(b) \quad (57)$$

$$\int_{[ab]} \chi_{ab}\,\chi_{ba} = -\partial_\gamma \mathcal{W}_{ba} \quad (58)$$

we finally get the spectral determinant (still up to a multiplicative constant):

$$\det(H+\gamma) = \prod_{[\alpha\beta]} \frac{1}{\mathcal{W}_{\alpha\beta}} \ \det(M)\cdot \tag{59}$$

Comparing the asymptotic behaviours of the right-hand sides of (35) and (59) when $\gamma \to \infty$, we establish the following equality that is valid in the presence of a potential $V(x)$ and for permutation-invariant boundary conditions:

$$\prod_{[\alpha\beta]} \frac{1}{W_{\alpha\beta}} \ \det(C+DN) = \prod_{[\alpha\beta]} \frac{1}{\mathcal{W}_{\alpha\beta}} \ \det(M)\cdot \tag{60}$$

Recall that, for such boundary conditions, C and D are block-diagonal matrices given by equations (6, 7).

4.2 Free case

Let us study the case $V(x) \equiv 0$ still with permutation-invariant boundary conditions.

With the notations

$$\eta_\alpha = \frac{c_\alpha + \sqrt{\gamma} d_\alpha}{c_\alpha - \sqrt{\gamma} d_\alpha} \tag{61}$$

$$\rho_\alpha = \frac{\mu_\alpha^- - \mu_\alpha^+}{1 + m_\alpha \mu_\alpha^-} \tag{62}$$

$$\mu_\alpha^\pm = \frac{t_\alpha \pm \sqrt{\gamma} w_\alpha}{c_\alpha \pm \sqrt{\gamma} d_\alpha} \tag{63}$$

(60, 37, 38) lead to:

$$\det(\mathbf{1} - QR) = 2^{-V} \prod_\alpha (\rho_\alpha \eta_\alpha) \prod_{[\alpha\beta]} \left(1 - \eta_\alpha \eta_\beta \mathrm{e}^{-2\sqrt{\gamma} l_{\alpha\beta}}\right) \ \det \widetilde{M} \tag{64}$$

with the $(V \times V)$ $\widetilde{M}$ matrix:

$$\widetilde{M}_{\alpha\alpha} = \frac{2}{\rho_\alpha \eta_\alpha} - \frac{m_\alpha}{\eta_\alpha} + \frac{1}{\eta_\alpha} \sum_{i=1}^{m_\alpha} \left(\frac{1 + \eta_\alpha \eta_{\beta_i} \mathrm{e}^{-2\sqrt{\gamma} l_{\alpha\beta_i}}}{1 - \eta_\alpha \eta_{\beta_i} \mathrm{e}^{-2\sqrt{\gamma} l_{\alpha\beta_i}}} \right) \tag{65}$$

$$\widetilde{M}_{\alpha\beta} = \frac{-2\mathrm{e}^{-\sqrt{\gamma} l_{\alpha\beta}}}{1 - \eta_\alpha \eta_\beta \mathrm{e}^{-2\sqrt{\gamma} l_{\alpha\beta}}} \qquad \text{if } [\alpha\beta\,] \text{ is a bond} \tag{66}$$
$$= 0 \qquad \text{otherwise.}$$

For permutation-invariant boundary conditions, the matrices C, D and Q (Eq. (38)) are block-diagonal. The block Q_α takes the simple form:

$$Q_\alpha = \eta_\alpha \left(-\mathbf{1} + \rho_\alpha F_\alpha\right). \tag{67}$$

The only non-vanishing elements of the QR matrix are:

$$(QR)_{(\alpha\beta)(\mu\alpha)} = (\rho_\alpha \eta_\alpha - \eta_\alpha \ \delta_{\beta\mu}) \ \mathrm{e}^{-\sqrt{\gamma} l_{\alpha\mu}}. \tag{68}$$

In view of the following application, we will say that $\rho_\alpha \eta_\alpha - \eta_\alpha$ is the reflection factor in α and $\rho_\alpha \eta_\alpha$ is the transmission factor.

Expanding

$$\ln \det(\mathbf{1} - QR) = -\sum_{n=1}^{\infty} \frac{1}{n} \ \mathrm{Tr}\ (QR)^n \tag{69}$$

and following the development of [8], we finally get:

$$\det(\mathbf{1} - QR) = \prod_{\widetilde{C}} \left(1 - \mu(\widetilde{C}) \mathrm{e}^{-\sqrt{\gamma} l(\widetilde{C})}\right) \tag{70}$$

where the product is taken over all primitive orbits $\widetilde{C}$. Recall that an orbit is said to be primitive if it cannot be decomposed as a repetition of any smaller orbit. $l(\widetilde{C})$ is the length of $\widetilde{C}$.

An orbit being a succession of arcs $\ldots(\tau\alpha)(\alpha\beta)\ldots$ with, in α, a reflection (if $\tau = \beta$) or a transmission (if $\tau \neq \beta$), the weight $\mu(\widetilde{C})$, in equation (70), will be the product of all the reflection – or transmission – factors along $\widetilde{C}$.

Henceforth, we will consider the situation where the spectral parameter γ is equal to 1 and, in addition:

$$\rho_\alpha \eta_\alpha = 1 \quad ; \quad \eta_\alpha = \eta \quad ; \quad l_{\alpha\beta} = l$$

for all the vertices and bonds of the graph.

With $u \equiv \mathrm{e}^{-l}$, (64) takes the simple form:

$$\prod_{\widetilde{C_m}} \left(1 - (1-\eta)^{n_R(\widetilde{C_m})} u^m\right) = (1 - \eta^2 u^2)^{B-V} \times \det\left((1-\eta^2u^2)\mathbf{1} + \eta u^2 \mathbf{Y} - u\mathbf{A}\right) \left(\equiv Z^{-1}\right) \tag{71}$$

m is the number of steps of the primitive orbit $\widetilde{C_m}$ and $n_R(\widetilde{C_m})$ is the number of reflections (backtrackings) occuring along $\widetilde{C_m}$.

$\mathbf{Y}$ is a $(V \times V)$ matrix with elements $Y_{\alpha\beta} = \delta_{\alpha\beta}\ m_\alpha$ and $\mathbf{A}$ is the adjacency matrix ($A_{\alpha\beta} = 1$ if $[\alpha\beta]$ is a bond, $= 0$ otherwise).

Setting $\eta = 1$ implies $n_R(\widetilde{C_m}) = 0$ in the left-hand side of (71): we recover Ihara's formula [15,16] where only primitive orbits without tails and backtrackings are kept. (Ihara [15] established this formula for a regular graph; the proof for a general graph is done in [16] using a direct – and somewhat tedious – counting technique).

Now, let us consider random walks with a given number of backtrackings. Equations (69) and (68) suggest an expansion in closed random walks on the graph. Taking Z in (71), we get:

$$u \ \frac{\mathrm{d} \ln Z}{\mathrm{d}u} = \sum_{m=2}^{\infty} \sum_{p=0}^{m} \sum_{\alpha=1}^{V} N_m^p(\alpha) \ (1-\eta)^p \ u^m \tag{72}$$

where $N_m^p(\alpha)$ is the number of m-steps closed random walks on the graph starting at α, with p backtrackings.

For the complete graph (each vertex α is linked to all the other vertices of the graph), we get the results:

$$\begin{aligned} N_2^0(\alpha) &= 0 \\ N_3^0(\alpha) &= (V-1)(V-2) \\ N_4^0(\alpha) &= (V-1)(V-2)(V-3) \\ N_5^0(\alpha) &= (V-1)(V-2)(V-3)(V-4) \\ N_6^0(\alpha) &= (V-1)(V-2)(V^3-9V^2+29V-32) \end{aligned} \quad (73)$$

and also:

$$\begin{aligned} N_2^1(\alpha) = N_3^1(\alpha) &= N_4^1(\alpha) = 0 \\ N_5^1(\alpha) &= 5(V-1)(V-2)(V-3) \\ N_6^1(\alpha) &= 6(V-1)(V-2)(V-3)^2. \end{aligned} \quad (74)$$

In [17], the same problem is studied with probabilistic methods but for open random walks. Closed walks are therefore obtained by identifying the starting and ending points but nothing is said about an eventual backtracking occurring at that point. So, the results of [17] (let us call them $\mathcal{N}_m^p(\alpha)$) will, in general, differ from ours. For instance, we checked for the complete graph, the relationship:

$$\mathcal{N}_m^0(\alpha) = N_m^0(\alpha) + \frac{1}{m} N_m^1(\alpha). \quad (75)$$

(This comes from the complete symmetry of this graph).

5 Conclusion

We have computed the spectral determinant for a Schrödinger operator on a graph with quite general boundary conditions. The result is expressed in terms of an arc matrix. When the conditions are permutation-invariant, another expression can be derived in terms of a vertex matrix. Comparison of both expressions allowed us to study reflection properties of random walks on any graph.

The expansion (70) of the spectral determinant in periodic orbits is the basis for obtaining a trace formula (see, for instance, [8] where this is done in great details for Neumann boundary conditions). Unfortunately, in the general case, the reflection and transmission factors are γ-dependent and technical difficulties prevent from getting a trace formula in an appealing form. So, this problem is still an open one.

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References

1. K. Rudenberg, C. Scherr, J. Chem. Phys. **21**, 1565 (1953).
2. S. Alexander, Phys. Rev. B **27**, 1541 (1983).
3. R. Rammal, J. Phys. I France **45**, 191 (1984).
4. B. Douçot, R. Rammal, Phys. Rev. Lett. **55**, 1148 (1985); J. Phys. France **47**, 973 (1986); G. Montambaux, in *Proceedings of the Les Houches Summer School, Session LXIII*, edited by S. Reynaud, E. Giacobino, J. Zinn-Justin (Elsevier, Amsterdam, 1996) p. 387.
5. T. Kottos, U. Smilansky, Phys. Rev. Lett. **79**, 4794 (1997); Ann. Phys. (N.Y.) **274**, 76 (1999).
6. J.P. Roth, C.R. Acad. Sc. Paris **296**, 793 (1983).
7. M. Pascaud, G. Montambaux, Phys. Rev. Lett. **82**, 4512 (1999); M. Pascaud, Ph.D. thesis, Université Paris XI, 1998.
8. E. Akkermans, A. Comtet, J. Desbois, G. Montambaux, C. Texier, Ann. of Phys. **284**, 10 (2000).
9. J. Desbois, J. Phys. A **33**, L63 (2000).
10. J. Desbois, Eur. Phys. J. B **15**, 201 (2000).
11. C. Texier, G. Montambaux, `cond-mat/0107104`.
12. J.E. Avron, P. Exner, Y. Last, Phys. Rev. Lett. **72**, 896 (1994).
13. P. Exner, Phys. Rev. Lett. **74**, 3503 (1995); J. Phys. A **29**, 87 (1996).
14. T. Kottos, H. Schanz, Physica E **9**, 523 (2001).
15. Y. Ihara, J. Math. Soc. Jpn **18**, 219 (1966).
16. H.M. Stark, A.A. Terras, Adv. in Math. **121**, 124 (1996).
17. F.Y. Wu, H. Kunz, Ann. Combin. **3**, 475 (1999), `cond-mat/9812203`.
18. V. Kostrykin, R. Schrader, J. Phys. A **32**, 595 (1999).
19. P. Exner, P. Šeba, Rep. Math. Phys. **28**, 7 (1989).